



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 10:01 AM BST

PDB ID : 4U56
Title : Crystal structure of Blasticidin S bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.45 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

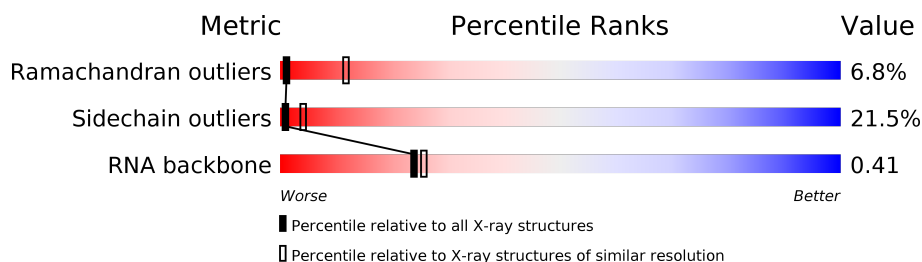
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)





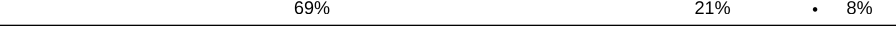
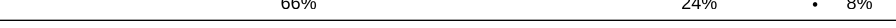

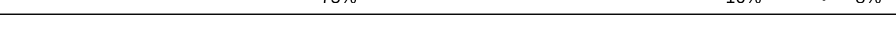
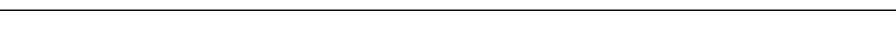
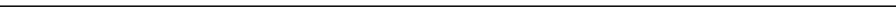















The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	60% 32% 5% .
1	6	1800	62% 32% 6%
2	S0	251	59% 22% . 18%
2	s0	251	65% 15% . 18%
3	S1	254	58% 23% . 16%
3	s1	254	64% 20% . 15%
4	S2	253	65% 19% . 14%
4	s2	253	62% 22% . 14%




















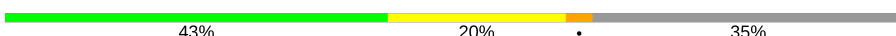





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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3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















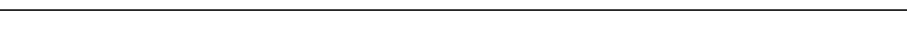




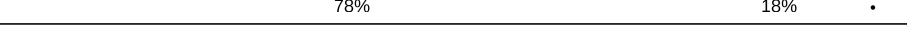





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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6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















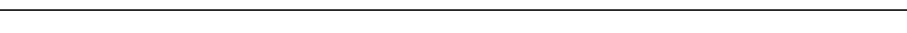




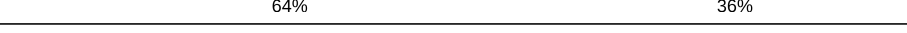





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Mol	Chain	Length	Quality of chain
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	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	120	
70	o4	120	
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	p0	311	 <div> <div></div> <div>38%</div> <div>7%</div> <div>54%</div> </div>
82	m2	160	 <div> <div></div> <div>94%</div> <div>6%</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 411214 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	S	0	0	0
			1481	951	265	265				
9	s7	186	Total	C	N	O	S	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			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			679	402	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	13	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	14	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	15	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	16	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	17	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			
45	18	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	19	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	S	0	0	0
			1053	675	199	177	2			
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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 60S acidic ribosomal protein P0.

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

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

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

- Molecule 83 is a protein called unknown protein chain 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 chain 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	2	Total	Mg	0	0
			2	2		
85	m6	2	Total	Mg	0	0
			2	2		
85	n8	3	Total	Mg	0	0
			3	3		
85	N5	1	Total	Mg	0	0
			1	1		
85	6	147	Total	Mg	0	0
			147	147		
85	sM	1	Total	Mg	0	0
			1	1		
85	m5	5	Total	Mg	0	0
			5	5		
85	l3	3	Total	Mg	0	0
			3	3		
85	C1	1	Total	Mg	0	0
			1	1		
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		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	n0	1	Total 1	Mg 1	0	0
85	L4	3	Total 3	Mg 3	0	0
85	l7	1	Total 1	Mg 1	0	0
85	M5	2	Total 2	Mg 2	0	0
85	c9	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	M9	1	Total 1	Mg 1	0	0
85	q0	2	Total 2	Mg 2	0	0
85	SM	1	Total 1	Mg 1	0	0
85	o4	3	Total 3	Mg 3	0	0
85	M0	3	Total 3	Mg 3	0	0
85	c1	1	Total 1	Mg 1	0	0
85	n6	2	Total 2	Mg 2	0	0
85	5	495	Total 495	Mg 495	0	0
85	c8	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	n9	2	Total 2	Mg 2	0	0
85	1	462	Total 462	Mg 462	0	0
85	c4	1	Total 1	Mg 1	0	0

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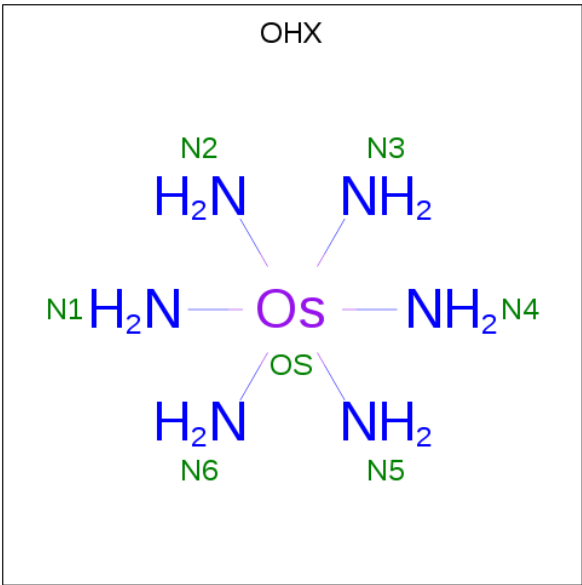
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	D0	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	3	Total 3	Mg 3	0	0
85	O2	2	Total 2	Mg 2	0	0
85	o7	1	Total 1	Mg 1	0	0
85	o3	2	Total 2	Mg 2	0	0
85	d3	3	Total 3	Mg 3	0	0
85	M3	2	Total 2	Mg 2	0	0
85	N3	3	Total 3	Mg 3	0	0
85	4	23	Total 23	Mg 23	0	0
85	D4	1	Total 1	Mg 1	0	0
85	S4	1	Total 1	Mg 1	0	0
85	L2	2	Total 2	Mg 2	0	0
85	m1	1	Total 1	Mg 1	0	0
85	l5	3	Total 3	Mg 3	0	0
85	d0	1	Total 1	Mg 1	0	0
85	M7	5	Total 5	Mg 5	0	0
85	m4	1	Total 1	Mg 1	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	O1	1	Total 1	Mg 1	0	0
85	s8	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	17	Total 17	Mg 17	0	0
85	n3	1	Total 1	Mg 1	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	4	Total 4	Mg 4	0	0
85	O5	1	Total 1	Mg 1	0	0
85	N6	2	Total 2	Mg 2	0	0
85	8	14	Total 14	Mg 14	0	0
85	l4	1	Total 1	Mg 1	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0
85	m0	1	Total 1	Mg 1	0	0
85	3	15	Total 15	Mg 15	0	0
85	m7	6	Total 6	Mg 6	0	0

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: H₁₂N₆Os).



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		

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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
			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		

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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		
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	C3	1	Total	N	Os	0	0
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86	C5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	D9	1	Total	N	Os	0	0
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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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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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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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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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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	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	M9	1	Total	N	Os	0	0
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86	N9	1	Total	N	Os	0	0
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86	O1	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	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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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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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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
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86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
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86	d4	1	Total 7	N 6	Os 1	0	0
86	d9	1	Total 7	N 6	Os 1	0	0
86	sR	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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		
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		

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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	7	1	Total	N	Os	0	0
			7	6	1		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	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	q2	1	Total	N	Os	0	0
			7	6	1		

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

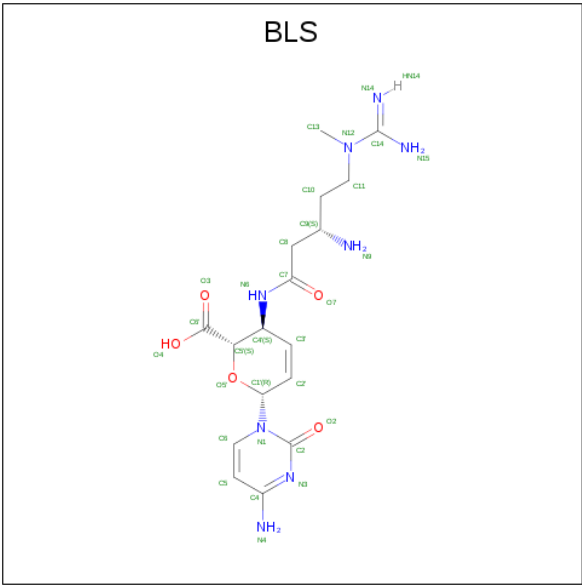
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	O7	1	Total	Zn	0	0
			1	1		
87	q2	1	Total	Zn	0	0
			1	1		

- Molecule 88 is BLASTICIDIN S (three-letter code: BLS) (formula: C₁₇H₂₆N₈O₅).



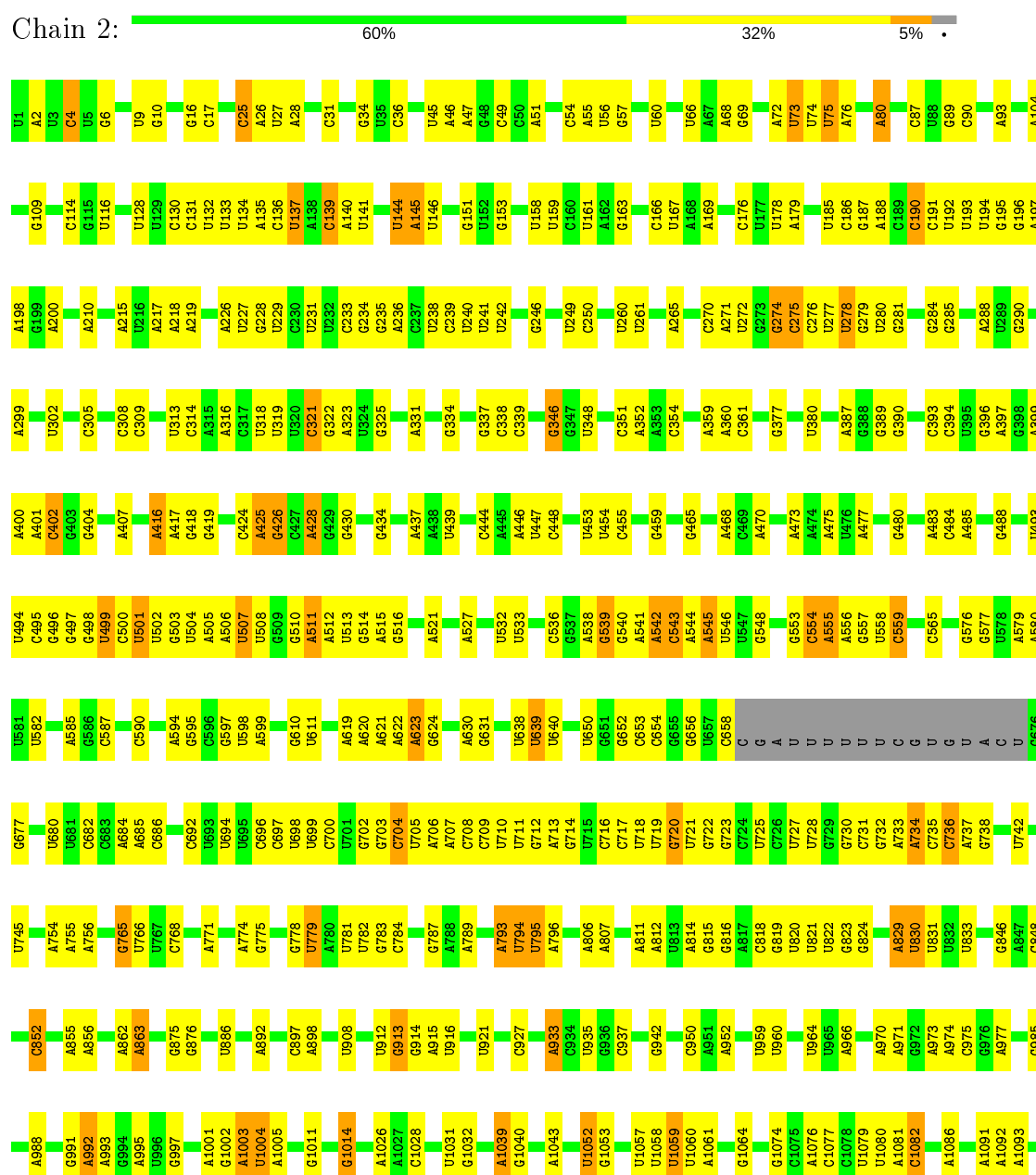
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	1	1	Total	C	N	O	0	0
			30	17	8	5		
88	5	1	Total	C	N	O	0	0
			30	17	8	5		

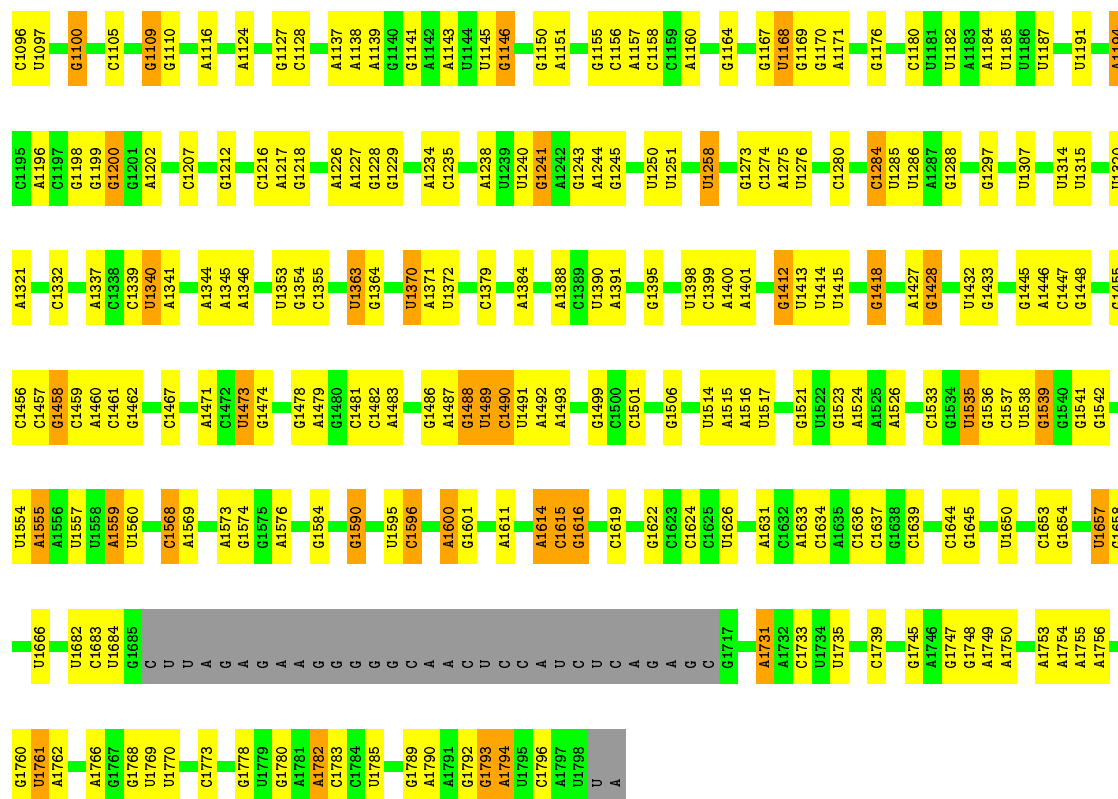
3 Residue-property plots

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.

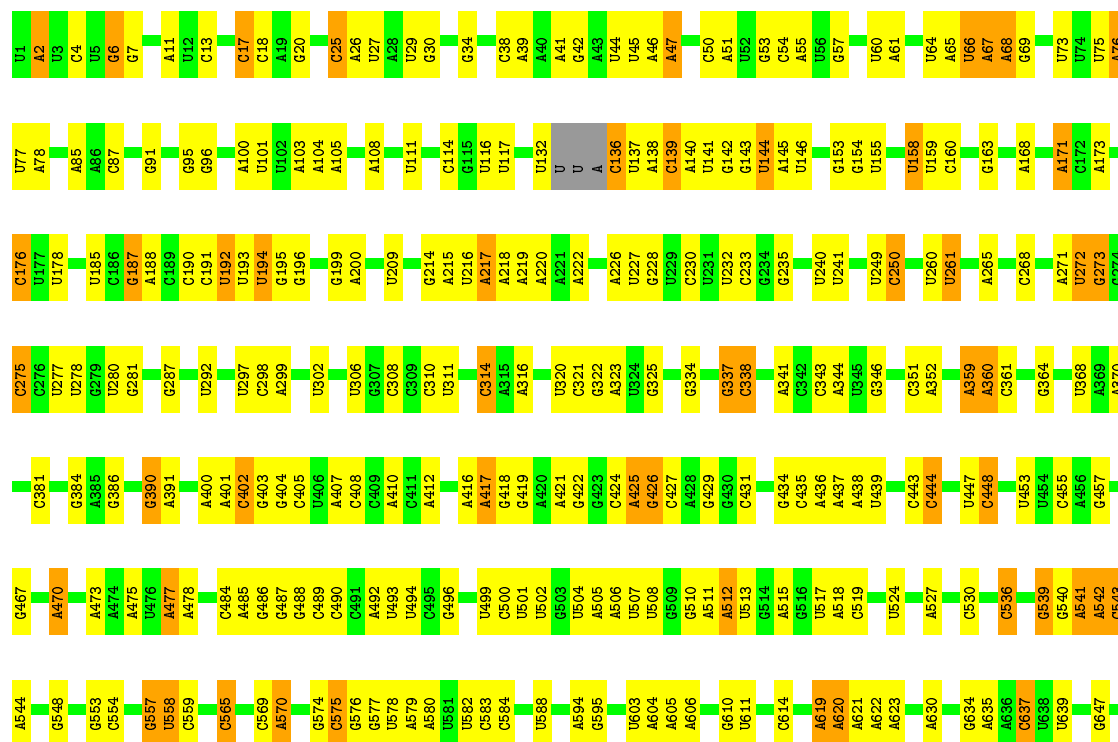
Note EDS failed to run properly.

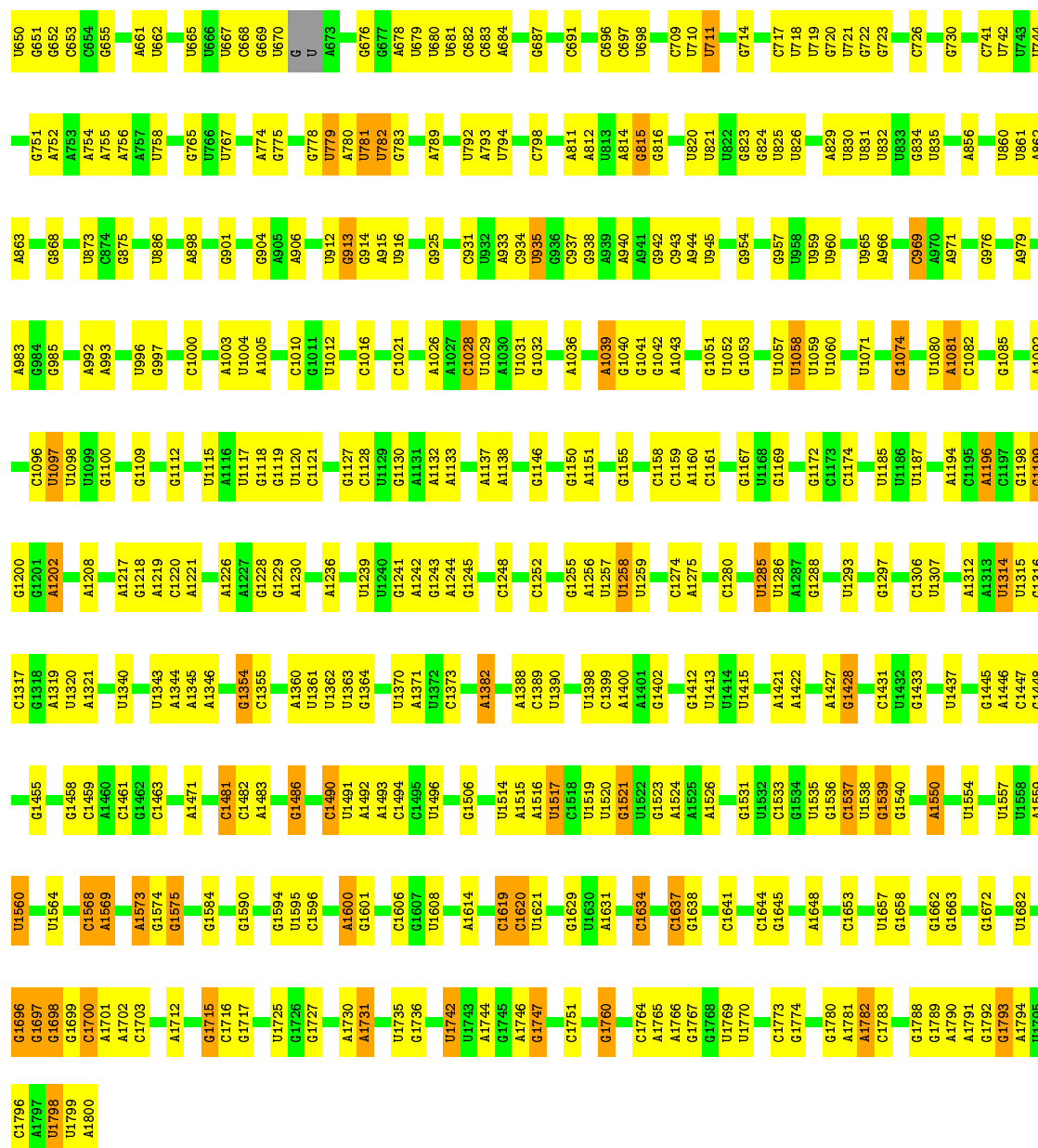
• Molecule 1: 18S ribosomal RNA





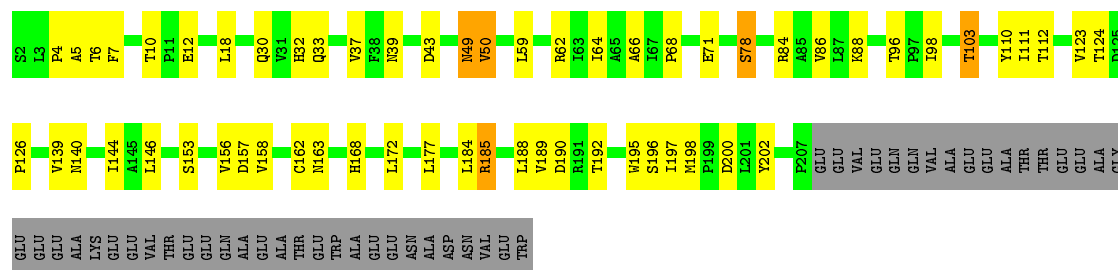
Chain 6:





• Molecule 2: 40S ribosomal protein S0-A

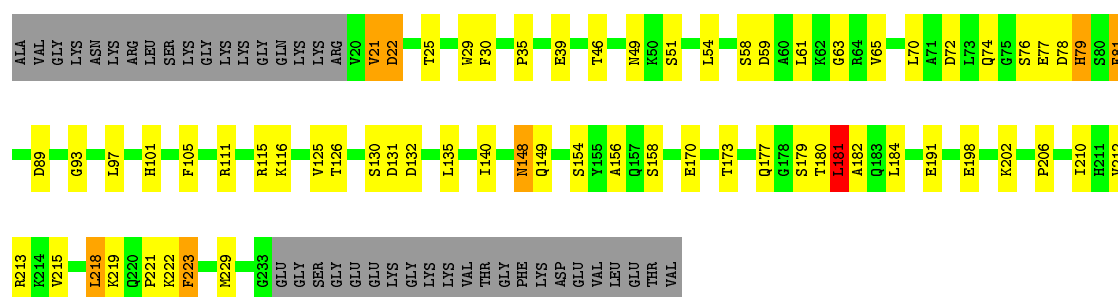
Chain S0: 59% 22% 18%



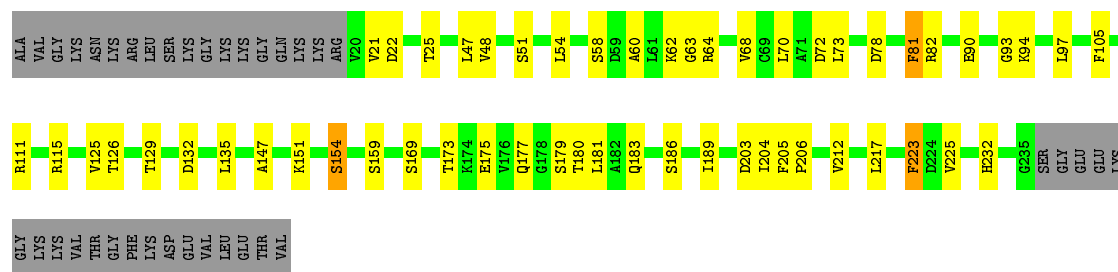
• Molecule 2: 40S ribosomal protein S0-A

ALA	L172	S2
ASP	L177	L3
ASN		P4
VAL		F7
GLU	R183	D8
TRP	L184	L9
	R185	T10
	G186	
		R27
	V189	V28
	D190	V29
	R191	Q30
		V31
	D200	H32
	L201	
	Y202	R41
	F203	
		V45
	D206	N49
	P207	V50
	GLU	
	GLU	L59
	VAL	
	GLU	P68
	GLN	
	GLN	D72
	VAL	
	ALA	T80
	GLU	
	GLU	Q83
	ALA	
	THR	L87
	THR	K88
	GLU	
	GLU	T96
	ALA	
	GLY	
	GLU	R101
	GLU	F102
	GLU	T103
	ALA	
	LYS	S114
	GLU	
	GLU	V139
	VAL	N140
	THR	I141
	GLU	
	GLU	P152
	GLN	S153
	ALA	E154
	GLU	
	ALA	V158
	THR	
	GLU	C162
	TRP	N163
	ALA	N164
	GLU	R165
	GLU	
	ASN	H169

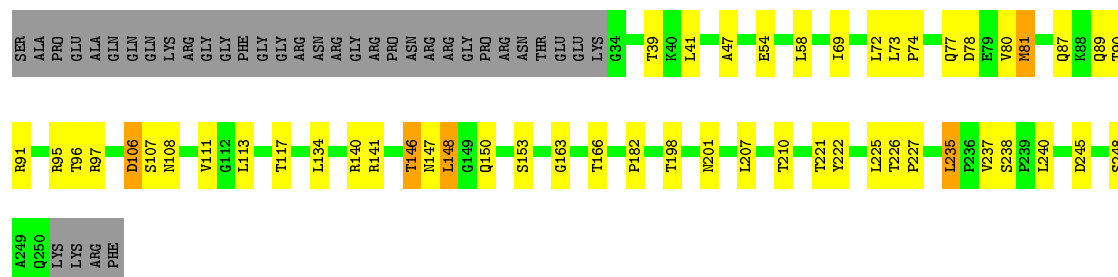
- Chain S1:



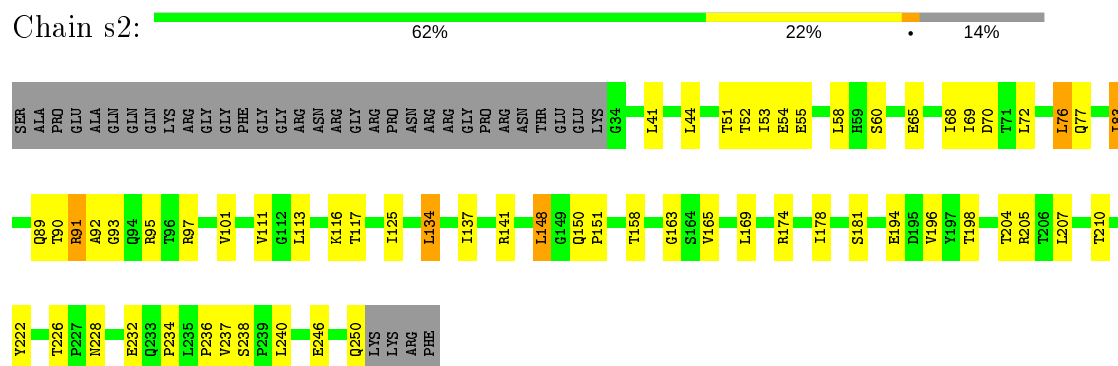
- Chain s1:



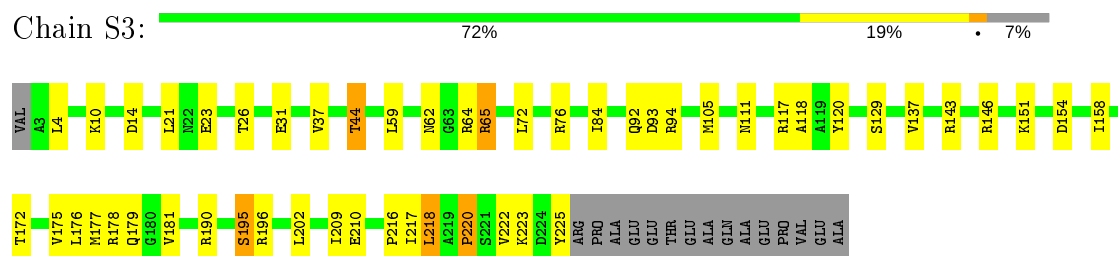
- Chain S2:



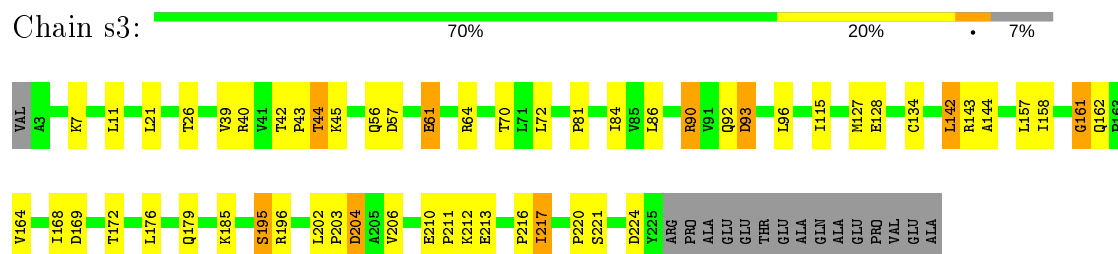
- Molecule 4: 40S ribosomal protein S2



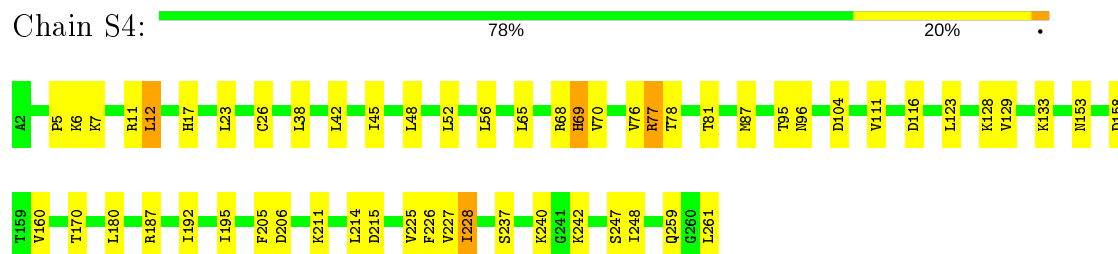
- Molecule 5: 40S ribosomal protein S3



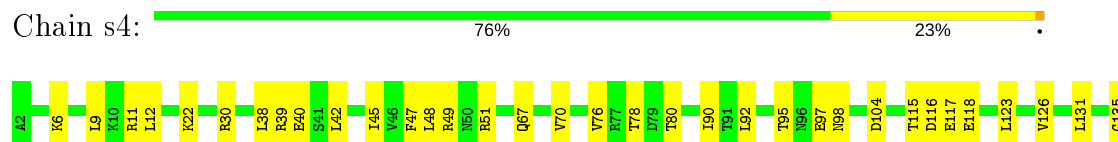
- Molecule 5: 40S ribosomal protein S3



- Molecule 6: 40S ribosomal protein S4-A



- Molecule 6: 40S ribosomal protein S4-A

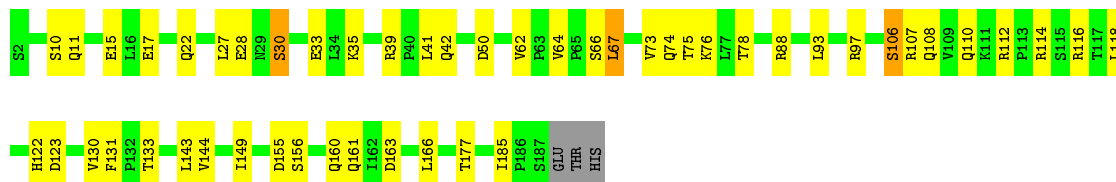






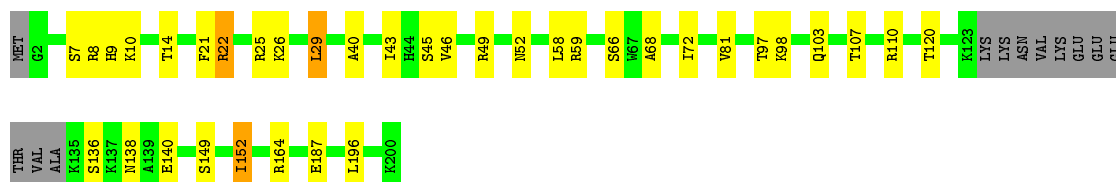
- Molecule 9: 40S ribosomal protein S7-A

Chain s7: 72% 25%



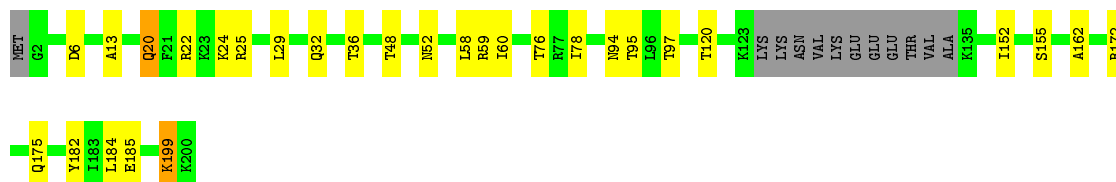
- Molecule 10: 40S ribosomal protein S8-A

Chain S8: 76% 17% 6%



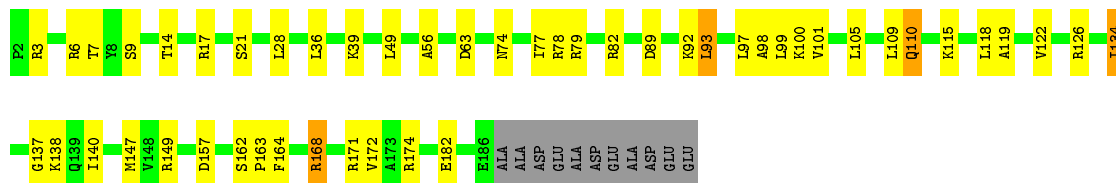
- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 80% 14% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain S9: 69% 23% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 75% 18% 6%



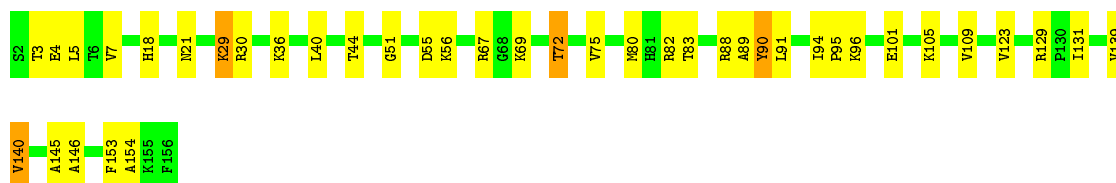
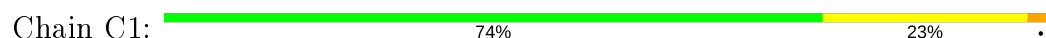
- Molecule 12: 40S ribosomal protein S10-A



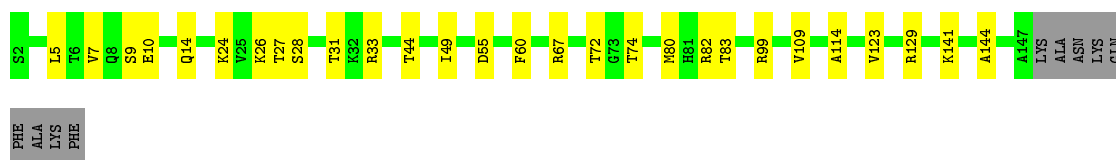
- Molecule 12: 40S ribosomal protein S10-A



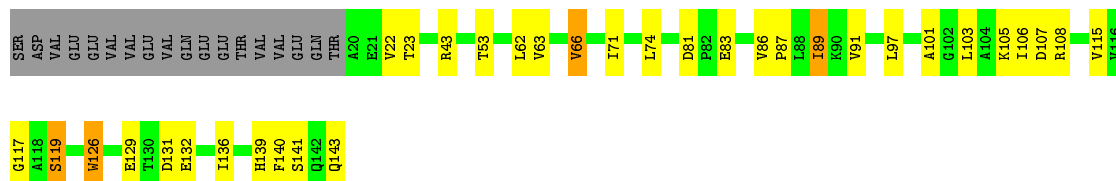
- Molecule 13: 40S ribosomal protein S11-A



- Molecule 13: 40S ribosomal protein S11-A

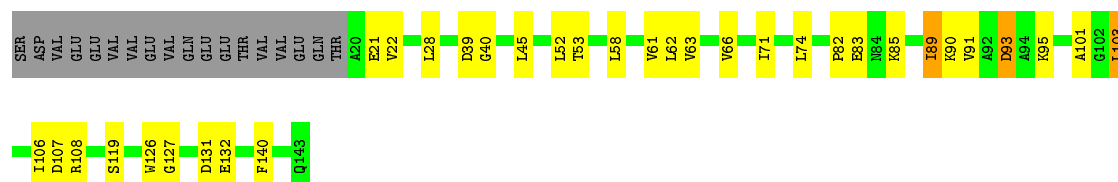


- Molecule 14: 40S ribosomal protein S12



- Molecule 14: 40S ribosomal protein S12





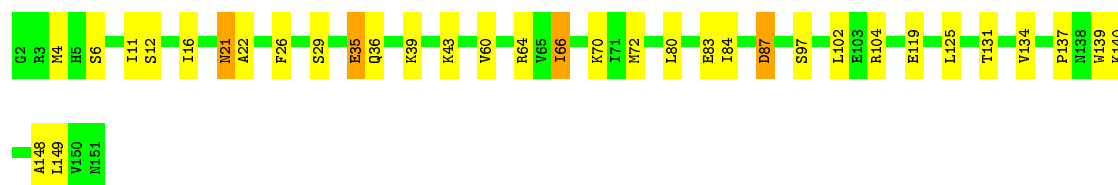
- Molecule 15: 40S ribosomal protein S13

Chain C3: 76% 22%



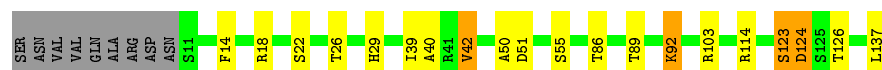
- Molecule 15: 40S ribosomal protein S13

Chain c3: 77% 20%



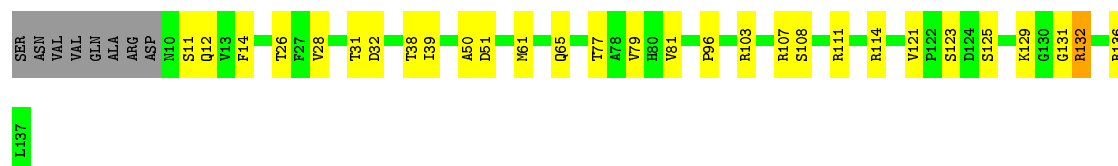
- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 79% 12% 7%



- Molecule 16: 40S ribosomal protein S14-A

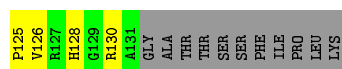
Chain c4: 73% 21% 6%



- Molecule 17: 40S ribosomal protein S15

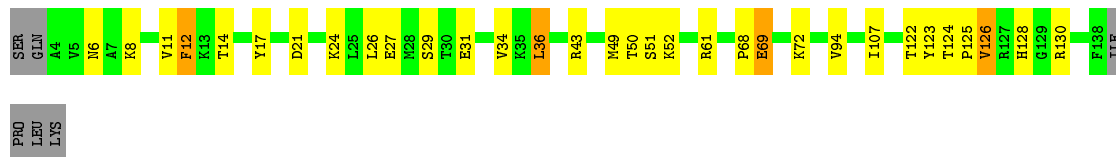
Chain C5: 63% 24% 12%






- Molecule 17: 40S ribosomal protein S15

Chain c5:  73% 20%



- Molecule 18: 40S ribosomal protein S16-A

Chain C6:  81% 17%



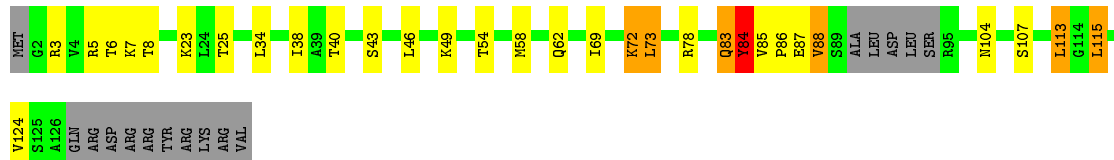
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:  77% 21%



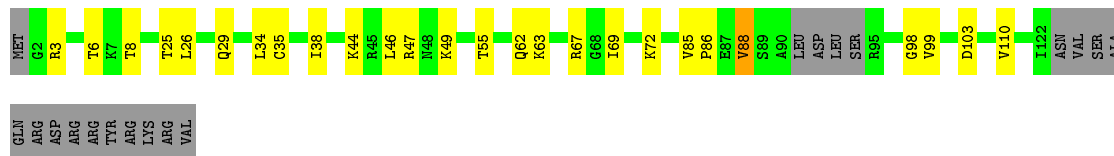
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:  65% 18% 12%



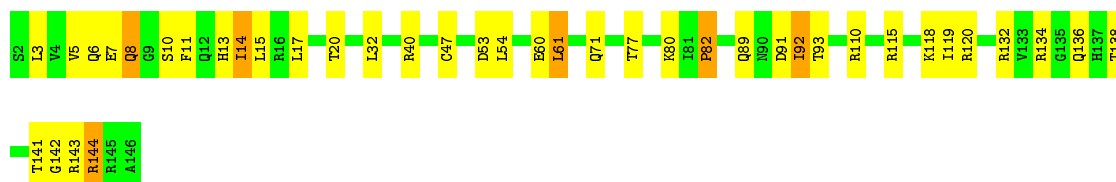
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:  67% 18% 14%



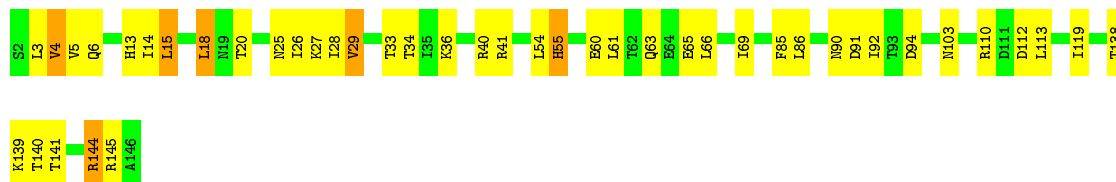
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:  72% 23%



- Molecule 20: 40S ribosomal protein S18-A

Chain c8: 70% 26%



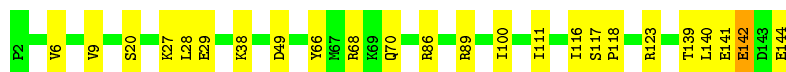
- Molecule 21: 40S ribosomal protein S19-A

Chain C9: 78% 20%



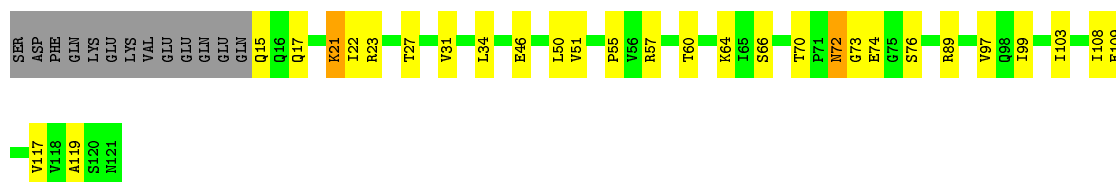
- Molecule 21: 40S ribosomal protein S19-A

Chain c9: 83% 16%



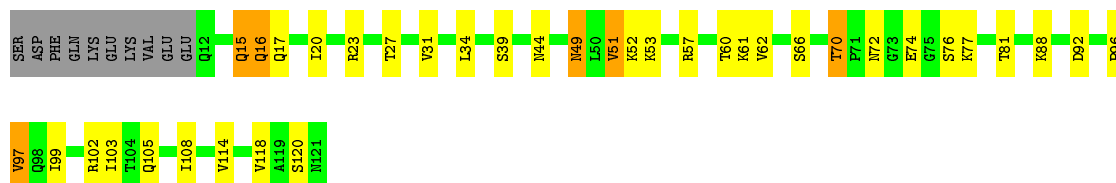
- Molecule 22: 40S ribosomal protein S20

Chain D0: 65% 23% 11%




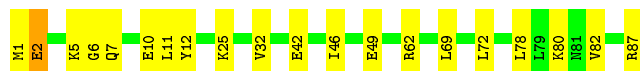
- Molecule 22: 40S ribosomal protein S20

Chain d0: 61% 26% 5% 8%



- Molecule 23: 40S ribosomal protein S21-A

Chain D1:  77% 22%




- Molecule 23: 40S ribosomal protein S21-A

Chain d1:  76% 24%




- Molecule 24: 40S ribosomal protein S22-A

Chain D2:  79% 21%




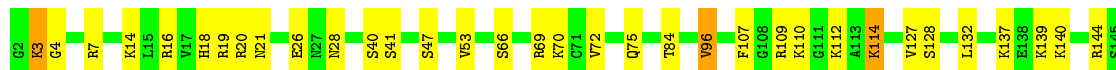
- Molecule 24: 40S ribosomal protein S22-A

Chain d2:  81% 18%




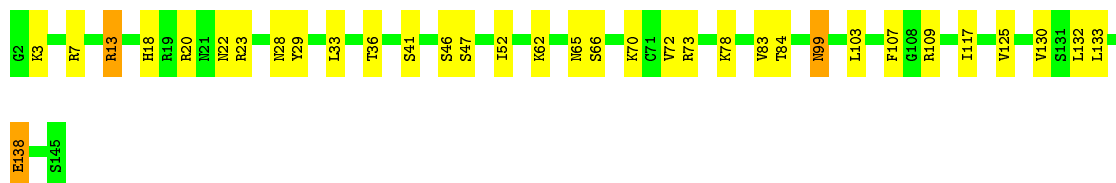
- Molecule 25: 40S ribosomal protein S23-A

Chain D3:  76% 22%




- Molecule 25: 40S ribosomal protein S23-A

Chain d3:  76% 22%

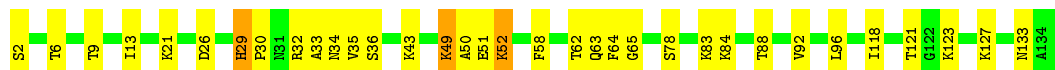
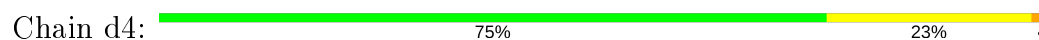


- Molecule 26: 40S ribosomal protein S24-A

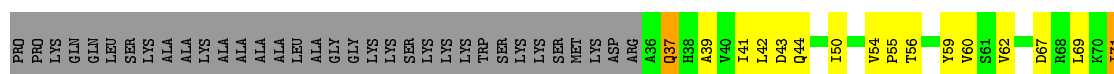
Chain D4:  79% 20%



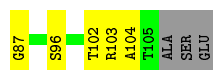
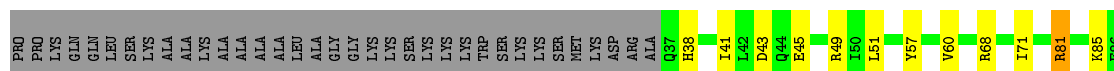
- Molecule 26: 40S ribosomal protein S24-A



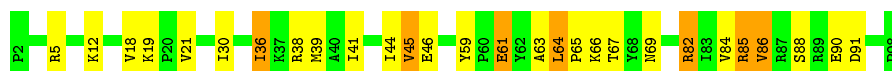
- Molecule 27: 40S ribosomal protein S25-A



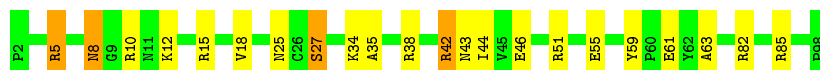
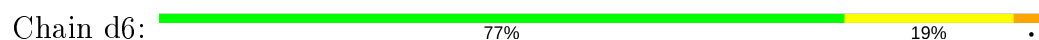
- Molecule 27: 40S ribosomal protein S25-A



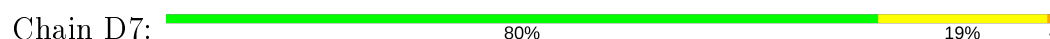
- Molecule 28: 40S ribosomal protein S26-B



- Molecule 28: 40S ribosomal protein S26-B

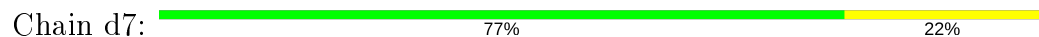


- Molecule 29: 40S ribosomal protein S27-A





- Molecule 29: 40S ribosomal protein S27-A



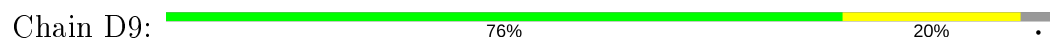
- Molecule 30: 40S ribosomal protein S28-A



- Molecule 30: 40S ribosomal protein S28-A



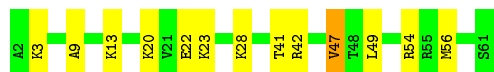
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A



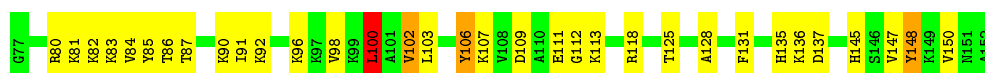
- Molecule 33: Ubiquitin-40S ribosomal protein S31





- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 57% 38%



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

Chain SR: 81% 18%



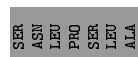
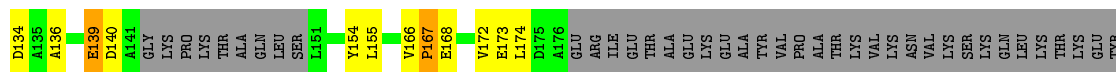
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR: 85% 14%



- Molecule 35: Suppressor protein STM1

Chain SM: 42% 14% 42%



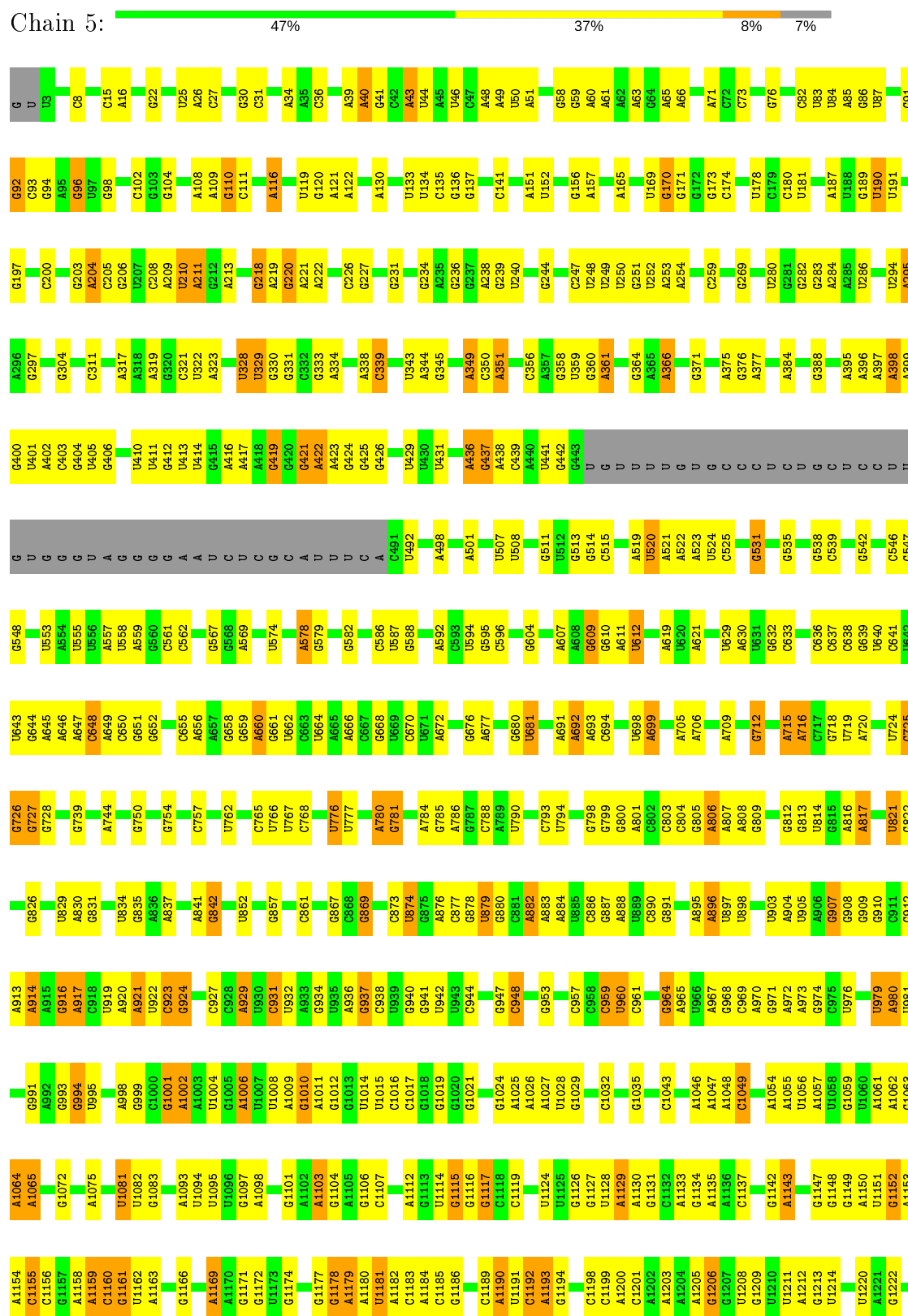
- Molecule 35: Suppressor protein STM1

Chain sM: 31% 7% 62%



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C3378	U3281	U3193	U3111	C3001	U2921	A2851	C2774	A2680	A2609	U2514	U	A2368	A2295	G2199
C3379	U3196	U3195	G3112	G3002	G2922	C2852	G2777	U2681	G2610	U2200	G	G2369	A2296	U2201
U3382	G3286	U3196	G3112	U3023	U2923	A2853	G2778	C2689	U2611	A2515	A	G2370	U2297	G2201
U3389	G3288	U3198	A3113	G3003	U2924	U2854	A2779	U2684	U2612	A2519	G	G2371	U2298	U2205
G3390	G3289	U3199	G3118	G3004	C2927	G2855	G2779	C2684	U2613	A2519	G	U2372	A2299	U2206
U3396	G3290	G3200	U3119	A3005	G2927	G2856	G2780	U2687	G2614	G2522	G	A2373	A2207	A2207
U3293	U3293	G3201	U3120	A3006	A2930	U2858	C2788	U2688	G2615	G2523	U	G2374	A2208	A2208
A3294	G3202	U3121	U3121	A3011	A2931	U2859	G2796	A2691	U2616	G2524	G	G2376	U2209	G2210
A3295	U3203	U3122	A3122	A3012	A2933	U2860	G2796	A2691	U2617	G2525	U	G2377	A2230	G2210
G3204	G3204	G3204	G3128	G3015	U2935	U2861	C2797	A2691	G2619	G2530	A	U2378	G2306	A2213
G3206	G3206	G3206	A3129	U2936	A2936	U2862	G2797	A2691	G2620	G2531	G	U2379	G2307	A2213
U3207	U3207	U3207	A3130	A3021	A2937	A2864	G2800	A2694	G2621	G2532	A	U2380	C2308	A2223
G3208	G3208	U3213	U3131	G3022	U2938	U2865	A2801	A2696	G2622	G2533	A	G2381	A2309	A2223
A3305	A3305	A3209	C3132	G3028	C2942	U2866	A2802	A2697	G2624	G2534	U	G2382	U2310	A2224
U3306	U3306	A3210	C3133	G3029	C2943	U2867	A2803	G2698	G2625	U2537	A	C2383	G2311	U2235
G3309	G3309	G3211	A3134	A3029	U2949	U2868	A2804	G2699	A2626	U2538	G	U2384	A2312	A2228
A3310	A3310	C3212	U3138	G3030	G2945	U2869	G2805	A2704	G2627	G2539	U	A2385	A2313	A2228
C3311	C3311	U3214	A3139	U3041	A2946	C2870	U2806	A2704	A2628	C2540	G	A2386	U2314	A2229
U3312	U3312	U3215	G3140	A3042	G2947	U2871	U2807	A2705	U2629	U2541	G	U2387	A2315	A2232
U3313	U3313	U3216	A3141	A3043	C2948	A2872	A2808	A2706	U2630	U2542	G	U2388	U2316	A2233
A3316	A3316	G3217	A3142	A3044	U2949	U2873	C2809	C2708	U2631	U2543	A	C2392	U2317	C2237
U3317	U3317	A3218	C3143	U3045	U2953	U2874	C2810	G2714	G2632	U2544	G	U2393	A2320	C2238
U3318	U3318	G3219	G3144	U3046	U2954	U2875	A2811	G2715	U2633	C2545	C	G2394	A2321	G2239
A3320	A3320	G3224	A3150	U3050	U2955	C2877	C2812	G2716	A2636	C2548	U	U2395	C2322	A2244
A3325	A3325	G3225	U3151	U3051	C2956	G2878	A2813	U2719	A2637	G2549	C	A2397	G2323	C2245
U3331	U3331	G3226	A3152	U3052	C2957	U2881	G2814	U2720	U2638	G2550	G	U2398	A2324	G2246
A3332	A3332	G3227	U3153	U3053	C2958	U2882	G2815	C2726	G2639	C2552	G	G2400	A2325	G2247
U3333	U3333	G3228	C3154	U3054	G2959	U2883	A2816	A2727	A2643	U2553	C	A2401	A2326	G2248
A3335	A3335	G3229	U3155	U3055	A2960	U2884	A2817	G2728	A2644	C2554	G	A2402	U2329	G2249
U3341	U3341	G3230	U3156	U3056	G2961	C2885	U2818	U2729	U2645	C2555	C	G2403	A2330	G2250
A3342	A3342	G3231	G3157	G3059	A2970	U2886	A2819	U2730	U2646	C2556	C	A2404	U2331	G2251
G3343	G3343	A3244	G3158	C3063	A2971	U2887	A2820	G2731	A2647	C2557	A	C2405	U2332	A2252
A3344	A3344	G3245	G3159	G3064	G2972	U2888	U2821	G2732	G2648	A2561	G	G2406	U2333	A2253
U3345	U3345	G3246	C3164	U3074	U2973	U2889	U2822	G2733	U2649	C2562	U	C2407	U2334	A2254
G3247	G3247	G3247	A3165	G3075	U2974	C2890	G2823	U2734	A2650	C2563	G	U2408	U2335	A2255
G3248	G3248	G3248	C3166	U3076	U2975	A2890	G2824	A2739	U2651	C2564	U	U2409	U2336	A2256
G3249	G3249	G3249	A3167	U3077	G2976	C2891	U2825	C2741	G2652	C2565	A	G2410	U2342	A2257
G3253	G3253	G3253	U3169	G3080	U2979	C2892	U2826	G2742	C2653	C2566	U	G2411	U2343	G2261
U3259	U3259	U3259	A3170	G3081	A2980	A2896	U2827	A2743	A2656	C2567	A	G2412	U2344	A2262
U3263	U3263	U3263	U3171	A3082	A2981	A2897	U2828	A2744	A2657	C2568	C	G2413	U2345	U2266
G3263	G3263	G3263	A3172	A3083	C2982	U2898	G2830	A2745	A2658	C2569	U	G2414	U2346	U2267
G3266	G3266	G3266	G3173	A3084	C2983	U2899	G2831	A2746	G2659	C2570	C	U2415	G2272	G2272
G3266	G3266	G3266	A3174	G3085	C2984	C2899	C2832	A2747	U2660	C2571	A	U2416	G2273	G2273
U3269	U3269	U3269	U3175	A3086	C2985	U2900	C2833	U2752	G2661	C2572	C	U2417	C2353	G2274
U3270	U3270	U3270	G3176	A3087	U2901	U2904	C2834	G2753	G2662	C2573	U	A2418	C2354	G2275
A3273	A3273	A3273	U3177	A3088	C2986	U2905	A2835	C2754	G2663	C2574	A	A2419	G2355	G2276
A3274	A3274	A3274	A3178	A3089	U2987	A2911	G2836	C2755	G2664	C2575	C	C2422	A2356	C2277
U3275	U3275	U3275	U3179	A3090	U2988	G2912	U2837	A2756	G2665	C2576	U	U2423	A2357	C2278
G3276	G3276	G3276	A3180	A3091	G2990	C2913	U2842	G2757	G2666	C2577	U	U2424	A2358	A2279
U3277	U3277	U3277	U3181	A3092	U2991	U2914	C2843	C2758	A2667	C2578	U	U2425	A2359	A2280
C3278	C3278	C3278	G3182	U3100	U2992	G2915	C2844	A2759	A2668	C2579	U	U2426	A2360	U2281
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C3279	C3279	C3279	A3184	U3102	U2994	U2917	C2846	A2761	G2670	C2581	U	U2428	A2362	U2283
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A3281	A3281	A3281	A3187	U3105	U2997	U2920	G2849	C2764	A2673	C2584	U	U2431	A2365	C2286
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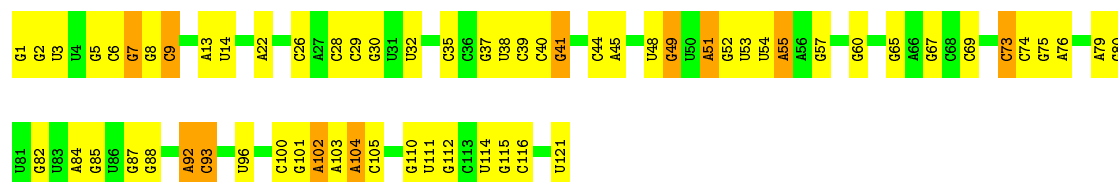
● Molecule 36: 25S ribosomal RNA



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G2435	A2363	U2289	A2198	C2101	G1892	A1797	A1667	C1563	A1467	C1392	G1319	U1235
U2436	C2364	C2290	G2199	U2102	U1893	A1810	A1683	G1564	A1468	G1393	G1321	G1236
G2437	C2365	A2291	C2204	U2102	A1894	A1810	A1684	G1565	G1473	A1393	U1324	G1237
A2438	A2368	A2295	U2205	G2111	A1895	A1814	G1685	U1566	A1474	G1394	U1325	G1238
G2440	G2369	U2297	U2209	U2112	G1896	U1815	U1686	U1567	A1475	G1395	A1326	C1239
G2441	G2370	U2298	G2210	A2113	G1897	U1816	U1687	U1568	G1476	U1398	U1241	U1240
A2443	A2372	A2299	U2211	C2114	G1898	A1817	U1688	U1570	A1477	A1399	G1243	G1242
G2442	G2373	G2300	G2215	G2115	A1900	U1818	U1695	U1572	G1480	G1400	A1330	A1244
C2444	C2374	U2301	A2223	G2116	A1901	U1821	U1696	U1573	G1481	G1404	A1331	A1245
A	C2375	G2302	A2224	G2121	U1902	U1822	A1704	G1574	A1482	U1405	A1332	G1246
U	A2376	A2303	U2225	G2122	G1903	G1830	A1704	A1575	G1483	A1406		
A	G2377	C2304	U2228	G2123	G1905	U1831	C1710	G1576	U1407	A1407	C1335	A1252
G	A2378		A2228	G2123	G1906	G1832	C1710	G1577	G1485	G1408		
G	U2379	G2307	C2231	C2128	U1909	G1833	A1713	C1578	U1494	G1409	U1258	
G	U2380	C2308	G2231	U2129	A1910	U1839	A1714	C1579	U1495	G1413		
U	A2381	A2309	G2234	G2130	A1911	U1840	U1715	A1580	A1482	U1341	G1262	
U	U2382	U2310	G2234	A2131	G1912	U1841	U1716	C1581	C1496	U1342	A1263	
G	A2383	C2312	C2237	C2132	A1913	A1842	U1717	C1582	C1497	C1416	G1264	
U	A2384	U2313	U2137	U2137	G1914	A1842	U1724	A1583	G1500	G1417	U1265	
A	A2385	G2314	A2138	A2138	A1915	G1845	U1724	A1584	U1501	A1418	U1266	
A	A2386	G2315	U2141	U2141	G1916	C1846	A1729	A1585	C1502	C1420	U1267	
A	U2387	G2316	A2142	A2142	C1917	A1847	G1733	A1586	G1507	G1421	G1268	
A	C2388		A2142	A2142	G1918	G1848	G1733	A1587	U1507		U1269	
U	A2389	A2320	A2244	A2244	G1919	U1849	G1736	A1588	A1428	A1428	C1275	
U	A2390	A2321	C2245	C2245	U1920	A1850	G1736	A1589	A1509	G1429		
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U	C2394	U2325	G2249	U2154	G	C1854	A1750	U1601	U1513	A1433	G1357	
G	A2397	U2326	U2155	G2155	G1927	U1855	G1751	G1604	G1514	G1434	C1358	C1284
G	A2398	C2329	C2156	C2156	U1944	C1856	A1752	A1605	G1517	U1436	C1359	G1285
G	C2400	C2330	G2157	G2157	U1944	C1857	A1752	U1606	U1518	U1437	G1362	C1292
C	A2401	C2331	U2158	U2158	U1944	A1858	A1760	U1607	U1519	C1437	U1293	U1293
U	U2402	U2334	U2159	U2159	G1948	A1858	C1761	C1608	G1528	U1438	A1294	A1294
U	G2335	G2335	G2160	G2160	G1953	A1866	C1762	C1609	G1529	U1439	G1295	G1295
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G	C2337	C2338	A2168	A2168	U	G1868	U1765	A1619	U1533	U1442	G1367	C1298
G	C2338	C2339	G2169	G2169	A	C1869	U1766	U1620	G1536	G1443	U1368	A1301
C	U2339	U2340	U2176	U2176	U	G1870	C1767	U1621	A1369	U1444	A1302	A1302
C	A2341	A2341	U2176	U2176	U	U1871	U1768	C1628	G1546	A1445	A1303	A1303
C	U2342	U2342	A2182	A2182	U	U1872	G1770	U1629	A1547	U1446	C1371	C1371
A	U2343	U2343	A2183	A2183	A	U1873	G1770	U1630	G1548	G1447	A1304	A1304
U	A2344	A2345	U2184	U2184	G	G1874	G1775	C1639	U1549	U1448	U1305	U1305
U	C2345	C2346	G2185	G2185	G	U1875	G1775	G1640	C1550	A1449	G1374	G1306
G	U2347	U2347	U2186	U2186	C	A1879	G1780	U1641	C1551	U1450	G1375	G1307
A	U2348	U2348	U2187	U2187	C	U1880	G1780	U1642	C1552	C1451	C1376	A1308
A	U2349	U2349	U2188	U2188	U	A1881	U1783	A1643	G1553	A1452	G1377	U1309
U	A2352	A2352	A2189	A2189	U	G1882	U1783	C1644	U1554	U1456	U1378	A1456
U	C2353	C2353	U2190	U2190	C	U1883	U1783	U1645	U1555	A1457	G1379	G1310
A	C2354	C2354	U2191	U2191	U	U1884	G1790	U1646	C1556	U1458	G1380	C1312
C	A2356	A2356	C2192	C2192	A	U1885	C1791	U1647	U1557	U1459	A1381	G1313
C	C2359	C2359	C2193	C2193	U	A1886	C1792	G1661	A1557		C1314	C1314
A	C2360	C2360	C2194	C2194	U	A1887	C1793	G1662	G1560	A1462	U1384	U1315
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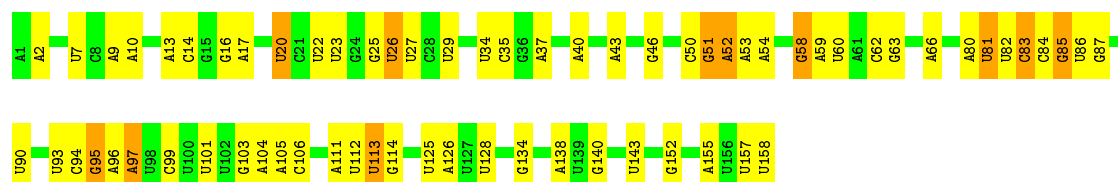
- Molecule 37: 5S ribosomal RNA

Chain 7: 



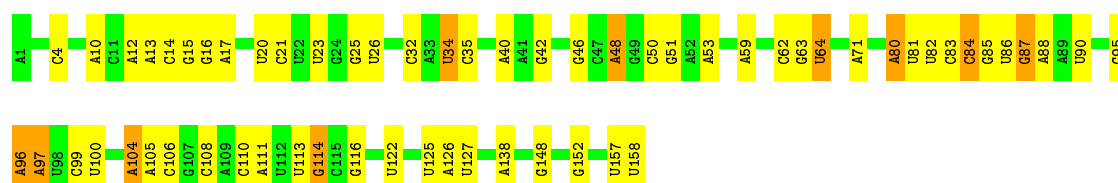
- Molecule 38: 5.8S ribosomal RNA

Chain 4: 




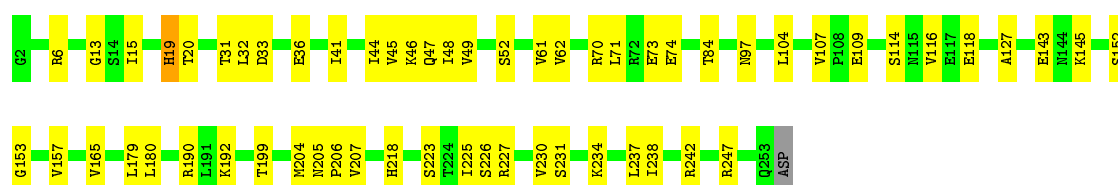
- Molecule 38: 5.8S ribosomal RNA

Chain 8: 




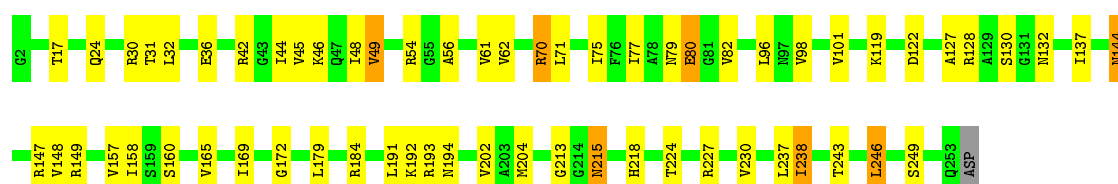
- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 




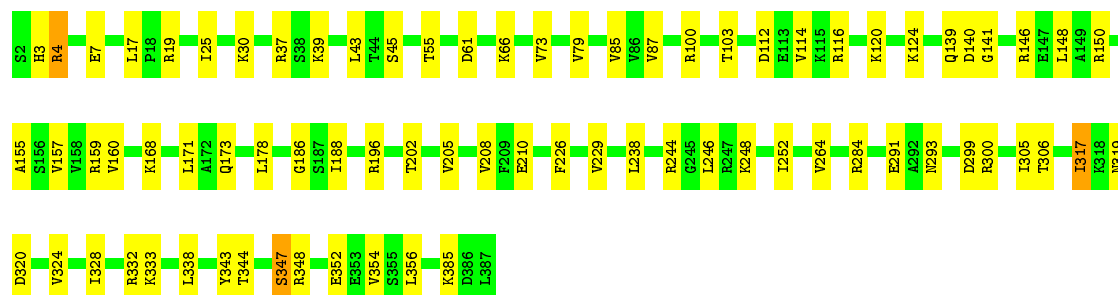
- Molecule 39: 60S ribosomal protein L2-A

Chain l2: 



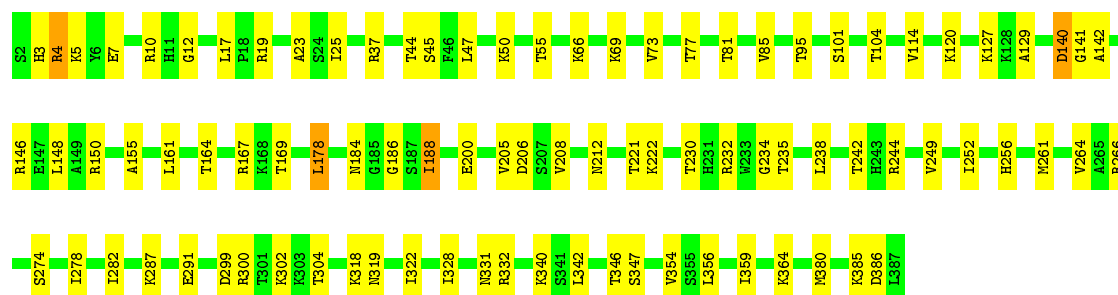
- Molecule 40: 60S ribosomal protein L3

Chain L3:  80% 19%

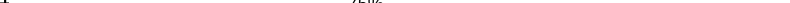


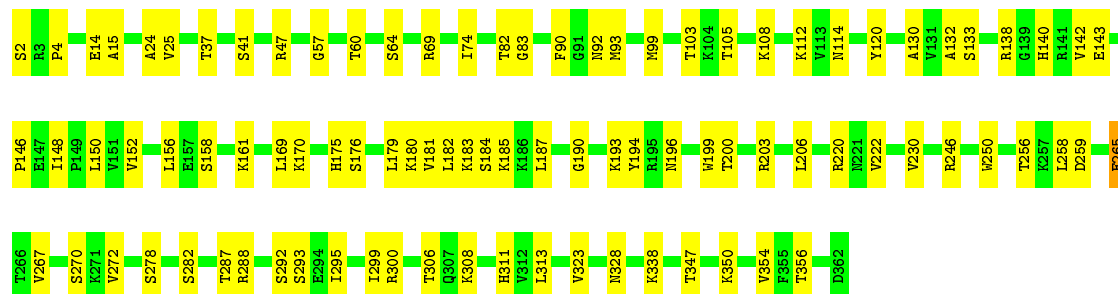
- Molecule 40: 60S ribosomal protein L3

Chain 13: 77% 22% .



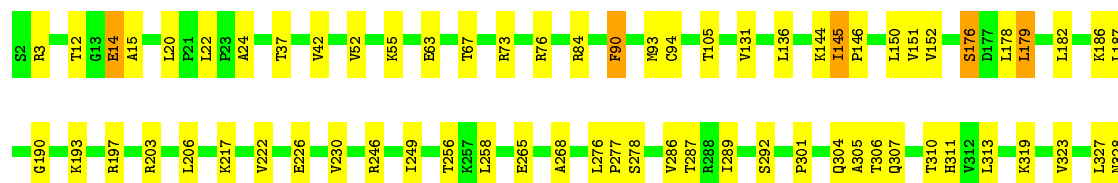
- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 



- Molecule 41: 60S ribosomal protein L4-A

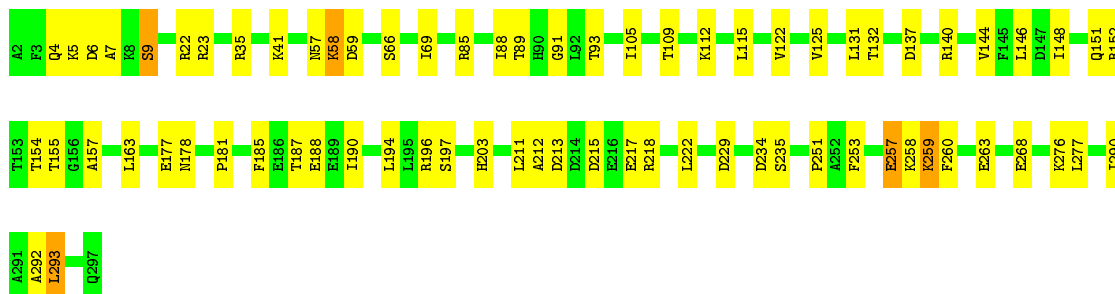
Chain 14: 77% 21% .





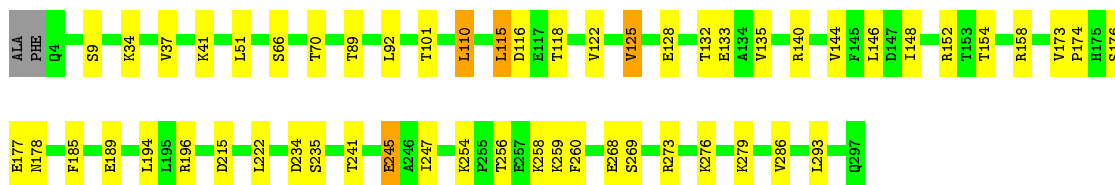
• Molecule 42: 60S ribosomal protein L5

Chain L5: 76% 23% .



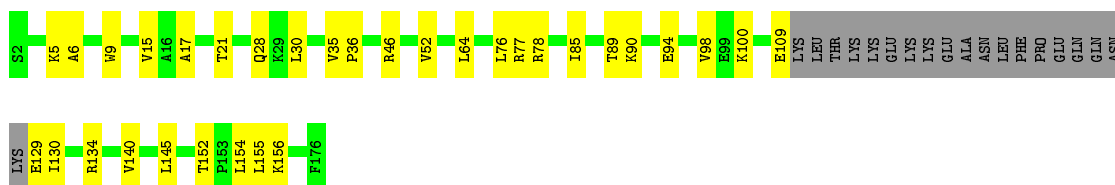
• Molecule 42: 60S ribosomal protein L5

Chain L5: 81% 17% ..



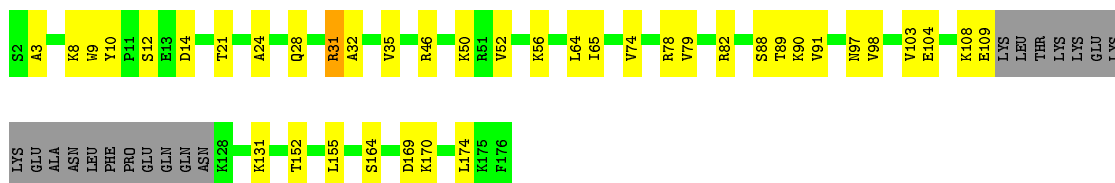
• Molecule 43: 60S ribosomal protein L6-A

Chain L6: 71% 18% 11%



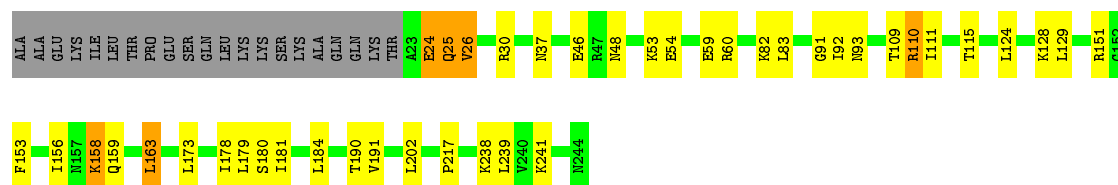
• Molecule 43: 60S ribosomal protein L6-A

Chain L6: 67% 22% 10%



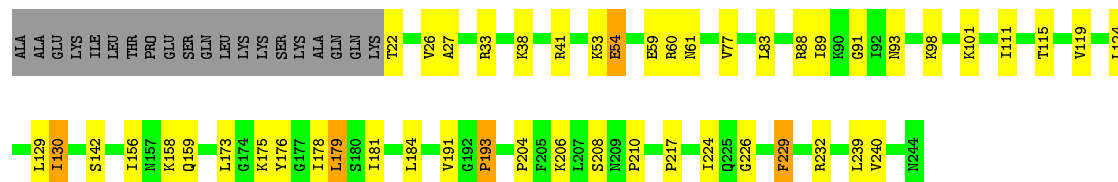
• Molecule 44: 60S ribosomal protein L7-A

Chain L7: 74% 15% 9%



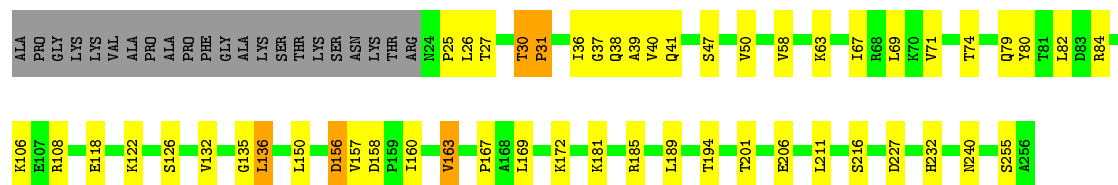
- Molecule 44: 60S ribosomal protein L7-A

Chain 17: 72% 18% 8%



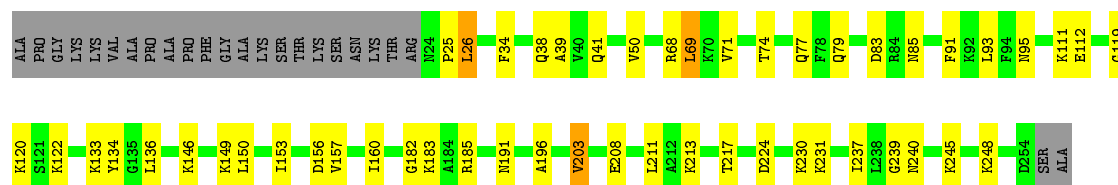
- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 71% 18% 9%



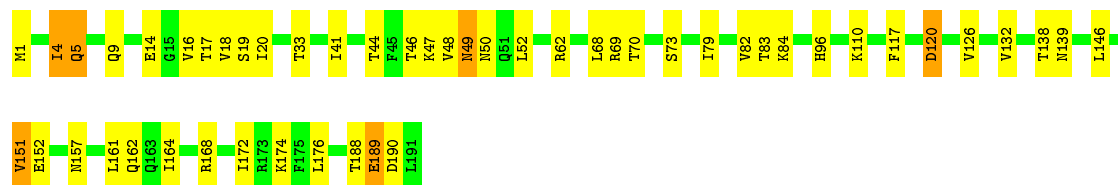
- Molecule 45: 60S ribosomal protein L8-A

Chain 18: 71% 19% 9%



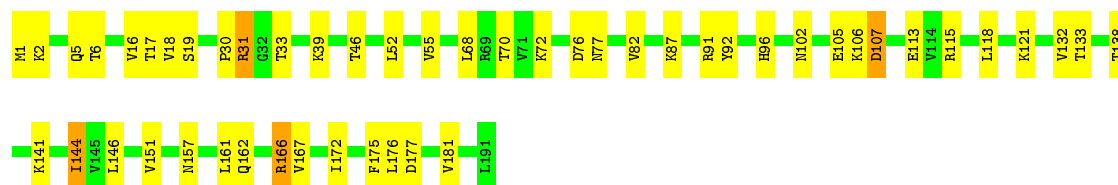
- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 74% 23% 3%



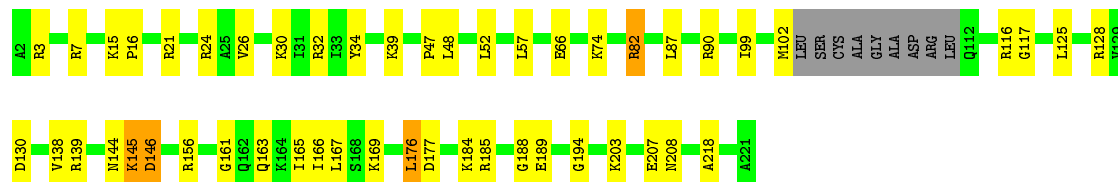
- Molecule 46: 60S ribosomal protein L9-A

Chain 19: 74% 24% 2%



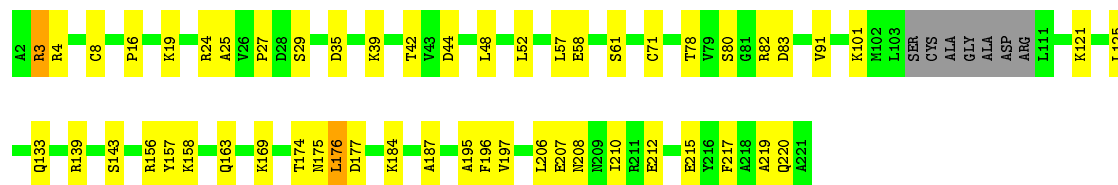
- Molecule 47: 60S ribosomal protein L10

Chain M0: 73% 21% . .



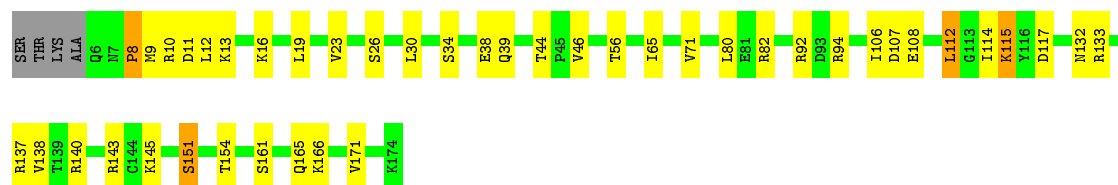
- Molecule 47: 60S ribosomal protein L10

Chain m0: 73% 23% . .



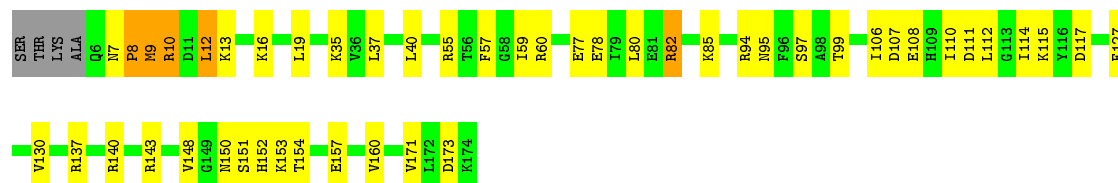
- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 73% 23% . .



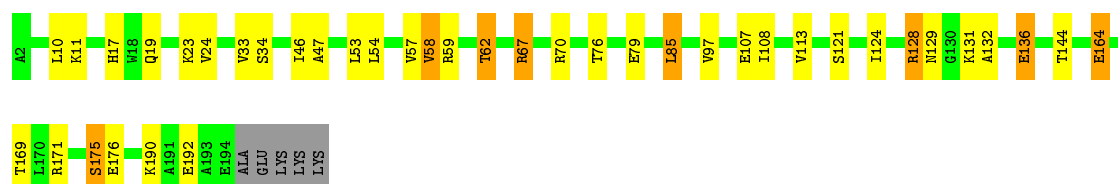
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 70% 25% . .



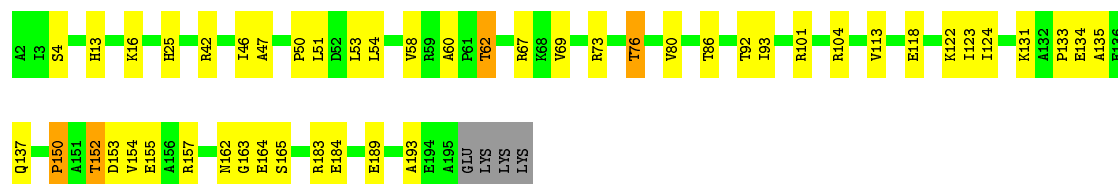
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 77% 16% . .



- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 74% 22% ..



- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 77% 21% ..



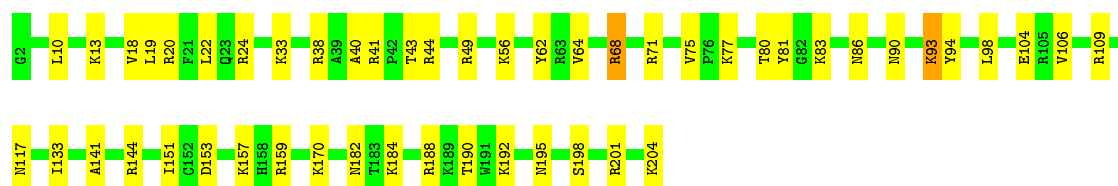
- Molecule 50: 60S ribosomal protein L14-A

Chain m4: 82% 16% .



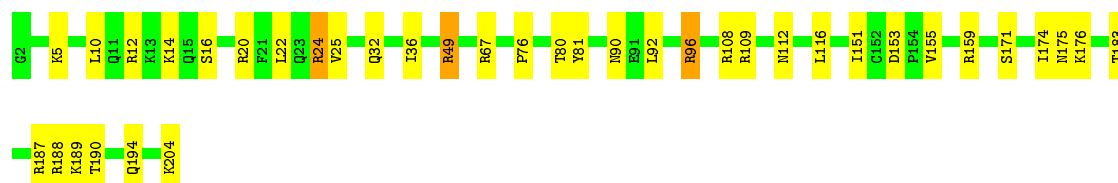
- Molecule 51: 60S ribosomal protein L15-A

Chain M5: 75% 24% .

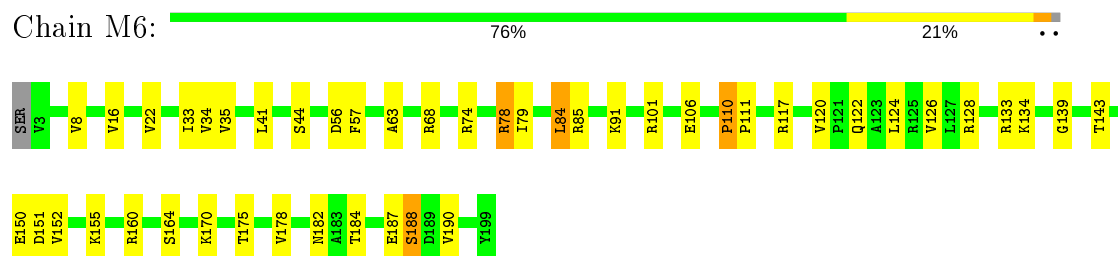


- Molecule 51: 60S ribosomal protein L15-A

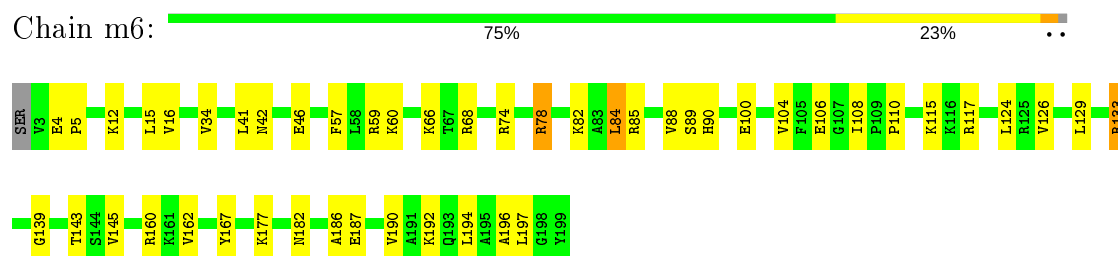
Chain m5: 81% 17% .



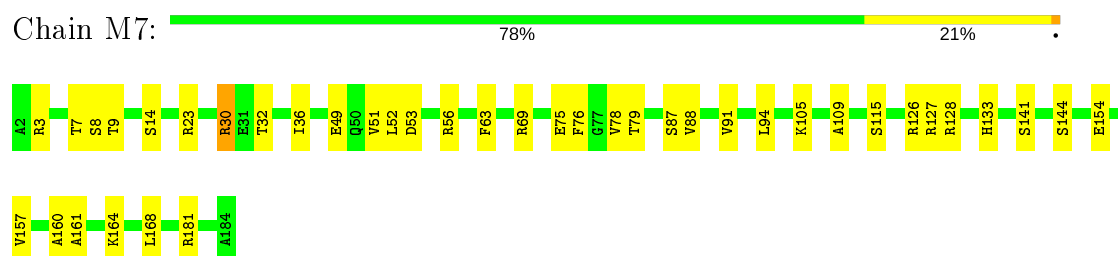
- Molecule 52: 60S ribosomal protein L16-A



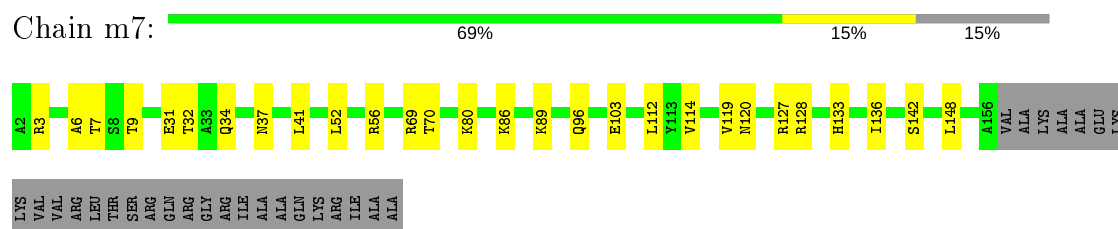
- Molecule 52: 60S ribosomal protein L16-A



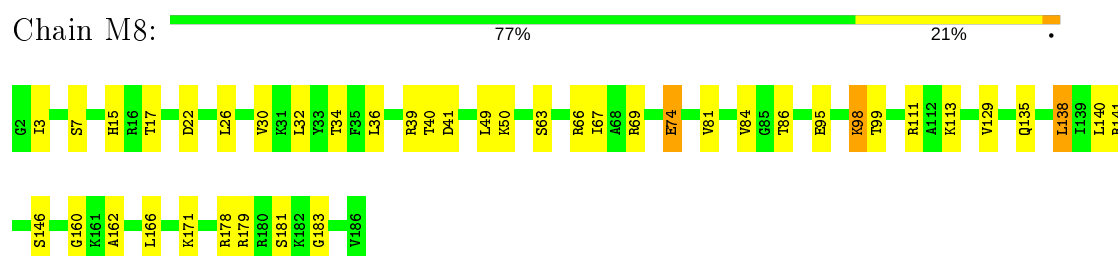
- Molecule 53: 60S ribosomal protein L17-A



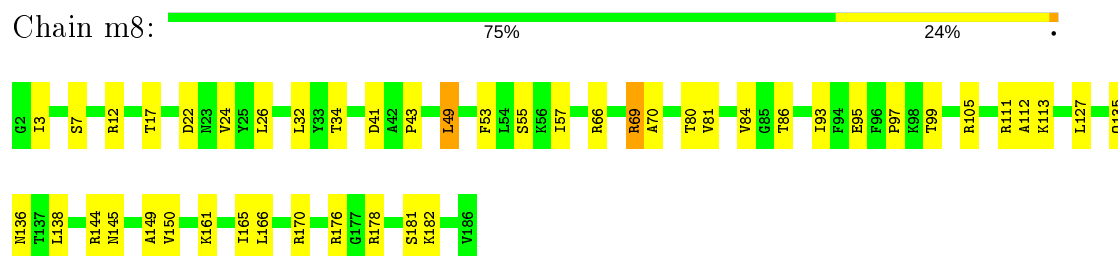
- Molecule 53: 60S ribosomal protein L17-A



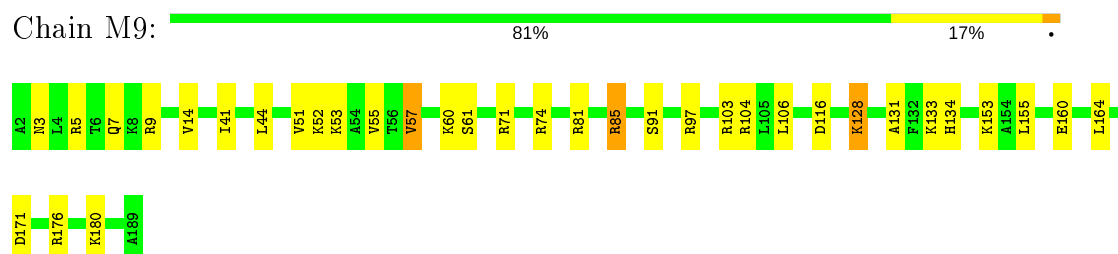
- Molecule 54: 60S ribosomal protein L18-A



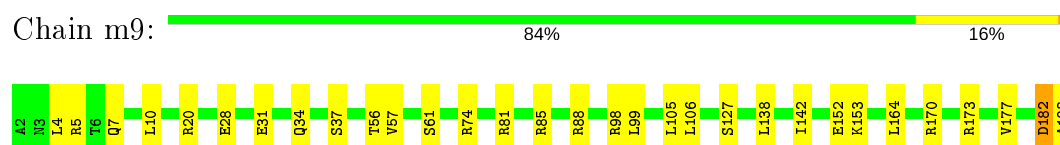
- Molecule 54: 60S ribosomal protein L18-A



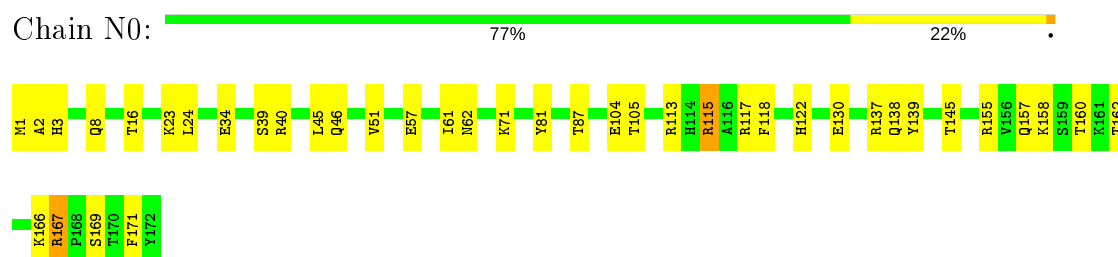
- Molecule 55: 60S ribosomal protein L19-A



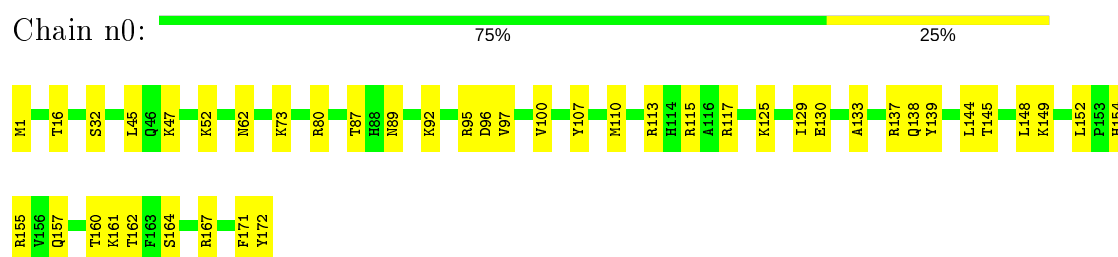
- Molecule 55: 60S ribosomal protein L19-A



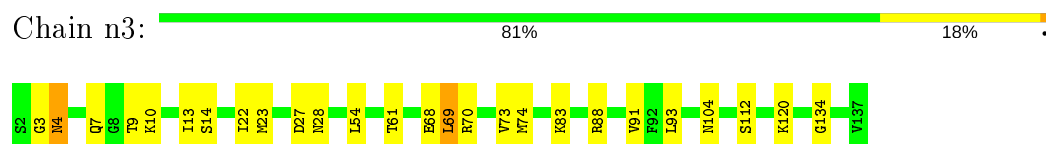
- Molecule 56: 60S ribosomal protein L20-A



- Molecule 56: 60S ribosomal protein L20-A

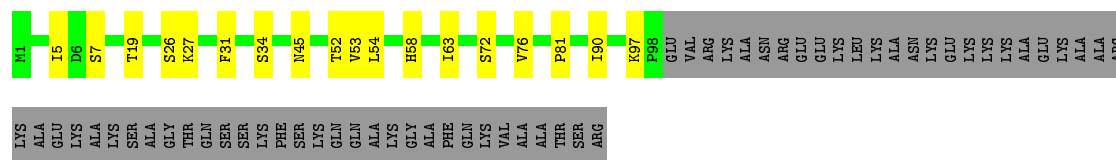


- Molecule 57: 60S ribosomal protein L21-A



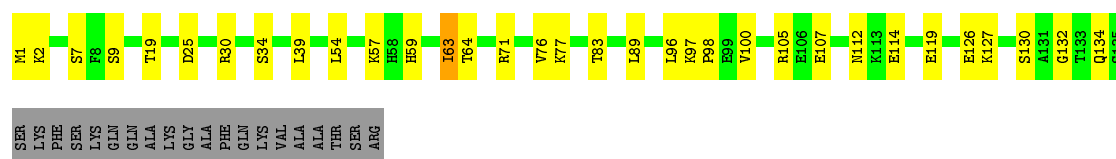
- Molecule 60: 60S ribosomal protein L24-A

Chain N4:  52% 12% 37%



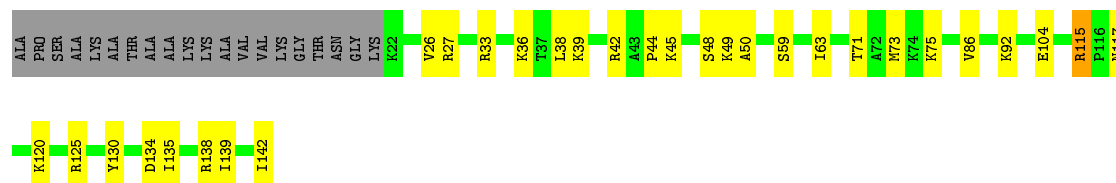
- Molecule 60: 60S ribosomal protein L24-A

Chain n4:  66% 21% 13%



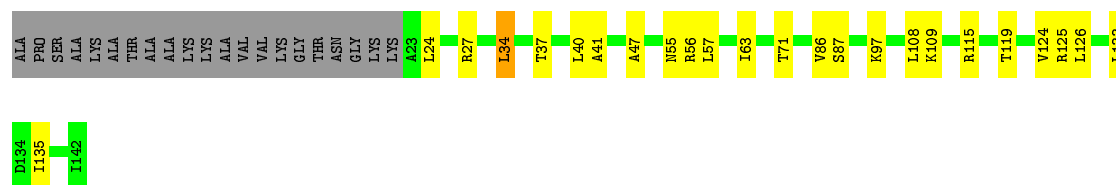
- Molecule 61: 60S ribosomal protein L25

Chain N5:  65% 21% 14%




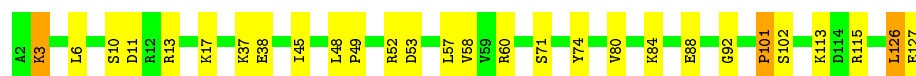
- Molecule 61: 60S ribosomal protein L25

Chain n5:  68% 16% 15%




- Molecule 62: 60S ribosomal protein L26-A

Chain N6:  78% 20% 2%

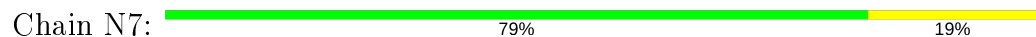


- Molecule 62: 60S ribosomal protein L26-A

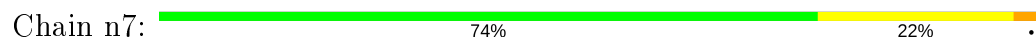
Chain n6:  76% 22% 2%



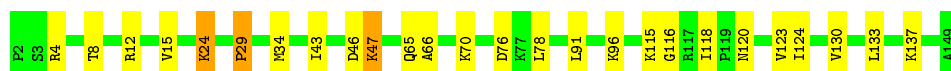
- Molecule 63: 60S ribosomal protein L27-A



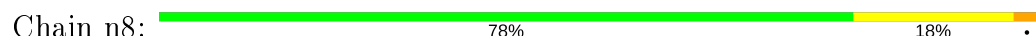
- Molecule 63: 60S ribosomal protein L27-A



- Molecule 64: 60S ribosomal protein L28



- Molecule 64: 60S ribosomal protein L28



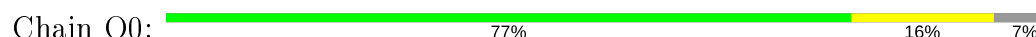
- Molecule 65: 60S ribosomal protein L29



- Molecule 65: 60S ribosomal protein L29

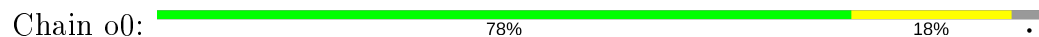


- Molecule 66: 60S ribosomal protein L30





- Molecule 66: 60S ribosomal protein L30



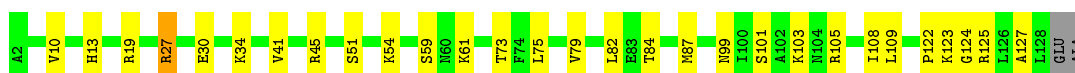
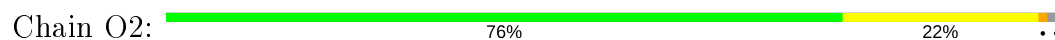
- Molecule 67: 60S ribosomal protein L31-A



- Molecule 67: 60S ribosomal protein L31-A



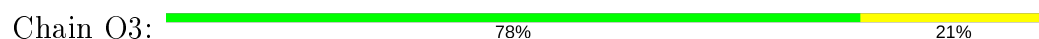
- Molecule 68: 60S ribosomal protein L32

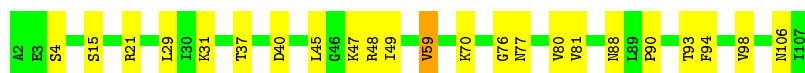


- Molecule 68: 60S ribosomal protein L32

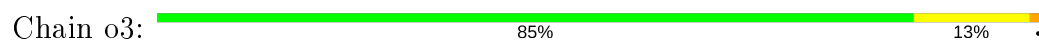


- Molecule 69: 60S ribosomal protein L33-A

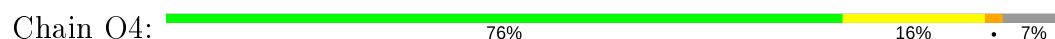




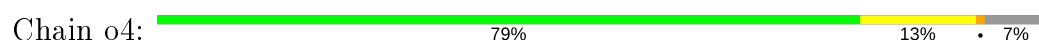
- Molecule 69: 60S ribosomal protein L33-A



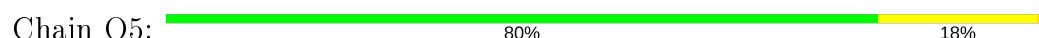
- Molecule 70: 60S ribosomal protein L34-A



- Molecule 70: 60S ribosomal protein L34-A



- Molecule 71: 60S ribosomal protein L35-A



- Molecule 71: 60S ribosomal protein L35-A

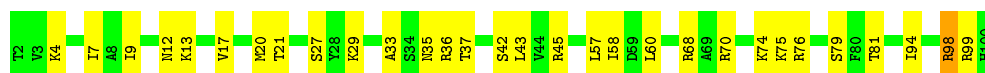


- Molecule 72: 60S ribosomal protein L36-A

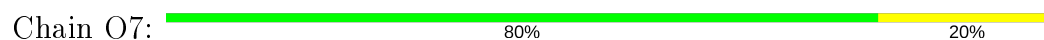


- Molecule 72: 60S ribosomal protein L36-A

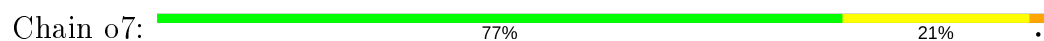




- Molecule 73: 60S ribosomal protein L37-A



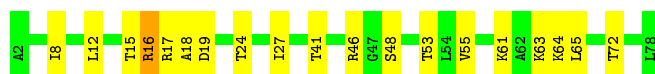
- Molecule 73: 60S ribosomal protein L37-A



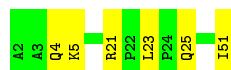
- Molecule 74: 60S ribosomal protein L38



- Molecule 74: 60S ribosomal protein L38



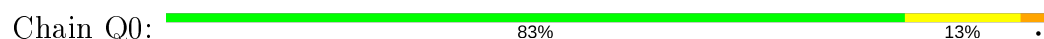
- Molecule 75: 60S ribosomal protein L39



- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40





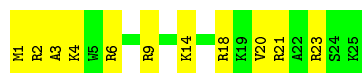
- Molecule 76: Ubiquitin-60S ribosomal protein L40



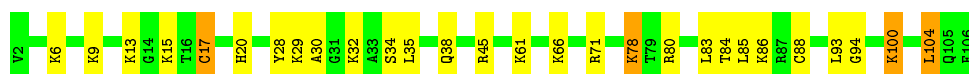
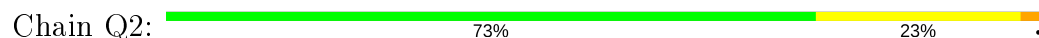
- Molecule 77: 60S ribosomal protein L41-A



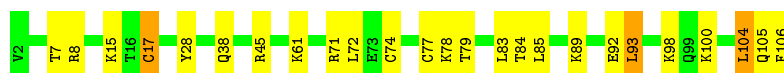
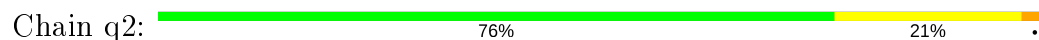
- Molecule 77: 60S ribosomal protein L41-A



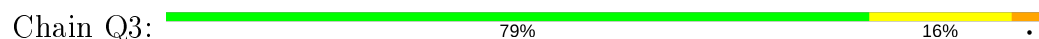
- Molecule 78: 60S ribosomal protein L42-A



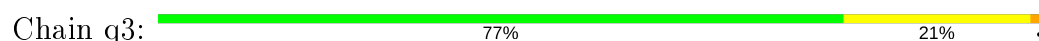
- Molecule 78: 60S ribosomal protein L42-A

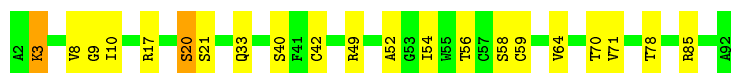


- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A





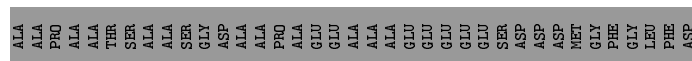
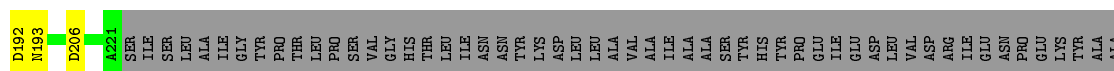
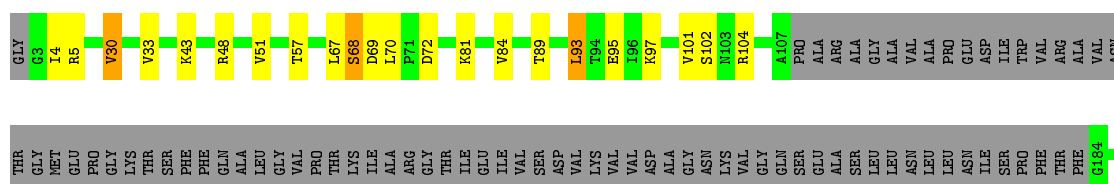
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:  68% 29% .



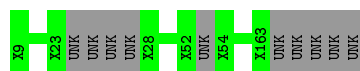
- Molecule 81: 60S acidic ribosomal protein P0

Chain p0: 38% 7% • 54%



- Molecule 82: unknown protein chain m2

Chain m2: 94% 6%



- Molecule 83: unknown protein chain p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

- Molecule 84: unknown protein chain p2

Chain p2: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.64Å 286.76Å 303.26Å 90.00° 98.72° 90.00°	Depositor
Resolution (Å)	299.76 – 3.45	Depositor
% Data completeness (in resolution range)	100.0 (299.76-3.45)	Depositor
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.196 , 0.260	Depositor
Wilson B-factor (Å ²)	93.1	Xtriage
Anisotropy	0.148	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411214	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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, BLS

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	0.74	4/41698 (0.0%)	1.34	362/64972 (0.6%)
1	6	0.83	14/42765 (0.0%)	1.39	467/66634 (0.7%)
2	S0	0.45	0/1617	0.68	0/2215
2	s0	0.47	0/1623	0.67	0/2222
3	S1	0.39	0/1735	0.66	1/2335 (0.0%)
3	s1	0.49	0/1748	0.68	0/2352
4	S2	0.49	0/1665	0.66	0/2263
4	s2	0.55	0/1665	0.77	0/2263
5	S3	0.50	0/1759	0.66	0/2368
5	s3	0.46	0/1759	0.64	1/2368 (0.0%)
6	S4	0.52	0/2109	0.73	0/2839
6	s4	0.53	0/2109	0.72	0/2839
7	S5	0.42	0/1629	0.64	0/2202
7	s5	0.45	0/1629	0.69	0/2202
8	S6	0.49	0/1823	0.65	0/2439
8	s6	0.59	1/1779 (0.1%)	0.72	1/2379 (0.0%)
9	S7	0.44	0/1506	0.68	0/2028
9	s7	0.45	0/1516	0.69	0/2043
10	S8	0.56	0/1514	0.74	1/2021 (0.0%)
10	s8	0.55	0/1514	0.71	0/2021
11	S9	0.48	0/1519	0.68	1/2035 (0.0%)
11	s9	0.54	0/1519	0.71	0/2035
12	C0	0.46	0/790	0.68	1/1069 (0.1%)
12	c0	0.41	0/777	0.69	3/1049 (0.3%)
13	C1	0.59	0/1240	0.76	1/1675 (0.1%)
13	c1	0.59	0/1194	0.76	0/1610
14	C2	0.41	0/900	0.65	0/1224
14	c2	0.32	0/900	0.60	0/1224
15	C3	0.52	0/1215	0.70	2/1638 (0.1%)
15	c3	0.55	0/1215	0.69	0/1638
16	C4	0.40	0/901	0.64	0/1217
16	c4	0.50	0/960	0.70	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.52	0/998	0.72	0/1341
17	c5	0.49	0/1060	0.69	1/1426 (0.1%)
18	C6	0.48	0/1125	0.68	2/1510 (0.1%)
18	c6	0.49	0/1131	0.71	0/1518
19	C7	0.48	0/935	0.68	1/1254 (0.1%)
19	c7	0.48	0/914	0.69	0/1224
20	C8	0.47	0/1211	0.70	0/1628
20	c8	0.50	0/1211	0.72	2/1628 (0.1%)
21	C9	0.44	0/1130	0.62	0/1517
21	c9	0.51	0/1130	0.67	0/1517
22	D0	0.45	0/865	0.71	1/1169 (0.1%)
22	d0	0.46	0/892	0.68	0/1205
23	D1	0.47	0/693	0.64	0/935
23	d1	0.51	0/693	0.68	0/935
24	D2	0.49	0/1038	0.71	0/1395
24	d2	0.59	0/1038	0.76	1/1395 (0.1%)
25	D3	0.61	0/1139	0.75	0/1518
25	d3	0.70	0/1139	0.83	1/1518 (0.1%)
26	D4	0.46	0/1087	0.65	0/1449
26	d4	0.55	0/1087	0.73	0/1449
27	D5	0.44	0/571	0.75	0/768
27	d5	0.45	0/566	0.68	0/761
28	D6	0.47	0/782	0.66	0/1047
28	d6	0.54	0/782	0.79	1/1047 (0.1%)
29	D7	0.42	0/620	0.65	0/838
29	d7	0.47	0/620	0.71	0/838
30	D8	0.42	0/499	0.64	0/670
30	d8	0.43	0/499	0.62	0/670
31	D9	0.53	0/452	0.67	0/600
31	d9	0.64	0/452	0.69	0/600
32	E0	0.48	0/483	0.65	0/643
33	E1	0.49	0/577	0.80	0/770
33	e1	0.42	0/619	0.75	1/822 (0.1%)
34	SR	0.40	0/2494	0.63	0/3393
34	sR	0.39	0/2495	0.58	0/3395
35	SM	0.53	0/1113	0.71	2/1502 (0.1%)
35	sM	0.49	0/682	0.69	1/921 (0.1%)
36	1	1.12	138/75394 (0.2%)	1.68	1938/117545 (1.6%)
36	5	1.11	157/75414 (0.2%)	1.68	1917/117575 (1.6%)
37	3	0.99	2/2883 (0.1%)	1.47	39/4491 (0.9%)
37	7	1.11	3/2883 (0.1%)	1.76	76/4491 (1.7%)
38	4	1.02	1/3746 (0.0%)	1.59	63/5832 (1.1%)
38	8	0.90	2/3746 (0.1%)	1.47	43/5832 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.68	0/1948	0.81	1/2617 (0.0%)
39	l2	0.60	0/1946	0.82	2/2614 (0.1%)
40	L3	0.74	0/3146	0.83	0/4228
40	l3	0.78	0/3146	0.86	2/4228 (0.0%)
41	L4	0.78	1/2800 (0.0%)	0.90	1/3790 (0.0%)
41	l4	0.73	1/2800 (0.0%)	0.88	3/3790 (0.1%)
42	L5	0.61	0/2425	0.73	0/3271
42	l5	0.72	0/2408	0.83	1/3248 (0.0%)
43	L6	0.78	0/1260	0.85	0/1694
43	l6	0.81	0/1269	0.87	0/1705
44	L7	0.83	0/1821	0.91	3/2451 (0.1%)
44	l7	0.87	0/1828	0.97	5/2461 (0.2%)
45	L8	0.54	0/1836	0.71	2/2481 (0.1%)
45	l8	0.48	0/1795	0.68	1/2429 (0.0%)
46	L9	0.69	0/1539	0.81	1/2073 (0.0%)
46	l9	0.76	0/1539	0.84	2/2073 (0.1%)
47	M0	0.76	0/1741	0.84	3/2335 (0.1%)
47	m0	0.76	1/1758 (0.1%)	0.82	0/2358
48	M1	0.56	0/1374	0.74	1/1842 (0.1%)
48	m1	0.70	0/1374	0.80	1/1842 (0.1%)
49	M3	0.72	0/1568	0.86	2/2106 (0.1%)
49	m3	0.64	0/1573	0.78	0/2113
50	M4	0.81	0/1068	0.88	1/1438 (0.1%)
50	m4	0.82	0/1074	0.84	1/1446 (0.1%)
51	M5	0.75	0/1757	0.86	2/2354 (0.1%)
51	m5	0.61	0/1757	0.79	2/2354 (0.1%)
52	M6	0.85	0/1585	0.92	4/2128 (0.2%)
52	m6	0.96	0/1585	0.98	4/2128 (0.2%)
53	M7	0.76	0/1443	0.83	0/1944
53	m7	0.83	0/1250	0.87	1/1683 (0.1%)
54	M8	0.75	0/1465	0.90	4/1965 (0.2%)
54	m8	0.72	0/1465	0.86	1/1965 (0.1%)
55	M9	0.60	0/1538	0.75	0/2050
55	m9	0.58	0/1538	0.69	0/2050
56	N0	0.78	0/1481	0.85	1/1990 (0.1%)
56	n0	0.88	0/1481	0.90	2/1990 (0.1%)
57	N1	0.74	0/1300	0.82	1/1743 (0.1%)
57	n1	0.81	1/1300 (0.1%)	0.88	0/1743
58	N2	0.48	0/812	0.63	0/1099
58	n2	0.49	0/794	0.68	0/1076
59	N3	0.69	0/1018	0.81	0/1369
59	n3	0.80	0/1018	0.82	0/1369
60	N4	0.62	0/712	0.74	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.65	0/1052	0.75	0/1398
61	N5	0.64	0/979	0.79	1/1321 (0.1%)
61	n5	0.60	0/974	0.77	1/1314 (0.1%)
62	N6	0.72	0/1004	0.86	1/1341 (0.1%)
62	n6	0.62	0/1004	0.81	0/1341
63	N7	0.54	0/1118	0.68	0/1497
63	n7	0.48	0/1118	0.66	0/1497
64	N8	0.73	0/1204	0.85	0/1612
64	n8	0.73	0/1204	0.84	1/1612 (0.1%)
65	N9	0.69	0/473	0.83	1/629 (0.2%)
65	n9	0.71	0/473	0.88	0/629
66	O0	0.49	0/751	0.68	0/1008
66	o0	0.53	0/775	0.69	0/1040
67	O1	0.65	0/890	0.80	0/1196
67	o1	0.71	0/897	0.86	2/1205 (0.2%)
68	O2	0.79	0/1041	0.87	0/1394
68	o2	0.87	0/1041	0.89	0/1394
69	O3	0.86	0/868	0.94	0/1168
69	o3	0.87	0/868	0.90	0/1168
70	O4	0.59	0/890	0.77	1/1189 (0.1%)
70	o4	0.52	0/890	0.74	0/1189
71	O5	0.67	0/978	0.78	0/1301
71	o5	0.58	0/974	0.77	2/1297 (0.2%)
72	O6	0.61	0/778	0.77	0/1034
72	o6	0.58	0/777	0.68	0/1033
73	O7	0.74	0/696	0.87	1/923 (0.1%)
73	o7	0.64	0/696	0.79	0/923
74	O8	0.53	0/618	0.66	0/826
74	o8	0.45	0/614	0.66	0/822
75	O9	0.64	0/443	0.82	0/588
75	o9	0.62	0/443	0.78	0/588
76	Q0	0.79	0/423	0.93	0/562
76	q0	0.90	1/423 (0.2%)	0.98	0/562
77	Q1	0.67	0/234	0.87	0/300
77	q1	0.58	0/234	0.89	0/300
78	Q2	0.83	1/860 (0.1%)	0.84	0/1136
78	q2	0.73	1/860 (0.1%)	0.83	2/1136 (0.2%)
79	Q3	0.71	0/701	0.83	0/934
79	q3	0.68	0/701	0.78	0/934
80	e0	0.51	0/499	0.75	0/665
81	p0	0.48	0/1091	0.64	0/1472
All	All	0.87	329/430072 (0.1%)	1.32	4999/631360 (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
3	S1	0	1
7	s5	0	2
9	S7	0	1
9	s7	0	1
10	S8	0	1
11	S9	0	1
16	C4	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	1
20	c8	0	1
22	d0	0	1
26	d4	0	1
27	D5	0	2
33	E1	0	1
39	L2	0	1
39	l2	0	1
40	L3	0	1
40	l3	0	1
42	L5	0	1
43	L6	0	1
44	l7	0	1
45	L8	0	1
47	M0	0	1
48	M1	0	1
48	m1	0	1
50	M4	0	1
52	M6	0	1
56	n0	0	2
64	n8	0	1
65	N9	0	1
67	O1	0	1
69	o3	0	1
80	e0	0	1
All	All	0	37

All (329) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	12.22	2.03	1.82
36	5	1152	G	N9-C4	-12.11	1.28	1.38
36	5	2145	A	N7-C5	-9.34	1.33	1.39
78	q2	17	CYS	CB-SG	9.04	1.97	1.82
36	5	3040	A	N9-C4	-8.70	1.32	1.37
36	5	1303	A	N9-C4	-8.37	1.32	1.37
36	5	1152	G	N3-C4	-8.29	1.29	1.35
37	3	66	A	N9-C4	-7.99	1.33	1.37
36	5	3040	A	N3-C4	-7.90	1.30	1.34
36	1	3000	A	N9-C4	-7.85	1.33	1.37
36	5	1159	A	N9-C4	-7.83	1.33	1.37
36	1	645	A	C6-N1	-7.71	1.30	1.35
36	1	2748	A	N9-C4	-7.70	1.33	1.37
36	1	1304	A	N9-C4	-7.60	1.33	1.37
36	1	3273	A	N3-C4	-7.58	1.30	1.34
36	1	2714	G	N9-C4	-7.49	1.31	1.38
36	5	607	A	N3-C4	-7.38	1.30	1.34
36	1	338	A	N7-C5	-7.35	1.34	1.39
47	m0	8	CYS	CB-SG	-7.33	1.69	1.82
36	5	706	A	N9-C4	-7.28	1.33	1.37
1	6	359	A	N9-C4	-7.17	1.33	1.37
36	5	924	G	N9-C4	-7.11	1.32	1.38
36	5	2879	C	N1-C6	-7.08	1.32	1.37
1	6	65	A	N9-C4	-7.02	1.33	1.37
36	5	1370	G	C6-N1	-7.02	1.34	1.39
36	1	1116	G	C5-C4	-7.00	1.33	1.38
36	5	3130	A	N3-C4	-6.98	1.30	1.34
36	5	397	A	N3-C4	-6.93	1.30	1.34
36	5	1135	A	N3-C4	-6.93	1.30	1.34
1	6	100	A	N7-C5	-6.91	1.35	1.39
76	q0	99	CYS	CB-SG	-6.91	1.70	1.82
36	5	522	A	N7-C5	-6.89	1.35	1.39
36	5	1205	A	N7-C5	-6.83	1.35	1.39
36	5	1432	C	N3-C4	-6.80	1.29	1.33
36	5	874	U	N1-C2	-6.75	1.32	1.38
36	5	936	A	N7-C5	-6.75	1.35	1.39
36	5	2860	U	N1-C2	6.74	1.44	1.38
36	5	924	G	N3-C4	-6.72	1.30	1.35
36	1	3091	A	N9-C4	-6.71	1.33	1.37
36	5	1192	C	N1-C2	6.68	1.46	1.40
36	5	2910	A	N3-C4	-6.68	1.30	1.34
36	1	2355	G	N7-C5	-6.66	1.35	1.39
36	5	1332	A	N7-C5	-6.63	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	806	A	N9-C4	-6.59	1.33	1.37
36	5	375	A	N9-C4	-6.59	1.33	1.37
36	1	1165	A	N9-C4	-6.56	1.33	1.37
36	5	2726	C	N3-C4	-6.54	1.29	1.33
36	5	2639	G	N7-C5	-6.54	1.35	1.39
36	5	1432	C	N1-C6	-6.52	1.33	1.37
36	1	1149	G	N3-C4	-6.51	1.30	1.35
36	1	342	A	N9-C4	-6.49	1.33	1.37
36	5	2368	A	N7-C5	-6.44	1.35	1.39
1	6	417	A	N9-C4	6.41	1.41	1.37
36	1	2823	G	N9-C8	-6.36	1.33	1.37
36	1	66	A	N9-C4	-6.31	1.34	1.37
36	1	972	A	C5-C4	-6.30	1.34	1.38
36	5	2358	A	N9-C4	-6.28	1.34	1.37
1	6	1746	A	N7-C5	-6.25	1.35	1.39
36	5	61	A	C6-N1	-6.25	1.31	1.35
36	1	71	A	N3-C4	-6.23	1.31	1.34
36	5	924	G	C2-N3	-6.22	1.27	1.32
36	5	2640	A	N9-C4	-6.22	1.34	1.37
36	1	1154	A	N7-C5	-6.21	1.35	1.39
36	5	647	A	N7-C5	-6.21	1.35	1.39
38	8	104	A	N9-C4	-6.20	1.34	1.37
36	1	2200	U	C4-O4	6.17	1.28	1.23
36	1	3006	A	N9-C4	-6.17	1.34	1.37
36	5	1172	G	N3-C4	-6.17	1.31	1.35
1	2	793	A	N9-C4	6.15	1.41	1.37
36	5	808	A	N3-C4	-6.15	1.31	1.34
37	7	102	A	N9-C4	-6.14	1.34	1.37
36	1	969	C	N1-C6	-6.13	1.33	1.37
36	1	2762	A	N3-C4	-6.12	1.31	1.34
36	1	936	A	N9-C4	-6.12	1.34	1.37
36	5	423	A	C5-C6	-6.12	1.35	1.41
36	1	1330	A	N9-C4	-6.11	1.34	1.37
36	5	2704	A	N9-C4	-6.11	1.34	1.37
36	5	1152	G	C5-C6	-6.10	1.36	1.42
36	1	1103	A	N7-C5	6.09	1.43	1.39
36	1	2679	A	N9-C4	-6.09	1.34	1.37
36	1	1406	A	C5-C6	-6.09	1.35	1.41
36	1	2363	A	N9-C4	-6.09	1.34	1.37
36	1	585	A	C6-N1	-6.08	1.31	1.35
36	1	1394	A	N9-C4	-6.07	1.34	1.37
36	1	1103	A	N9-C4	6.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2971	A	N9-C4	6.06	1.41	1.37
37	7	85	G	N7-C5	-6.05	1.35	1.39
36	1	71	A	N9-C4	-6.03	1.34	1.37
36	1	355	A	N9-C4	-6.02	1.34	1.37
36	1	2409	G	N9-C8	-6.02	1.33	1.37
36	5	1348	U	N1-C2	6.00	1.44	1.38
36	1	647	A	N7-C5	-6.00	1.35	1.39
36	5	1103	A	N3-C4	5.99	1.38	1.34
36	5	519	A	C5-C6	-5.99	1.35	1.41
36	1	3006	A	N3-C4	-5.97	1.31	1.34
36	5	2932	U	C2-N3	-5.97	1.33	1.37
36	5	1149	G	N3-C4	-5.96	1.31	1.35
36	5	2138	A	N7-C5	-5.96	1.35	1.39
1	2	1124	A	N9-C4	-5.95	1.34	1.37
36	1	1103	A	N3-C4	5.94	1.38	1.34
36	5	343	U	N1-C2	-5.94	1.33	1.38
36	1	638	C	N1-C6	-5.92	1.33	1.37
36	5	1467	A	N9-C4	-5.92	1.34	1.37
41	L4	199	TRP	CB-CG	-5.91	1.39	1.50
36	1	953	G	C5-C6	-5.91	1.36	1.42
36	1	2656	A	N7-C5	-5.91	1.35	1.39
36	5	807	A	N7-C5	-5.89	1.35	1.39
36	5	2377	G	C6-N1	-5.88	1.35	1.39
36	1	1476	G	C6-N1	-5.88	1.35	1.39
36	5	522	A	C5-C6	-5.87	1.35	1.41
36	5	1370	G	N3-C4	-5.86	1.31	1.35
36	1	668	G	N3-C4	-5.86	1.31	1.35
36	5	2282	U	N1-C2	-5.86	1.33	1.38
36	5	2643	A	N9-C4	-5.85	1.34	1.37
36	1	659	G	C5-C4	-5.85	1.34	1.38
36	1	2207	A	N9-C4	5.84	1.41	1.37
36	5	1130	A	C5-C4	-5.83	1.34	1.38
36	1	1148	G	N7-C5	-5.83	1.35	1.39
36	5	2994	A	N3-C4	-5.82	1.31	1.34
36	5	917	A	N7-C5	-5.80	1.35	1.39
36	5	921	A	N3-C4	-5.79	1.31	1.34
36	5	1432	C	C2-N3	-5.79	1.31	1.35
36	1	45	A	N3-C4	-5.78	1.31	1.34
36	1	2333	C	N3-C4	-5.78	1.29	1.33
36	1	676	G	N9-C4	5.76	1.42	1.38
36	5	1306	G	C5-C6	-5.74	1.36	1.42
36	1	2986	U	N1-C2	-5.72	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	1047	A	N3-C4	-5.72	1.31	1.34
36	1	2147	A	N9-C4	-5.72	1.34	1.37
36	5	1159	A	N3-C4	-5.72	1.31	1.34
36	5	40	A	N7-C5	-5.72	1.35	1.39
36	5	3245	A	C5-C6	-5.72	1.35	1.41
36	1	695	C	N1-C6	-5.72	1.33	1.37
36	5	652	G	N3-C4	-5.72	1.31	1.35
36	1	2200	U	C2-N3	5.71	1.41	1.37
36	5	1849	C	N1-C2	-5.70	1.34	1.40
37	7	96	U	N1-C2	-5.70	1.33	1.38
36	5	1135	A	C6-N1	-5.70	1.31	1.35
36	1	1369	A	N7-C5	-5.70	1.35	1.39
36	5	884	A	N9-C4	-5.70	1.34	1.37
36	5	931	C	N3-C4	-5.69	1.29	1.33
36	5	652	G	N1-C2	-5.68	1.33	1.37
36	1	947	G	N7-C5	-5.67	1.35	1.39
36	1	2313	A	N9-C4	-5.67	1.34	1.37
36	1	928	C	N3-C4	-5.67	1.29	1.33
36	5	2295	A	C5-C6	-5.65	1.35	1.41
36	5	2851	A	N9-C4	-5.65	1.34	1.37
36	1	970	A	N3-C4	-5.64	1.31	1.34
36	1	653	A	C5-C6	-5.64	1.35	1.41
36	5	2970	C	N1-C6	-5.63	1.33	1.37
36	5	1152	G	N7-C5	-5.62	1.35	1.39
57	n1	104	GLU	CB-CG	5.61	1.62	1.52
36	1	2352	A	N9-C4	5.61	1.41	1.37
36	5	2248	C	N1-C6	-5.61	1.33	1.37
36	5	2113	A	N9-C4	-5.60	1.34	1.37
36	5	2377	G	N1-C2	-5.59	1.33	1.37
36	5	2966	G	N7-C5	-5.58	1.35	1.39
36	1	585	A	N3-C4	-5.58	1.31	1.34
36	1	2983	C	N3-C4	-5.58	1.30	1.33
36	1	979	U	N1-C2	5.58	1.43	1.38
36	1	908	G	N7-C5	-5.56	1.35	1.39
36	5	1462	A	N9-C4	-5.56	1.34	1.37
36	5	1902	G	N3-C4	-5.56	1.31	1.35
36	5	880	G	N7-C5	-5.55	1.35	1.39
36	5	2279	A	N9-C4	-5.55	1.34	1.37
36	1	187	A	N9-C4	5.55	1.41	1.37
36	1	1119	C	N3-C4	-5.55	1.30	1.33
36	1	2812	C	N1-C6	-5.55	1.33	1.37
36	1	2422	C	N3-C4	-5.54	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1200	A	N7-C5	-5.54	1.35	1.39
36	1	1371	G	N3-C4	-5.54	1.31	1.35
36	1	940	G	C6-N1	-5.53	1.35	1.39
36	1	2296	A	N9-C4	-5.52	1.34	1.37
36	1	1891	A	N9-C4	-5.48	1.34	1.37
36	5	3000	A	N9-C4	-5.48	1.34	1.37
36	5	3209	A	C5-C4	5.48	1.42	1.38
36	1	1304	A	N3-C4	-5.48	1.31	1.34
36	1	218	G	N9-C8	-5.47	1.34	1.37
36	1	342	A	N3-C4	-5.47	1.31	1.34
36	1	1119	C	N1-C6	-5.47	1.33	1.37
36	5	3094	A	N9-C4	-5.47	1.34	1.37
36	1	1159	A	N9-C4	-5.46	1.34	1.37
36	5	3052	G	C6-N1	-5.46	1.35	1.39
36	1	100	A	N3-C4	-5.46	1.31	1.34
36	1	925	A	N3-C4	-5.46	1.31	1.34
36	5	672	A	N3-C4	-5.45	1.31	1.34
36	5	2840	C	N1-C6	-5.44	1.33	1.37
1	6	1137	A	N9-C4	-5.43	1.34	1.37
36	5	2626	A	N9-C4	-5.43	1.34	1.37
36	5	1429	G	N9-C4	-5.43	1.33	1.38
36	5	1143	A	N9-C4	-5.42	1.34	1.37
36	5	1370	G	N9-C8	-5.42	1.34	1.37
36	5	1081	U	N1-C2	5.42	1.43	1.38
36	5	2386	A	N7-C5	-5.41	1.36	1.39
36	5	2131	A	N7-C5	-5.40	1.36	1.39
36	5	942	U	C4-O4	5.40	1.27	1.23
36	5	3091	A	N3-C4	-5.40	1.31	1.34
36	1	2401	A	N3-C4	5.39	1.38	1.34
36	5	2872	A	N9-C4	-5.39	1.34	1.37
36	1	1153	A	C6-N1	-5.39	1.31	1.35
36	5	34	A	N9-C4	-5.37	1.34	1.37
36	5	1432	C	N1-C2	-5.37	1.34	1.40
36	5	3209	A	C5-C6	5.37	1.45	1.41
36	5	1174	G	C5-C4	-5.37	1.34	1.38
36	1	585	A	N9-C4	-5.37	1.34	1.37
1	6	337	G	C2-N3	5.36	1.37	1.32
36	5	2891	U	C2-N3	-5.36	1.34	1.37
1	6	542	A	N7-C5	-5.35	1.36	1.39
36	5	2386	A	C5-C6	-5.35	1.36	1.41
36	5	2610	G	N7-C5	-5.35	1.36	1.39
36	1	2386	A	N7-C5	-5.35	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	645	A	C6-N6	-5.34	1.29	1.33
36	1	1143	A	N7-C5	-5.34	1.36	1.39
36	5	947	G	N3-C4	-5.34	1.31	1.35
36	5	2910	A	N9-C4	-5.33	1.34	1.37
36	5	519	A	N7-C5	-5.33	1.36	1.39
36	5	655	C	N3-C4	-5.33	1.30	1.33
36	5	349	A	C5-C4	-5.33	1.35	1.38
36	1	635	G	C5-C4	-5.33	1.34	1.38
36	1	1714	A	N9-C4	-5.33	1.34	1.37
36	1	1351	U	N1-C2	5.32	1.43	1.38
36	5	2873	U	N1-C2	5.31	1.43	1.38
36	5	2918	G	N7-C5	-5.31	1.36	1.39
36	5	965	A	C6-N1	-5.30	1.31	1.35
36	1	98	G	N3-C4	-5.30	1.31	1.35
36	1	965	A	N9-C4	-5.30	1.34	1.37
36	1	1116	G	C6-N1	-5.29	1.35	1.39
36	5	43	A	N9-C4	-5.28	1.34	1.37
36	1	218	G	N7-C5	-5.28	1.36	1.39
41	14	94	CYS	CB-SG	-5.28	1.73	1.81
36	1	921	A	N3-C4	-5.28	1.31	1.34
36	1	2811	A	C6-N1	-5.27	1.31	1.35
36	1	1116	G	N3-C4	-5.26	1.31	1.35
36	1	642	U	C4-O4	5.26	1.27	1.23
36	1	3209	A	C5-C4	5.26	1.42	1.38
36	1	610	G	N9-C4	-5.25	1.33	1.38
36	1	2875	U	N1-C2	5.25	1.43	1.38
36	1	1149	G	N9-C8	-5.25	1.34	1.37
36	5	929	A	N3-C4	-5.25	1.31	1.34
36	1	1148	G	N9-C8	-5.24	1.34	1.37
36	5	3245	A	N3-C4	-5.24	1.31	1.34
36	5	3209	A	N7-C5	5.24	1.42	1.39
36	1	2244	A	N3-C4	-5.24	1.31	1.34
36	5	2976	A	N3-C4	-5.24	1.31	1.34
36	1	2386	A	C5-C6	-5.23	1.36	1.41
36	1	2627	C	N1-C6	-5.23	1.34	1.37
36	5	2131	A	C5-C6	-5.23	1.36	1.41
36	5	1061	A	N3-C4	-5.23	1.31	1.34
36	5	3081	C	N3-C4	-5.22	1.30	1.33
36	5	2302	G	C6-N1	-5.22	1.35	1.39
36	1	39	A	N9-C4	-5.21	1.34	1.37
36	5	2866	U	N1-C2	5.21	1.43	1.38
36	1	2986	U	C2-N3	-5.21	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2524	A	N9-C4	-5.21	1.34	1.37
36	5	3091	A	C6-N1	-5.21	1.31	1.35
1	2	971	A	N7-C5	-5.20	1.36	1.39
36	1	1165	A	N3-C4	-5.20	1.31	1.34
36	5	887	G	C5-C6	-5.20	1.37	1.42
36	5	2910	A	C5-C4	-5.20	1.35	1.38
1	6	390	G	N7-C5	-5.20	1.36	1.39
1	6	436	A	N7-C5	-5.20	1.36	1.39
36	1	98	G	C6-N1	-5.20	1.35	1.39
36	1	2797	C	N1-C6	-5.19	1.34	1.37
36	1	670	C	N1-C6	-5.19	1.34	1.37
36	5	2813	A	N7-C5	-5.19	1.36	1.39
36	1	2232	A	N9-C4	-5.17	1.34	1.37
36	5	1107	C	N1-C6	-5.17	1.34	1.37
36	5	980	A	C5-C6	5.17	1.45	1.41
36	5	2610	G	N3-C4	-5.17	1.31	1.35
36	5	2917	G	C5-C4	-5.16	1.34	1.38
36	1	970	A	N9-C4	-5.16	1.34	1.37
36	1	1001	G	C6-N1	5.16	1.43	1.39
36	5	2403	G	C6-N1	5.15	1.43	1.39
36	1	360	G	N7-C5	-5.15	1.36	1.39
1	6	1746	A	N9-C4	-5.15	1.34	1.37
37	3	39	C	N3-C4	-5.15	1.30	1.33
1	6	384	G	N9-C4	-5.15	1.33	1.38
36	1	2682	C	N3-C4	-5.14	1.30	1.33
36	5	3012	A	N9-C4	-5.14	1.34	1.37
36	5	921	A	C6-N1	-5.13	1.31	1.35
36	1	35	A	N3-C4	-5.13	1.31	1.34
36	1	1116	G	N7-C5	-5.12	1.36	1.39
36	5	2814	G	C6-N1	-5.12	1.35	1.39
36	1	2762	A	C6-N1	-5.11	1.31	1.35
1	2	863	A	N9-C4	-5.11	1.34	1.37
36	1	2365	C	N1-C6	-5.11	1.34	1.37
36	5	424	G	N7-C5	-5.09	1.36	1.39
36	5	3294	A	N3-C4	-5.09	1.31	1.34
36	5	607	A	C6-N1	-5.09	1.31	1.35
36	5	2698	G	N9-C4	-5.09	1.33	1.38
36	1	817	A	N9-C4	5.08	1.40	1.37
36	5	2145	A	C5-C6	-5.08	1.36	1.41
36	5	1126	G	N7-C5	-5.08	1.36	1.39
36	5	3008	A	N3-C4	-5.08	1.31	1.34
36	1	1153	A	C5-C6	-5.08	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	1903	U	C4-O4	5.08	1.27	1.23
36	1	2620	G	C5-C4	-5.07	1.34	1.38
36	5	957	C	N3-C4	-5.07	1.30	1.33
1	6	1746	A	C5-C4	-5.07	1.35	1.38
36	5	1134	G	N3-C4	-5.06	1.31	1.35
36	1	2377	G	N9-C4	-5.06	1.33	1.38
36	5	1332	A	C5-C6	-5.06	1.36	1.41
38	4	37	A	N3-C4	5.06	1.37	1.34
36	5	2385	G	N9-C4	-5.06	1.33	1.38
36	1	584	G	N7-C5	-5.06	1.36	1.39
36	1	2309	A	C5-C6	-5.05	1.36	1.41
36	1	962	A	N3-C4	-5.05	1.31	1.34
36	1	2247	G	N7-C5	-5.05	1.36	1.39
36	5	1200	A	C5-C6	-5.05	1.36	1.41
36	5	1161	G	N3-C4	5.04	1.39	1.35
36	5	2826	U	C2-N3	-5.04	1.34	1.37
36	1	806	A	C5-C4	-5.04	1.35	1.38
36	5	2338	C	N1-C6	-5.04	1.34	1.37
36	5	567	G	N7-C5	-5.04	1.36	1.39
36	1	1330	A	N3-C4	-5.04	1.31	1.34
36	1	2601	A	N9-C4	-5.03	1.34	1.37
36	5	2703	A	N7-C5	-5.03	1.36	1.39
36	5	2911	A	N7-C5	-5.03	1.36	1.39
36	1	343	U	C2-N3	-5.02	1.34	1.37
36	5	2359	C	N1-C6	-5.02	1.34	1.37
38	8	20	U	N1-C2	-5.02	1.34	1.38
1	6	100	A	C5-C6	-5.02	1.36	1.41
36	1	1192	C	N1-C2	5.01	1.45	1.40
36	5	650	C	N3-C4	-5.01	1.30	1.33
36	5	1189	C	N1-C6	-5.01	1.34	1.37
36	1	2358	A	C5-C6	-5.01	1.36	1.41
8	s6	83	CYS	CB-SG	-5.01	1.73	1.81
36	1	1890	U	N1-C2	-5.01	1.34	1.38
36	1	2178	A	N3-C4	-5.01	1.31	1.34

All (4999) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-19.38	114.37	126.00
36	5	1152	G	N3-C4-C5	17.87	137.53	128.60
36	5	1152	G	C2-N3-C4	-16.63	103.58	111.90
36	1	645	A	N1-C6-N6	-16.45	108.73	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	343	U	O5'-P-OP2	-14.33	92.80	105.70
36	5	1437	C	C6-N1-C2	-13.92	114.73	120.30
36	5	2818	U	O5'-P-OP1	-13.76	93.32	105.70
36	5	1192	C	N1-C2-O2	13.27	126.86	118.90
36	5	1200	A	N1-C6-N6	12.86	126.31	118.60
36	1	2714	G	N3-C4-C5	12.71	134.95	128.60
36	1	959	C	C6-N1-C2	12.63	125.35	120.30
36	5	1129	A	O5'-P-OP2	-12.62	94.34	105.70
36	5	2760	C	N3-C4-C5	12.60	126.94	121.90
36	1	2819	A	O5'-P-OP2	-12.44	94.51	105.70
36	5	1587	A	C8-N9-C4	12.21	110.68	105.80
36	1	369	A	C8-N9-C4	-12.17	100.93	105.80
36	5	1897	G	N1-C6-O6	12.09	127.15	119.90
36	5	1433	A	C8-N9-C4	-11.97	101.01	105.80
36	5	1192	C	N3-C2-O2	-11.95	113.54	121.90
36	5	344	A	O5'-P-OP1	-11.92	94.97	105.70
36	5	715	A	N1-C6-N6	-11.85	111.49	118.60
36	5	917	A	O5'-P-OP2	-11.75	95.13	105.70
36	5	940	G	O5'-P-OP1	-11.69	95.18	105.70
36	5	1152	G	C5-N7-C8	-11.67	98.47	104.30
36	1	1433	A	C8-N9-C4	-11.55	101.18	105.80
36	1	424	G	C5-C6-O6	-11.46	121.73	128.60
36	1	2374	C	C6-N1-C2	-11.45	115.72	120.30
36	5	211	A	O5'-P-OP1	-11.39	95.45	105.70
36	5	2283	G	N1-C6-O6	11.35	126.71	119.90
36	5	424	G	C5-C6-O6	-11.30	121.82	128.60
36	5	2129	U	O5'-P-OP1	-11.27	95.56	105.70
36	1	2996	U	C2-N1-C1'	11.19	131.12	117.70
36	1	3092	C	C6-N1-C2	11.11	124.74	120.30
36	1	2814	G	O5'-P-OP1	-11.10	95.71	105.70
36	1	963	G	O5'-P-OP2	-11.09	95.72	105.70
36	1	1166	G	N1-C6-O6	11.08	126.55	119.90
36	1	645	A	N9-C4-C5	11.06	110.23	105.80
36	5	1311	G	O5'-P-OP2	-10.98	95.82	105.70
36	5	923	C	C6-N1-C2	10.97	124.69	120.30
36	1	1166	G	C5-C6-O6	-10.92	122.05	128.60
36	5	2760	C	C6-N1-C2	10.90	124.66	120.30
36	5	2400	G	N1-C6-O6	10.87	126.42	119.90
1	2	553	G	N1-C6-O6	10.85	126.41	119.90
36	1	2714	G	N3-C4-N9	-10.81	119.52	126.00
36	1	1151	U	C6-N1-C2	-10.80	114.52	121.00
36	1	2374	C	N3-C2-O2	-10.80	114.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2709	C	C6-N1-C2	10.75	124.60	120.30
36	1	2344	U	O5'-P-OP2	-10.72	96.05	105.70
1	2	1082	C	C2-N1-C1'	10.71	130.58	118.80
36	5	924	G	N3-C4-N9	-10.68	119.59	126.00
1	6	1537	C	C6-N1-C2	-10.67	116.03	120.30
36	1	637	C	N1-C2-O2	10.67	125.30	118.90
36	5	3245	A	C2-N3-C4	-10.65	105.27	110.60
36	1	1369	A	O5'-P-OP1	-10.64	96.12	105.70
36	1	2899	C	C6-N1-C2	-10.62	116.05	120.30
36	1	1323	G	C5-C6-O6	-10.62	122.23	128.60
37	7	93	C	O5'-P-OP2	-10.61	96.15	105.70
36	5	2607	G	N1-C6-O6	10.59	126.25	119.90
36	5	907	G	C5-C6-O6	-10.56	122.26	128.60
36	5	1306	G	C5-C6-O6	-10.53	122.28	128.60
36	1	1323	G	C4-C5-N7	10.50	115.00	110.80
36	1	1303	A	N1-C6-N6	10.49	124.90	118.60
36	1	940	G	N1-C6-O6	-10.46	113.62	119.90
36	5	1152	G	N1-C6-O6	10.45	126.17	119.90
38	4	13	A	O5'-P-OP1	-10.44	96.31	105.70
1	6	1773	C	C6-N1-C2	-10.41	116.14	120.30
36	1	2355	G	N1-C6-O6	10.40	126.14	119.90
36	5	422	A	O5'-P-OP2	-10.40	96.34	105.70
1	2	577	G	N1-C6-O6	10.38	126.13	119.90
36	5	2655	U	O5'-P-OP2	-10.37	96.36	105.70
36	1	979	U	N3-C2-O2	-10.35	114.95	122.20
36	5	567	G	C6-C5-N7	-10.31	124.21	130.40
36	5	2880	U	C6-N1-C2	-10.30	114.82	121.00
36	1	1307	G	N9-C4-C5	10.28	109.51	105.40
36	5	2707	C	C6-N1-C2	10.27	124.41	120.30
36	5	887	G	C4-C5-N7	10.22	114.89	110.80
37	7	1	G	N3-C4-C5	-10.22	123.49	128.60
36	1	2869	U	O5'-P-OP1	-10.18	96.54	105.70
36	5	1149	G	N1-C6-O6	10.14	125.98	119.90
36	1	2200	U	N3-C4-O4	10.10	126.47	119.40
36	1	676	G	N3-C4-N9	10.09	132.06	126.00
36	5	2607	G	C5-C6-O6	-10.09	122.55	128.60
36	5	1507	G	O5'-P-OP1	-10.03	96.67	105.70
36	5	924	G	N3-C4-C5	9.99	133.60	128.60
36	5	410	U	C6-N1-C2	-9.99	115.01	121.00
36	5	567	G	N1-C6-O6	9.99	125.89	119.90
36	5	715	A	N9-C4-C5	9.99	109.80	105.80
36	5	1604	G	C4-N9-C1'	9.98	139.48	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2899	C	C2-N1-C1'	9.97	129.77	118.80
36	1	3344	A	N7-C8-N9	9.97	118.78	113.80
36	1	3022	G	C5-C6-O6	-9.95	122.63	128.60
36	5	2726	C	C6-N1-C2	-9.94	116.32	120.30
36	5	1306	G	C4-C5-N7	9.92	114.77	110.80
36	1	676	G	N3-C4-C5	-9.87	123.67	128.60
36	5	693	A	O5'-P-OP1	-9.84	96.84	105.70
36	5	1200	A	C6-C5-N7	-9.84	125.41	132.30
36	1	2412	G	O5'-P-OP2	-9.84	96.85	105.70
36	1	1151	U	C5-C6-N1	9.83	127.62	122.70
36	1	2395	G	N1-C6-O6	9.83	125.80	119.90
36	1	921	A	N1-C6-N6	-9.74	112.75	118.60
36	5	1604	G	C8-N9-C1'	-9.74	114.34	127.00
36	5	874	U	O5'-P-OP1	-9.72	96.95	105.70
36	5	3092	C	C6-N1-C2	9.71	124.18	120.30
36	5	2385	G	O5'-P-OP1	-9.70	96.97	105.70
36	1	709	A	N1-C6-N6	9.68	124.41	118.60
36	5	1200	A	C4-C5-C6	9.67	121.84	117.00
36	1	2881	C	C6-N1-C2	9.64	124.16	120.30
36	1	2996	U	C6-N1-C1'	-9.63	107.71	121.20
1	2	1794	A	O5'-P-OP1	-9.62	97.04	105.70
36	1	3382	U	C2-N1-C1'	9.62	129.24	117.70
36	5	2797	C	C6-N1-C2	-9.62	116.45	120.30
36	5	812	G	O5'-P-OP2	-9.61	97.05	105.70
36	5	720	A	N1-C6-N6	9.60	124.36	118.60
36	1	1192	C	C6-N1-C2	-9.59	116.46	120.30
36	1	3217	C	C2-N1-C1'	9.58	129.34	118.80
36	5	424	G	N1-C6-O6	9.58	125.65	119.90
36	5	2272	G	O4'-C1'-N9	9.56	115.85	108.20
36	1	1166	G	C4-C5-N7	9.56	114.62	110.80
36	5	3245	A	N1-C6-N6	9.55	124.33	118.60
36	5	2385	G	N1-C6-O6	9.52	125.61	119.90
36	1	1365	G	O5'-P-OP1	-9.51	97.14	105.70
36	5	2197	C	C6-N1-C2	9.50	124.10	120.30
1	6	1773	C	N3-C4-C5	-9.47	118.11	121.90
36	1	2287	C	C6-N1-C2	-9.46	116.52	120.30
36	5	1869	C	C6-N1-C2	9.45	124.08	120.30
36	1	1307	G	P-O3'-C3'	9.44	131.03	119.70
36	1	1160	C	C6-N1-C2	9.44	124.07	120.30
36	1	580	C	N1-C2-O2	-9.43	113.24	118.90
36	1	1442	U	N3-C2-O2	9.43	128.80	122.20
36	5	3245	A	C6-C5-N7	-9.42	125.70	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	1	G	N3-C4-N9	9.42	131.65	126.00
36	5	1152	G	C8-N9-C1'	9.40	139.23	127.00
36	1	421	G	N1-C6-O6	-9.40	114.26	119.90
36	5	519	A	N1-C6-N6	9.40	124.24	118.60
36	5	1896	A	O5'-P-OP1	-9.40	97.24	105.70
36	1	2882	U	O5'-P-OP2	-9.40	97.24	105.70
36	1	2200	U	N3-C4-C5	-9.37	108.98	114.60
36	1	948	C	C6-N1-C2	9.36	124.04	120.30
36	1	3204	C	N3-C2-O2	-9.35	115.35	121.90
36	1	676	G	C4-N9-C1'	9.33	138.63	126.50
36	1	2247	G	N1-C6-O6	9.33	125.50	119.90
36	1	1001	G	N9-C4-C5	-9.32	101.67	105.40
36	5	1055	A	O5'-P-OP2	-9.30	97.33	105.70
36	1	1495	U	C5-C6-N1	-9.29	118.06	122.70
36	1	1367	G	C8-N9-C4	9.28	110.11	106.40
36	5	1447	G	O5'-P-OP1	-9.27	97.36	105.70
36	5	1149	G	N3-C2-N2	-9.25	113.42	119.90
36	5	1152	G	C5-C6-N1	-9.23	106.88	111.50
36	1	2406	C	C6-N1-C2	9.22	123.99	120.30
36	1	2968	G	N1-C6-O6	9.22	125.43	119.90
36	1	358	G	N1-C6-O6	9.21	125.43	119.90
36	1	1389	G	N9-C4-C5	-9.21	101.72	105.40
36	1	901	G	N1-C6-O6	9.21	125.42	119.90
1	2	1773	C	C6-N1-C2	-9.20	116.62	120.30
36	1	1314	C	C6-N1-C2	-9.20	116.62	120.30
36	5	668	G	C8-N9-C4	9.18	110.07	106.40
38	4	53	A	N1-C6-N6	-9.17	113.10	118.60
36	1	3362	A	C8-N9-C4	-9.15	102.14	105.80
1	6	337	G	N3-C4-C5	-9.13	124.04	128.60
36	5	2282	U	C5-C6-N1	-9.13	118.14	122.70
36	5	1433	A	N9-C4-C5	9.10	109.44	105.80
36	1	1904	C	C6-N1-C2	-9.10	116.66	120.30
36	1	921	A	N9-C4-C5	9.05	109.42	105.80
36	5	2392	C	C6-N1-C2	9.05	123.92	120.30
36	1	1949	G	O5'-P-OP1	-9.04	97.57	105.70
36	5	2389	C	O5'-P-OP1	-9.04	97.57	105.70
36	5	2416	U	O5'-P-OP2	-9.03	97.58	105.70
38	8	26	U	N3-C2-O2	-9.02	115.89	122.20
36	5	800	G	C6-C5-N7	-9.02	124.99	130.40
36	1	690	A	N1-C6-N6	-9.01	113.19	118.60
36	1	2355	G	C6-C5-N7	-9.01	125.00	130.40
36	1	39	A	N1-C6-N6	-9.01	113.20	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2639	G	C6-C5-N7	-9.00	125.00	130.40
36	5	2413	A	C8-N9-C4	9.00	109.40	105.80
36	1	421	G	C5-C6-N1	8.99	116.00	111.50
36	5	2971	A	C2-N3-C4	8.99	115.10	110.60
36	5	1437	C	C5-C6-N1	8.98	125.49	121.00
36	1	1001	G	C5-C6-O6	-8.97	123.22	128.60
36	1	2395	G	C5-C6-O6	-8.96	123.22	128.60
36	1	3344	A	C8-N9-C4	-8.96	102.22	105.80
36	1	3243	A	N1-C6-N6	8.95	123.97	118.60
36	1	3362	A	N7-C8-N9	8.95	118.28	113.80
36	5	1417	G	C8-N9-C4	-8.94	102.82	106.40
36	5	1124	U	N3-C2-O2	-8.93	115.95	122.20
36	1	1311	G	C5-C6-O6	-8.93	123.24	128.60
36	5	965	A	C8-N9-C4	-8.93	102.23	105.80
36	5	2283	G	C5-C6-O6	-8.93	123.24	128.60
36	5	967	A	C8-N9-C4	-8.93	102.23	105.80
36	1	1314	C	C5-C6-N1	8.92	125.46	121.00
36	5	2322	C	C6-N1-C2	-8.92	116.73	120.30
36	5	1849	C	N1-C2-O2	-8.92	113.55	118.90
36	5	2973	G	O5'-P-OP1	-8.90	97.69	105.70
36	5	907	G	N9-C4-C5	-8.89	101.84	105.40
36	1	608	A	N1-C6-N6	8.87	123.92	118.60
36	5	3154	C	N1-C2-O2	8.87	124.22	118.90
36	1	2995	A	O5'-P-OP2	-8.86	97.73	105.70
36	1	2885	C	C6-N1-C2	8.85	123.84	120.30
36	5	942	U	N3-C4-O4	8.85	125.60	119.40
36	5	1897	G	C5-C6-N1	-8.84	107.08	111.50
36	5	2327	U	C6-N1-C2	8.84	126.30	121.00
36	5	398	A	O5'-P-OP2	-8.84	97.75	105.70
36	1	1843	C	C6-N1-C2	-8.83	116.77	120.30
36	1	1001	G	N1-C6-O6	8.83	125.20	119.90
36	1	609	G	C5-C6-O6	-8.82	123.31	128.60
36	1	1323	G	N9-C4-C5	-8.82	101.87	105.40
36	5	2637	A	O5'-P-OP1	-8.82	97.76	105.70
36	5	3177	G	C2-N3-C4	-8.82	107.49	111.90
36	1	1124	U	OP1-P-O3'	8.82	124.61	105.20
38	4	94	C	C6-N1-C2	8.81	123.83	120.30
1	6	1744	A	N1-C6-N6	8.81	123.89	118.60
36	1	1323	G	N1-C6-O6	8.79	125.18	119.90
1	2	426	G	C8-N9-C1'	-8.79	115.58	127.00
36	5	2285	C	C6-N1-C2	-8.78	116.79	120.30
1	6	390	G	N1-C6-O6	8.78	125.17	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1301	A	N1-C6-N6	8.76	123.86	118.60
36	1	933	A	N1-C6-N6	8.76	123.85	118.60
36	1	2400	G	N1-C6-O6	8.75	125.15	119.90
1	6	338	C	C6-N1-C2	-8.72	116.81	120.30
1	6	1614	A	C2-N3-C4	-8.72	106.24	110.60
36	1	2726	C	N3-C2-O2	-8.72	115.80	121.90
36	5	2936	A	C2-N3-C4	8.70	114.95	110.60
36	1	2741	C	N1-C2-O2	8.68	124.11	118.90
36	5	803	C	C6-N1-C2	-8.68	116.83	120.30
36	1	66	A	O5'-P-OP1	-8.67	97.90	105.70
36	1	1848	G	N1-C6-O6	-8.66	114.70	119.90
36	1	3154	C	C6-N1-C2	-8.66	116.83	120.30
36	1	2417	U	N1-C2-O2	-8.66	116.74	122.80
36	1	1192	C	N3-C4-C5	-8.65	118.44	121.90
36	5	414	U	O5'-P-OP2	-8.65	97.91	105.70
36	1	3217	C	N3-C2-O2	-8.65	115.85	121.90
36	5	1149	G	C5-C6-N1	-8.65	107.18	111.50
36	1	1433	A	N9-C4-C5	8.64	109.25	105.80
36	1	711	A	C8-N9-C4	8.61	109.25	105.80
1	2	971	A	C4-C5-C6	8.60	121.30	117.00
36	1	2726	C	C5-C4-N4	8.60	126.22	120.20
1	2	830	U	N3-C2-O2	-8.59	116.18	122.20
36	1	2818	U	O5'-P-OP2	-8.59	97.97	105.70
36	5	82	C	N3-C4-C5	-8.58	118.47	121.90
36	1	3022	G	N1-C6-O6	8.58	125.05	119.90
36	5	1367	G	C5-C6-N1	-8.56	107.22	111.50
1	2	453	U	C2-N1-C1'	8.55	127.96	117.70
36	5	1306	G	N1-C6-O6	8.54	125.02	119.90
36	1	809	G	C5-C6-O6	-8.53	123.48	128.60
36	5	2327	U	C5-C6-N1	-8.53	118.44	122.70
1	6	553	G	N1-C6-O6	8.53	125.02	119.90
36	5	3108	G	C5-C6-N1	-8.53	107.24	111.50
1	2	426	G	C4-N9-C1'	8.52	137.58	126.50
36	1	635	G	C5-C6-N1	8.52	115.76	111.50
37	7	5	G	C8-N9-C4	8.52	109.81	106.40
1	2	1212	G	N1-C6-O6	8.52	125.01	119.90
36	5	607	A	N1-C6-N6	-8.52	113.49	118.60
36	1	406	G	O4'-C1'-N9	8.51	115.01	108.20
36	5	2843	U	N3-C2-O2	-8.51	116.25	122.20
36	5	3002	C	C6-N1-C2	8.51	123.70	120.30
36	5	2866	U	N3-C2-O2	-8.50	116.25	122.20
36	1	860	G	N1-C6-O6	8.49	125.00	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1179	A	O5'-P-OP1	-8.49	98.06	105.70
36	5	800	G	C5-C6-O6	-8.48	123.51	128.60
36	5	2421	U	N1-C2-N3	8.48	119.99	114.90
36	5	2726	C	N3-C2-O2	-8.47	115.97	121.90
36	5	2726	C	C5-C4-N4	8.47	126.13	120.20
36	1	645	A	C5-C6-N6	8.47	130.48	123.70
36	5	515	C	C6-N1-C2	8.47	123.69	120.30
36	1	2811	A	C6-N1-C2	-8.46	113.52	118.60
36	5	655	C	C6-N1-C2	-8.45	116.92	120.30
36	1	718	G	N7-C8-N9	8.45	117.33	113.10
36	1	1049	C	O5'-P-OP1	-8.45	98.10	105.70
36	1	1437	C	C6-N1-C2	-8.45	116.92	120.30
36	1	979	U	C6-N1-C2	-8.44	115.94	121.00
36	1	780	A	O4'-C1'-N9	-8.43	101.45	108.20
52	M6	78	ARG	NE-CZ-NH1	8.43	124.52	120.30
36	1	3344	A	C6-C5-N7	-8.43	126.40	132.30
36	5	2290	C	C6-N1-C2	8.43	123.67	120.30
1	2	1761	U	C5-C4-O4	8.43	130.96	125.90
36	5	2383	C	C6-N1-C2	-8.43	116.93	120.30
36	1	2875	U	N3-C2-O2	-8.43	116.30	122.20
36	5	226	C	C6-N1-C2	-8.43	116.93	120.30
36	1	953	G	C4-C5-N7	8.42	114.17	110.80
1	2	73	U	O4'-C1'-N1	8.41	114.93	108.20
36	1	1104	G	O5'-P-OP1	-8.40	98.14	105.70
1	6	95	G	N1-C6-O6	-8.40	114.86	119.90
36	5	1319	G	C8-N9-C4	8.40	109.76	106.40
36	1	1792	C	C6-N1-C2	-8.40	116.94	120.30
36	1	1450	G	N1-C6-O6	8.38	124.93	119.90
36	5	1200	A	C5-C6-N6	-8.38	117.00	123.70
36	5	672	A	N9-C4-C5	8.36	109.14	105.80
36	5	1437	C	C2-N1-C1'	8.37	128.00	118.80
36	5	2341	A	C8-N9-C4	8.36	109.14	105.80
36	5	2827	U	N1-C2-O2	8.36	128.65	122.80
36	5	345	G	N1-C6-O6	8.35	124.91	119.90
1	2	380	U	N3-C2-O2	-8.35	116.35	122.20
36	1	2374	C	C2-N1-C1'	8.35	127.98	118.80
36	5	817	A	O5'-P-OP1	-8.34	98.19	105.70
36	1	648	C	C2-N1-C1'	8.34	127.97	118.80
36	5	2142	A	N1-C6-N6	-8.34	113.60	118.60
38	8	17	A	N1-C6-N6	8.33	123.60	118.60
36	1	959	C	C5-C6-N1	-8.33	116.84	121.00
36	5	2295	A	C5-C6-N6	-8.33	117.04	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	12	246	LEU	CA-CB-CG	8.33	134.46	115.30
1	2	577	G	C4-C5-N7	8.32	114.13	110.80
36	1	287	G	C5-C6-N1	-8.32	107.34	111.50
36	5	2398	A	N1-C6-N6	-8.32	113.61	118.60
36	1	2881	C	N3-C4-C5	8.32	125.23	121.90
36	1	2959	C	N1-C2-O2	-8.31	113.91	118.90
36	5	3172	A	N1-C6-N6	8.30	123.58	118.60
36	1	1351	U	N3-C2-O2	-8.30	116.39	122.20
36	5	888	A	N1-C6-N6	8.29	123.58	118.60
1	6	583	C	C6-N1-C2	-8.29	116.98	120.30
36	5	48	A	C5-C6-N1	8.29	121.84	117.70
36	5	1437	C	N3-C4-C5	-8.29	118.59	121.90
36	5	2157	G	C8-N9-C4	8.28	109.71	106.40
36	1	1192	C	N1-C2-O2	8.28	123.87	118.90
36	5	2777	G	N3-C4-N9	-8.28	121.03	126.00
36	5	718	G	C4-N9-C1'	8.27	137.26	126.50
36	1	612	U	C5-C4-O4	8.27	130.86	125.90
36	5	1012	G	C4-N9-C1'	-8.27	115.75	126.50
36	1	2679	A	C2-N3-C4	-8.27	106.47	110.60
36	5	3141	A	O5'-P-OP1	-8.27	98.26	105.70
36	1	609	G	O5'-P-OP2	-8.27	98.26	105.70
36	5	1404	G	C8-N9-C4	8.27	109.71	106.40
36	1	2797	C	N3-C4-C5	-8.25	118.60	121.90
36	1	2714	G	C2-N3-C4	-8.24	107.78	111.90
1	2	1039	A	O4'-C1'-N9	8.24	114.79	108.20
36	5	2364	G	N1-C6-O6	-8.23	114.96	119.90
36	1	282	G	C8-N9-C4	-8.23	103.11	106.40
36	1	2606	G	C4-N9-C1'	8.23	137.19	126.50
44	17	229	PHE	CB-CG-CD1	8.23	126.56	120.80
36	1	690	A	N9-C4-C5	8.22	109.09	105.80
36	5	410	U	N3-C4-C5	-8.22	109.67	114.60
36	1	3022	G	C4-C5-N7	8.22	114.09	110.80
1	6	1537	C	N3-C4-C5	-8.21	118.62	121.90
1	2	1212	G	C5-C6-O6	-8.20	123.68	128.60
36	1	1323	G	C6-C5-N7	-8.20	125.48	130.40
36	1	28	C	C6-N1-C2	8.20	123.58	120.30
1	2	190	C	O4'-C1'-N1	8.19	114.75	108.20
36	1	2610	G	N1-C6-O6	8.19	124.81	119.90
36	5	3154	C	C2-N1-C1'	8.19	127.81	118.80
36	5	1607	U	P-O3'-C3'	8.19	129.53	119.70
36	1	1508	C	C6-N1-C2	-8.19	117.03	120.30
36	1	229	G	N3-C2-N2	-8.18	114.17	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2996	U	N1-C2-O2	8.18	128.53	122.80
36	1	1389	G	C4-C5-N7	8.18	114.07	110.80
36	1	2175	U	N1-C2-N3	8.18	119.81	114.90
36	5	942	U	N3-C4-C5	-8.17	109.70	114.60
36	5	2420	C	N1-C2-O2	-8.17	114.00	118.90
36	1	3143	C	C6-N1-C2	8.16	123.56	120.30
36	5	3181	C	C6-N1-C2	-8.16	117.03	120.30
36	1	3181	C	C6-N1-C2	-8.16	117.03	120.30
36	5	907	G	C4-C5-N7	8.16	114.06	110.80
36	5	2635	A	O5'-P-OP2	-8.15	98.37	105.70
36	1	2811	A	N1-C6-N6	-8.14	113.72	118.60
36	1	699	A	C2-N3-C4	-8.14	106.53	110.60
37	7	105	C	N3-C4-C5	-8.14	118.65	121.90
1	2	577	G	C5-C6-O6	-8.13	123.72	128.60
36	1	1414	G	C5-C6-O6	-8.13	123.72	128.60
36	5	1604	G	N3-C4-N9	8.12	130.88	126.00
36	5	1178	G	C8-N9-C4	-8.12	103.15	106.40
36	5	1152	G	N3-C2-N2	-8.12	114.22	119.90
36	5	1150	A	O5'-P-OP2	-8.11	98.40	105.70
36	5	1149	G	C4-C5-C6	8.11	123.67	118.80
36	1	2811	A	C5-C6-N1	8.10	121.75	117.70
36	1	1595	U	C5-C6-N1	-8.10	118.65	122.70
36	1	635	G	C5-C6-O6	-8.09	123.74	128.60
36	5	2736	A	N1-C6-N6	8.09	123.45	118.60
36	5	1452	A	N1-C6-N6	8.09	123.45	118.60
36	1	1113	G	C8-N9-C4	-8.08	103.17	106.40
36	1	3278	C	N1-C2-O2	8.08	123.75	118.90
36	5	226	C	N3-C4-C5	-8.08	118.67	121.90
36	5	1152	G	O5'-P-OP1	-8.08	98.42	105.70
36	1	2279	A	N1-C6-N6	8.08	123.45	118.60
1	2	1761	U	C6-N1-C2	-8.07	116.16	121.00
36	5	2885	C	N1-C2-O2	-8.07	114.06	118.90
36	5	1184	A	N1-C6-N6	-8.07	113.76	118.60
36	5	670	C	N3-C4-C5	-8.06	118.68	121.90
36	1	1207	G	C5-C6-O6	-8.05	123.77	128.60
36	5	2864	A	N1-C6-N6	8.05	123.43	118.60
36	1	2819	A	C8-N9-C4	-8.04	102.59	105.80
36	5	1142	G	N3-C4-C5	-8.04	124.58	128.60
36	5	694	C	C6-N1-C2	-8.03	117.09	120.30
36	5	3029	A	N1-C6-N6	-8.03	113.78	118.60
36	1	637	C	O5'-P-OP1	-8.03	98.47	105.70
1	6	337	G	C2-N3-C4	8.03	115.92	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1901	A	N1-C6-N6	-8.03	113.78	118.60
36	5	2777	G	C4-C5-N7	-8.02	107.59	110.80
36	1	355	A	C2-N3-C4	-8.02	106.59	110.60
36	5	2819	A	O5'-P-OP2	-8.02	98.49	105.70
36	5	2842	U	O5'-P-OP1	-8.02	98.49	105.70
1	2	1636	C	C6-N1-C2	-8.01	117.10	120.30
37	7	80	G	C6-C5-N7	-8.01	125.59	130.40
36	1	2380	U	N1-C2-N3	8.00	119.70	114.90
36	5	2777	G	N9-C4-C5	8.00	108.60	105.40
36	5	1192	C	C2-N1-C1'	8.00	127.60	118.80
36	5	3245	A	C5-C6-N1	-8.00	113.70	117.70
36	5	1008	U	C5-C6-N1	-7.99	118.70	122.70
36	5	2880	U	C5-C6-N1	7.99	126.70	122.70
36	1	1113	G	N7-C8-N9	7.98	117.09	113.10
36	5	798	G	C8-N9-C4	-7.98	103.21	106.40
36	5	1377	G	N3-C4-C5	-7.97	124.61	128.60
36	5	2113	A	C8-N9-C4	7.97	108.99	105.80
36	1	2636	A	C8-N9-C4	-7.97	102.61	105.80
36	1	218	G	C5-C6-O6	-7.97	123.82	128.60
1	6	630	A	C8-N9-C4	7.96	108.99	105.80
36	5	826	G	N1-C6-O6	7.96	124.68	119.90
36	1	2379	U	N1-C2-O2	-7.96	117.23	122.80
36	5	567	G	C4-C5-N7	7.96	113.98	110.80
36	5	1321	G	N1-C6-O6	7.95	124.67	119.90
36	1	1166	G	C6-C5-N7	-7.95	125.63	130.40
36	5	874	U	C2-N1-C1'	-7.95	108.16	117.70
1	2	93	A	C8-N9-C4	-7.95	102.62	105.80
36	1	676	G	C8-N9-C1'	-7.94	116.68	127.00
36	5	923	C	N3-C4-C5	7.94	125.08	121.90
36	1	1124	U	N3-C2-O2	-7.93	116.64	122.20
36	5	1161	G	O5'-P-OP1	-7.93	98.56	105.70
36	5	2552	C	N1-C2-O2	7.93	123.66	118.90
36	1	914	A	N1-C6-N6	-7.93	113.84	118.60
36	5	2295	A	C4-C5-N7	7.93	114.67	110.70
36	5	2707	C	N3-C4-C5	7.93	125.07	121.90
36	1	595	G	O5'-P-OP1	-7.92	98.57	105.70
36	5	1483	G	O4'-C1'-N9	7.92	114.54	108.20
36	1	2836	C	C4-C5-C6	7.92	121.36	117.40
36	5	2811	A	O5'-P-OP1	-7.91	98.58	105.70
36	1	2795	U	O5'-P-OP1	-7.91	98.58	105.70
36	5	2199	G	C8-N9-C4	-7.91	103.24	106.40
36	5	2959	C	N3-C4-C5	-7.91	118.74	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2960	C	C6-N1-C2	-7.90	117.14	120.30
1	6	163	G	C2-N3-C4	-7.90	107.95	111.90
36	1	2916	U	N1-C2-N3	-7.89	110.16	114.90
36	5	2145	A	C8-N9-C4	-7.89	102.64	105.80
36	1	326	U	O5'-P-OP2	-7.89	98.60	105.70
36	5	800	G	C4-C5-N7	7.88	113.95	110.80
36	1	2374	C	N1-C2-O2	7.88	123.63	118.90
36	1	94	G	O5'-P-OP1	-7.88	98.61	105.70
36	1	2726	C	C6-N1-C2	-7.87	117.15	120.30
36	5	1371	G	C8-N9-C4	7.87	109.55	106.40
36	5	1900	A	N1-C6-N6	7.87	123.32	118.60
36	5	2383	C	C5-C6-N1	7.87	124.93	121.00
36	1	2409	G	N3-C4-C5	-7.86	124.67	128.60
36	1	24	G	C5-C6-N1	-7.85	107.57	111.50
36	5	776	U	N3-C2-O2	-7.85	116.70	122.20
36	1	991	G	C8-N9-C4	-7.85	103.26	106.40
36	5	1443	G	N1-C6-O6	7.85	124.61	119.90
36	5	661	G	C8-N9-C4	-7.84	103.27	106.40
36	1	2852	C	C6-N1-C2	7.83	123.43	120.30
36	5	1301	A	C6-C5-N7	-7.83	126.82	132.30
36	5	522	A	N1-C6-N6	7.82	123.29	118.60
36	5	364	G	N1-C6-O6	7.82	124.59	119.90
36	1	2899	C	N3-C2-O2	-7.82	116.43	121.90
36	5	887	G	C5-C6-O6	-7.81	123.91	128.60
1	6	782	U	N3-C2-O2	-7.81	116.73	122.20
36	5	924	G	C5-C6-N1	-7.81	107.59	111.50
36	1	2356	A	N1-C6-N6	7.81	123.28	118.60
36	1	3217	C	C6-N1-C2	-7.80	117.18	120.30
36	1	2617	U	C5-C4-O4	7.80	130.58	125.90
1	2	639	U	N1-C2-O2	7.79	128.26	122.80
36	5	1592	G	C8-N9-C4	-7.79	103.28	106.40
1	6	798	C	C6-N1-C2	7.79	123.41	120.30
36	1	718	G	C8-N9-C4	-7.78	103.29	106.40
36	5	2373	A	O5'-P-OP1	-7.78	98.70	105.70
36	1	3212	C	C6-N1-C2	7.77	123.41	120.30
36	5	2403	G	C8-N9-C4	7.76	109.50	106.40
36	5	668	G	N7-C8-N9	-7.76	109.22	113.10
36	5	2392	C	N3-C4-C5	7.76	125.00	121.90
36	1	933	A	C5-N7-C8	-7.76	100.02	103.90
36	1	2281	A	O5'-P-OP2	-7.76	98.72	105.70
36	5	2199	G	N7-C8-N9	7.76	116.98	113.10
36	1	2662	G	N1-C6-O6	7.75	124.55	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1187	C	N3-C4-C5	7.75	125.00	121.90
1	6	1150	G	N3-C4-C5	7.75	132.48	128.60
36	5	960	U	N3-C2-O2	-7.75	116.77	122.20
36	1	689	U	N1-C2-O2	7.75	128.22	122.80
38	8	25	G	N3-C4-C5	-7.75	124.73	128.60
36	5	980	A	N1-C6-N6	-7.74	113.95	118.60
36	5	2994	A	C6-N1-C2	-7.74	113.95	118.60
36	1	590	G	C5-C6-O6	-7.74	123.95	128.60
36	1	2194	G	N1-C6-O6	7.74	124.54	119.90
36	5	2295	A	C5-N7-C8	-7.74	100.03	103.90
36	5	2797	C	N3-C4-C5	-7.73	118.81	121.90
36	1	948	C	C5-C6-N1	-7.73	117.13	121.00
36	5	388	G	C8-N9-C4	-7.72	103.31	106.40
36	5	1148	G	C5-C6-O6	-7.72	123.97	128.60
36	1	145	G	C4-C5-N7	7.72	113.89	110.80
36	1	2730	G	N3-C4-N9	-7.72	121.37	126.00
36	1	1351	U	N1-C2-O2	7.72	128.20	122.80
1	2	830	U	N1-C2-O2	7.71	128.20	122.80
36	5	1127	G	O5'-P-OP2	-7.71	98.77	105.70
36	1	689	U	N3-C2-O2	-7.70	116.81	122.20
36	1	2617	U	N3-C2-O2	-7.70	116.81	122.20
36	1	644	G	C5-C6-O6	7.70	133.22	128.60
36	1	957	C	N1-C2-O2	-7.70	114.28	118.90
36	1	637	C	N3-C2-O2	-7.70	116.51	121.90
36	5	2906	C	C6-N1-C2	7.69	123.38	120.30
36	1	398	A	C8-N9-C4	7.69	108.88	105.80
36	1	676	G	C6-C5-N7	-7.69	125.79	130.40
36	5	3149	G	C5-C6-N1	-7.69	107.66	111.50
1	2	1340	U	C5-C4-O4	7.69	130.51	125.90
1	2	1636	C	N3-C4-C5	-7.69	118.83	121.90
36	1	1001	G	N3-C4-N9	7.69	130.61	126.00
36	5	82	C	C4-C5-C6	7.68	121.24	117.40
1	6	337	G	N3-C4-N9	7.68	130.61	126.00
36	1	2968	G	C6-C5-N7	-7.68	125.79	130.40
1	2	1539	G	C4-N9-C1'	7.68	136.48	126.50
36	1	1113	G	C5-N7-C8	-7.67	100.46	104.30
37	7	1	G	C4-N9-C1'	7.67	136.47	126.50
36	5	2733	A	O5'-P-OP2	-7.67	98.80	105.70
36	1	3054	U	N3-C4-C5	-7.66	110.00	114.60
36	5	2869	U	C5-C4-O4	7.66	130.50	125.90
36	5	3078	U	N3-C2-O2	-7.66	116.84	122.20
36	1	1414	G	N1-C6-O6	7.65	124.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	304	G	C5-C6-O6	7.65	133.19	128.60
36	1	2697	A	N1-C6-N6	-7.65	114.01	118.60
38	4	26	U	N3-C2-O2	-7.65	116.85	122.20
36	5	2271	A	N1-C6-N6	-7.65	114.01	118.60
36	1	1904	C	N3-C4-C5	-7.65	118.84	121.90
36	1	3201	C	C6-N1-C2	-7.64	117.24	120.30
38	4	52	A	N1-C6-N6	-7.64	114.02	118.60
1	2	1200	G	N1-C6-O6	7.64	124.48	119.90
36	1	287	G	N1-C6-O6	7.64	124.48	119.90
36	5	1152	G	C4-N9-C1'	-7.64	116.57	126.50
36	1	808	A	N1-C6-N6	7.63	123.18	118.60
36	1	232	G	N3-C4-C5	-7.63	124.78	128.60
36	1	2948	C	C6-N1-C2	7.63	123.35	120.30
36	1	1607	U	P-O3'-C3'	7.63	128.85	119.70
36	1	1175	C	C6-N1-C2	7.62	123.35	120.30
36	1	3344	A	C5-N7-C8	-7.62	100.09	103.90
36	5	2865	U	C5-C6-N1	7.62	126.51	122.70
36	1	1888	U	N3-C2-O2	-7.62	116.87	122.20
44	17	232	ARG	NE-CZ-NH1	-7.62	116.49	120.30
36	1	1149	G	C4-C5-C6	7.61	123.37	118.80
36	1	1307	G	N3-C4-N9	-7.61	121.44	126.00
36	1	2912	G	O5'-P-OP1	-7.61	98.86	105.70
1	6	621	A	O5'-P-OP1	-7.61	98.85	105.70
36	5	2629	U	C5-C4-O4	-7.61	121.34	125.90
36	5	2817	A	C2-N3-C4	7.61	114.40	110.60
36	1	638	C	O5'-P-OP2	-7.60	98.86	105.70
36	5	1171	G	O5'-P-OP2	-7.60	98.86	105.70
1	6	390	G	C6-C5-N7	-7.60	125.84	130.40
36	5	2364	G	C5-C6-O6	7.60	133.16	128.60
36	1	1367	G	N9-C4-C5	-7.60	102.36	105.40
36	1	963	G	O5'-P-OP1	7.59	119.81	110.70
36	1	1495	U	N1-C2-N3	7.59	119.46	114.90
1	2	17	C	C6-N1-C2	-7.59	117.27	120.30
36	1	645	A	C4-C5-N7	-7.59	106.91	110.70
36	5	2942	C	C5-C6-N1	7.59	124.79	121.00
36	5	2353	G	N1-C6-O6	7.58	124.45	119.90
36	1	2418	G	OP1-P-O3'	7.58	121.88	105.20
36	1	397	A	N7-C8-N9	-7.58	110.01	113.80
36	1	1386	A	N1-C6-N6	7.58	123.15	118.60
36	1	1389	G	C5-C6-O6	-7.58	124.05	128.60
36	5	2413	A	O5'-P-OP1	-7.58	98.88	105.70
36	5	2761	G	C5-C6-N1	7.58	115.29	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2190	U	N3-C4-C5	-7.57	110.06	114.60
36	1	937	G	N1-C6-O6	7.57	124.44	119.90
36	1	2549	G	N3-C4-N9	7.57	130.54	126.00
36	1	3344	A	O4'-C1'-N9	7.57	114.26	108.20
1	6	1744	A	C4-C5-N7	7.57	114.48	110.70
36	5	519	A	C5-C6-N6	-7.57	117.64	123.70
36	5	2421	U	N1-C2-O2	-7.57	117.50	122.80
36	5	1127	G	N1-C6-O6	-7.57	115.36	119.90
36	5	672	A	C8-N9-C4	-7.57	102.77	105.80
36	5	1306	G	C5-N7-C8	-7.56	100.52	104.30
36	5	514	G	N1-C6-O6	7.56	124.44	119.90
36	5	1190	A	C8-N9-C4	-7.56	102.78	105.80
36	5	437	G	C8-N9-C4	-7.56	103.38	106.40
36	1	1004	U	C6-N1-C2	-7.56	116.47	121.00
36	1	3382	U	C6-N1-C1'	-7.56	110.62	121.20
36	5	2375	G	O4'-C1'-N9	7.56	114.25	108.20
36	1	287	G	O5'-P-OP1	-7.55	98.90	105.70
36	1	2117	A	O5'-P-OP1	-7.55	98.91	105.70
36	1	2827	U	C5-C4-O4	7.55	130.43	125.90
36	1	358	G	C4-C5-N7	7.55	113.82	110.80
36	1	2870	C	C2-N1-C1'	-7.55	110.50	118.80
36	5	2616	C	O5'-P-OP1	-7.54	98.91	105.70
36	1	880	G	O4'-C1'-N9	7.54	114.23	108.20
36	1	611	A	O5'-P-OP2	-7.54	98.92	105.70
36	1	913	A	C8-N9-C4	-7.54	102.79	105.80
1	6	779	U	N1-C2-O2	7.54	128.07	122.80
36	1	1192	C	N3-C2-O2	-7.53	116.63	121.90
36	1	690	A	C5-C6-N6	7.53	129.72	123.70
36	1	1888	U	N1-C2-N3	7.53	119.42	114.90
36	1	2358	A	N1-C6-N6	7.53	123.12	118.60
1	2	779	U	O4'-C1'-N1	7.53	114.22	108.20
36	1	715	A	O5'-P-OP2	-7.52	98.93	105.70
36	5	364	G	C4-C5-N7	7.52	113.81	110.80
36	1	1435	A	C8-N9-C4	-7.52	102.79	105.80
36	1	283	G	O4'-C1'-N9	-7.52	102.19	108.20
36	5	806	A	C8-N9-C4	7.52	108.81	105.80
36	5	1012	G	N3-C4-N9	-7.52	121.49	126.00
36	5	1198	C	C2-N1-C1'	-7.51	110.53	118.80
36	5	800	G	N1-C6-O6	7.51	124.41	119.90
36	1	1329	U	C2-N1-C1'	7.50	126.70	117.70
1	2	971	A	C8-N9-C4	-7.50	102.80	105.80
36	1	3022	G	N9-C4-C5	-7.50	102.40	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1321	G	C6-C5-N7	-7.49	125.91	130.40
36	1	1115	G	C8-N9-C4	-7.49	103.40	106.40
36	1	2296	A	C8-N9-C4	7.49	108.80	105.80
36	5	1160	C	C2-N1-C1'	-7.49	110.56	118.80
36	1	3110	C	C6-N1-C2	-7.49	117.30	120.30
36	5	2866	U	N1-C2-O2	7.49	128.04	122.80
36	1	2643	A	N1-C6-N6	7.49	123.09	118.60
36	5	2186	U	O5'-P-OP2	-7.49	98.96	105.70
36	1	727	G	N3-C4-C5	-7.48	124.86	128.60
1	6	337	G	C4-N9-C1'	7.48	136.23	126.50
36	5	2777	G	C5-C6-O6	7.48	133.09	128.60
78	q2	93	LEU	CA-CB-CG	7.48	132.50	115.30
36	1	2309	A	N1-C6-N6	7.48	123.08	118.60
1	6	1600	A	O4'-C1'-N9	7.48	114.18	108.20
36	5	1917	C	C6-N1-C2	7.47	123.29	120.30
36	1	1389	G	N3-C4-N9	7.47	130.48	126.00
38	4	81	U	N3-C2-O2	-7.47	116.97	122.20
36	1	940	G	O5'-P-OP1	-7.47	98.98	105.70
1	2	1489	U	N3-C2-O2	-7.47	116.97	122.20
36	1	3078	U	N3-C2-O2	-7.47	116.97	122.20
1	6	543	C	C6-N1-C2	-7.47	117.31	120.30
36	5	877	C	N3-C4-C5	7.47	124.89	121.90
36	5	2890	A	O5'-P-OP1	-7.46	98.98	105.70
36	1	2344	U	C5-C6-N1	-7.46	118.97	122.70
36	1	709	A	C5-C6-N6	-7.46	117.74	123.70
36	1	2619	G	O5'-P-OP1	-7.46	98.99	105.70
36	1	1838	G	C5-C6-O6	-7.45	124.13	128.60
36	1	2298	U	C5-C4-O4	7.45	130.37	125.90
1	6	542	A	C8-N9-C4	-7.45	102.82	105.80
37	7	55	A	O5'-P-OP1	-7.45	99.00	105.70
36	5	1152	G	C8-N9-C4	-7.44	103.42	106.40
36	1	49	A	C8-N9-C4	7.44	108.78	105.80
36	1	14	U	O5'-P-OP2	-7.44	99.00	105.70
36	5	3245	A	C5-N7-C8	-7.44	100.18	103.90
36	1	2889	C	N1-C2-O2	7.44	123.36	118.90
10	S8	29	LEU	CA-CB-CG	7.44	132.41	115.30
36	5	670	C	C6-N1-C2	-7.44	117.33	120.30
36	5	1160	C	N1-C2-O2	-7.44	114.44	118.90
36	5	1012	G	N3-C4-C5	7.43	132.32	128.60
36	1	1450	G	C5-C6-O6	-7.43	124.14	128.60
36	1	2585	G	N3-C4-C5	-7.43	124.89	128.60
36	5	587	U	C6-N1-C2	7.43	125.46	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1156	C	C6-N1-C2	-7.43	117.33	120.30
36	1	714	G	C6-C5-N7	-7.42	125.95	130.40
36	1	2247	G	C6-C5-N7	-7.42	125.95	130.40
36	5	2189	U	O5'-P-OP1	-7.42	99.02	105.70
36	1	2376	G	C5-N7-C8	-7.42	100.59	104.30
36	5	2400	G	C8-N9-C4	7.42	109.37	106.40
36	1	1151	U	N3-C4-O4	7.42	124.59	119.40
1	6	453	U	C2-N1-C1'	7.42	126.60	117.70
1	6	435	C	N1-C2-O2	7.41	123.35	118.90
36	5	1126	G	C8-N9-C4	-7.41	103.44	106.40
36	5	2197	C	N1-C2-N3	-7.41	114.01	119.20
36	5	1849	C	N3-C2-O2	7.41	127.09	121.90
36	1	1484	U	P-O3'-C3'	7.41	128.59	119.70
51	m5	24	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	6	524	U	O5'-P-OP2	-7.40	99.04	105.70
1	2	736	C	C5-C6-N1	7.40	124.70	121.00
36	1	1595	U	C2-N1-C1'	-7.40	108.82	117.70
36	5	1317	A	N1-C2-N3	-7.40	125.60	129.30
36	1	1166	G	N9-C4-C5	-7.40	102.44	105.40
36	1	2279	A	C5-C6-N6	-7.39	117.78	123.70
36	5	2550	U	N3-C2-O2	-7.39	117.03	122.20
1	2	1280	C	C6-N1-C2	-7.39	117.34	120.30
36	1	318	A	O5'-P-OP1	-7.39	99.05	105.70
36	5	2345	A	N1-C6-N6	7.39	123.03	118.60
36	1	1522	U	C2-N3-C4	-7.38	122.57	127.00
36	5	2981	U	N3-C2-O2	-7.38	117.03	122.20
37	7	40	C	C6-N1-C2	7.38	123.25	120.30
36	5	776	U	C5-C6-N1	-7.38	119.01	122.70
37	7	93	C	C6-N1-C2	-7.38	117.35	120.30
36	1	1556	C	N1-C2-O2	7.37	123.32	118.90
36	1	2179	C	N1-C2-O2	7.37	123.32	118.90
36	1	1407	A	O5'-P-OP2	-7.37	99.06	105.70
36	5	2199	G	C5-N7-C8	-7.37	100.61	104.30
36	1	2403	G	N1-C6-O6	7.37	124.32	119.90
36	5	2281	A	N9-C4-C5	-7.37	102.85	105.80
36	1	1151	U	N3-C4-C5	-7.36	110.18	114.60
36	1	397	A	C8-N9-C4	7.36	108.74	105.80
36	5	715	A	C5-C6-N6	7.35	129.58	123.70
36	5	1212	A	C5-C6-N6	-7.35	117.82	123.70
36	1	974	G	C5-C6-N1	7.35	115.18	111.50
36	5	3197	G	N3-C2-N2	-7.35	114.75	119.90
36	5	3309	G	C4-N9-C1'	7.35	136.05	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	901	G	C5-C6-N1	-7.34	107.83	111.50
36	1	2606	G	C8-N9-C1'	-7.34	117.45	127.00
36	1	2822	U	O5'-P-OP1	-7.34	99.09	105.70
36	5	1321	G	C4-C5-N7	7.34	113.74	110.80
36	5	2699	G	N1-C6-O6	7.34	124.31	119.90
36	1	1201	C	C5-C6-N1	7.34	124.67	121.00
36	1	388	G	C8-N9-C4	-7.34	103.46	106.40
36	1	870	G	N9-C4-C5	7.34	108.34	105.40
36	5	98	G	N3-C4-N9	7.34	130.40	126.00
36	1	432	G	C5-C6-N1	-7.33	107.83	111.50
36	5	1868	G	C6-C5-N7	-7.33	126.00	130.40
38	4	99	C	N1-C2-O2	7.33	123.30	118.90
36	5	718	G	C6-C5-N7	-7.32	126.01	130.40
36	5	339	C	N3-C2-O2	7.32	127.02	121.90
1	2	1082	C	C6-N1-C2	-7.32	117.37	120.30
1	2	1082	C	C6-N1-C1'	-7.32	112.02	120.80
36	5	2899	C	C6-N1-C2	-7.32	117.37	120.30
36	5	2976	A	N9-C4-C5	7.32	108.73	105.80
36	1	3362	A	O4'-C1'-N9	7.32	114.05	108.20
36	5	197	G	C4-C5-N7	7.32	113.73	110.80
36	5	2351	U	N3-C2-O2	-7.32	117.08	122.20
37	7	51	A	C6-C5-N7	-7.32	127.18	132.30
36	5	1449	A	N9-C4-C5	-7.31	102.88	105.80
36	5	2610	G	C8-N9-C4	-7.31	103.47	106.40
1	2	1761	U	N3-C2-O2	-7.31	117.08	122.20
36	1	631	U	N3-C2-O2	7.31	127.32	122.20
38	4	83	C	N1-C2-O2	7.31	123.29	118.90
36	5	1848	G	C8-N9-C4	7.31	109.32	106.40
36	5	646	A	C2-N3-C4	-7.31	106.95	110.60
36	1	1303	A	C5-C6-N6	-7.30	117.86	123.70
36	1	1403	C	C6-N1-C2	7.30	123.22	120.30
36	1	711	A	N7-C8-N9	-7.30	110.15	113.80
1	2	1241	G	C6-C5-N7	-7.30	126.02	130.40
36	1	51	A	C5-N7-C8	-7.30	100.25	103.90
36	5	1347	U	C2-N1-C1'	-7.30	108.94	117.70
36	1	2989	U	N3-C4-O4	7.30	124.51	119.40
36	5	437	G	N9-C4-C5	7.30	108.32	105.40
36	1	2624	G	C5-C6-O6	-7.30	124.22	128.60
1	6	542	A	O5'-P-OP1	-7.29	99.14	105.70
36	5	2893	C	N3-C4-C5	-7.29	118.98	121.90
36	5	3130	A	N1-C2-N3	7.29	132.94	129.30
36	5	1316	C	N1-C2-O2	-7.28	114.53	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1392	G	C8-N9-C4	7.28	109.31	106.40
36	5	1404	G	C2-N3-C4	-7.28	108.26	111.90
36	5	2723	U	C6-N1-C2	-7.28	116.63	121.00
36	5	961	C	O5'-P-OP1	-7.28	99.15	105.70
36	1	51	A	N1-C6-N6	7.27	122.97	118.60
1	2	970	A	N1-C6-N6	7.27	122.96	118.60
36	1	716	A	N9-C4-C5	-7.27	102.89	105.80
1	2	1731	A	N1-C6-N6	7.27	122.96	118.60
36	1	3078	U	N1-C2-O2	7.27	127.89	122.80
36	5	2936	A	N1-C6-N6	-7.26	114.24	118.60
36	5	2385	G	C2-N3-C4	-7.26	108.27	111.90
36	1	1493	G	N1-C6-O6	-7.26	115.54	119.90
36	5	2863	G	C5-C6-O6	7.26	132.96	128.60
36	1	2935	U	C5-C6-N1	7.25	126.33	122.70
36	5	2283	G	C4-C5-N7	7.25	113.70	110.80
36	5	304	G	N1-C6-O6	-7.25	115.55	119.90
36	5	2351	U	C6-N1-C2	-7.25	116.65	121.00
36	5	1404	G	N3-C4-C5	7.25	132.22	128.60
36	1	637	C	P-O3'-C3'	7.25	128.40	119.70
36	5	2391	G	C5-C6-N1	7.25	115.12	111.50
36	5	423	A	N9-C4-C5	-7.24	102.90	105.80
1	2	970	A	C5-C6-N6	-7.24	117.91	123.70
1	6	543	C	N1-C2-O2	7.24	123.24	118.90
36	1	558	U	C2-N1-C1'	7.24	126.38	117.70
36	1	803	C	C2-N1-C1'	7.24	126.76	118.80
36	5	1169	A	C8-N9-C4	7.24	108.69	105.80
36	1	2960	C	N3-C2-O2	-7.23	116.84	121.90
36	5	1006	A	O5'-P-OP2	-7.23	99.19	105.70
36	5	1468	A	N1-C6-N6	7.23	122.94	118.60
36	1	1437	C	C2-N1-C1'	7.22	126.75	118.80
1	2	1241	G	N7-C8-N9	7.22	116.71	113.10
36	1	1192	C	C2-N1-C1'	7.22	126.74	118.80
36	5	806	A	C4-C5-C6	-7.22	113.39	117.00
36	5	3278	C	C6-N1-C2	7.22	123.19	120.30
36	5	1452	A	N9-C4-C5	-7.22	102.91	105.80
36	1	692	A	C4-C5-C6	7.21	120.61	117.00
36	5	612	U	OP2-P-O3'	7.21	121.07	105.20
36	1	906	A	N1-C6-N6	7.21	122.92	118.60
36	5	360	G	C8-N9-C4	-7.21	103.52	106.40
1	2	1489	U	C2-N1-C1'	7.21	126.35	117.70
36	1	2369	G	C8-N9-C4	-7.20	103.52	106.40
36	5	2156	C	C6-N1-C2	7.20	123.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3217	C	N1-C2-O2	7.20	123.22	118.90
36	1	947	G	C6-C5-N7	-7.20	126.08	130.40
36	1	2175	U	C5-C4-O4	7.20	130.22	125.90
38	4	93	U	C5-C4-O4	7.20	130.22	125.90
36	1	1733	G	N3-C4-C5	-7.19	125.00	128.60
38	4	66	A	C8-N9-C4	-7.19	102.92	105.80
36	1	3000	A	C2-N3-C4	-7.19	107.00	110.60
36	5	3131	U	N3-C4-C5	7.19	118.91	114.60
36	1	105	C	C6-N1-C2	7.19	123.17	120.30
36	5	1158	A	O5'-P-OP2	-7.19	99.23	105.70
38	8	20	U	N1-C2-O2	-7.19	117.77	122.80
36	1	690	A	C4-C5-N7	-7.18	107.11	110.70
36	1	912	G	N3-C4-N9	7.18	130.31	126.00
36	5	2419	A	C8-N9-C4	-7.18	102.93	105.80
37	7	48	U	N3-C4-O4	7.18	124.42	119.40
36	5	1114	U	OP1-P-O3'	7.17	120.98	105.20
1	6	1130	G	C8-N9-C4	7.17	109.27	106.40
36	5	2758	A	N9-C4-C5	7.17	108.67	105.80
36	5	720	A	C6-C5-N7	-7.17	127.28	132.30
36	1	2882	U	N3-C2-O2	-7.17	117.19	122.20
36	5	1010	G	O5'-P-OP2	-7.17	99.25	105.70
37	7	69	C	C6-N1-C2	7.17	123.17	120.30
36	1	586	C	N1-C2-O2	-7.16	114.60	118.90
36	5	1198	C	C6-N1-C1'	7.16	129.40	120.80
38	8	4	C	N3-C2-O2	-7.16	116.89	121.90
36	5	3091	A	O5'-P-OP1	-7.16	99.25	105.70
1	6	1744	A	N9-C4-C5	-7.16	102.94	105.80
36	5	948	C	C6-N1-C2	7.16	123.16	120.30
36	1	860	G	C5-C6-O6	-7.16	124.31	128.60
36	1	3054	U	C6-N1-C2	-7.16	116.70	121.00
36	5	1373	A	N1-C6-N6	7.15	122.89	118.60
36	1	833	G	C4-C5-N7	-7.15	107.94	110.80
36	1	2920	U	C5-C6-N1	-7.15	119.12	122.70
36	1	1831	U	C6-N1-C2	-7.15	116.71	121.00
36	5	48	A	C6-N1-C2	-7.15	114.31	118.60
36	1	2871	G	O5'-P-OP2	-7.14	99.27	105.70
36	1	1480	G	N3-C4-C5	7.14	132.17	128.60
1	2	639	U	N3-C2-O2	-7.14	117.20	122.20
36	1	586	C	N3-C2-O2	7.14	126.90	121.90
36	1	2870	C	C6-N1-C1'	7.14	129.37	120.80
1	6	979	A	C8-N9-C4	-7.14	102.94	105.80
36	5	2709	C	C5-C6-N1	-7.14	117.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1541	G	N3-C4-C5	-7.14	125.03	128.60
36	5	1301	A	C5-C6-N6	-7.14	117.99	123.70
36	5	2816	G	C8-N9-C4	7.14	109.25	106.40
36	1	590	G	N1-C6-O6	7.13	124.18	119.90
36	5	205	C	O5'-P-OP1	-7.13	99.28	105.70
36	5	905	U	O5'-P-OP1	-7.13	99.28	105.70
36	5	2400	G	N3-C4-C5	7.13	132.17	128.60
1	2	346	G	C8-N9-C4	7.13	109.25	106.40
36	1	1373	A	O5'-P-OP2	-7.13	99.28	105.70
36	5	1364	C	OP2-P-O3'	7.13	120.89	105.20
36	5	2281	A	C8-N9-C4	7.13	108.65	105.80
36	5	715	A	O4'-C1'-N9	7.13	113.90	108.20
36	5	2662	G	N3-C4-N9	7.13	130.28	126.00
36	1	123	A	N1-C6-N6	7.13	122.88	118.60
36	5	921	A	OP2-P-O3'	7.13	120.88	105.20
36	5	1587	A	N7-C8-N9	-7.13	110.24	113.80
38	8	48	A	C5-N7-C8	-7.13	100.34	103.90
36	5	3309	G	N3-C4-C5	-7.12	125.04	128.60
36	5	887	G	N9-C4-C5	-7.12	102.55	105.40
1	6	136	C	C2-N1-C1'	7.12	126.63	118.80
36	1	684	G	N1-C6-O6	7.12	124.17	119.90
36	1	1885	U	C5-C6-N1	-7.12	119.14	122.70
1	6	55	A	C8-N9-C4	-7.12	102.95	105.80
36	5	364	G	C6-C5-N7	-7.12	126.13	130.40
1	6	1032	G	C8-N9-C4	7.12	109.25	106.40
36	5	2316	G	N3-C4-C5	-7.12	125.04	128.60
1	2	559	C	C6-N1-C2	-7.12	117.45	120.30
49	M3	85	LEU	CA-CB-CG	7.12	131.66	115.30
37	7	101	G	C4-C5-N7	7.12	113.65	110.80
1	2	553	G	C5-C6-O6	-7.11	124.33	128.60
36	5	1317	A	C2-N3-C4	7.11	114.16	110.60
36	5	3000	A	C8-N9-C4	7.11	108.64	105.80
36	1	3362	A	C6-C5-N7	-7.11	127.32	132.30
36	1	421	G	N3-C2-N2	7.11	124.88	119.90
1	6	1744	A	C5-C6-N6	-7.11	118.01	123.70
12	c0	97	PRO	N-CA-CB	7.11	111.83	103.30
1	6	1653	C	N1-C2-O2	-7.10	114.64	118.90
36	1	808	A	C5-C6-N6	-7.10	118.02	123.70
36	5	1163	A	O5'-P-OP2	-7.10	99.31	105.70
36	1	645	A	C8-N9-C4	-7.09	102.96	105.80
36	1	2827	U	N1-C2-N3	7.09	119.16	114.90
36	5	3315	G	C6-C5-N7	-7.09	126.14	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2874	G	C5-C6-N1	-7.09	107.96	111.50
36	1	612	U	N3-C4-O4	-7.09	114.44	119.40
36	1	1269	U	C2-N1-C1'	7.09	126.20	117.70
36	1	2329	C	N3-C4-C5	7.09	124.73	121.90
36	5	519	A	C4-C5-N7	7.09	114.24	110.70
36	5	2283	G	O5'-P-OP2	-7.09	99.32	105.70
36	1	1157	G	N1-C2-N3	7.08	128.15	123.90
37	7	101	G	C6-C5-N7	-7.08	126.15	130.40
36	1	1421	G	OP2-P-O3'	7.08	120.79	105.20
36	5	781	G	N1-C6-O6	-7.08	115.65	119.90
36	1	2298	U	N3-C4-O4	-7.08	114.44	119.40
36	5	610	G	C8-N9-C4	-7.08	103.57	106.40
37	3	93	C	N3-C4-C5	7.08	124.73	121.90
1	2	1182	U	N3-C2-O2	-7.08	117.25	122.20
36	5	1496	C	C2-N1-C1'	7.08	126.58	118.80
36	1	1328	C	C6-N1-C2	-7.08	117.47	120.30
1	6	1172	G	N3-C4-C5	-7.08	125.06	128.60
36	1	912	G	N3-C4-C5	-7.07	125.06	128.60
48	M1	112	LEU	CA-CB-CG	7.07	131.56	115.30
36	5	3092	C	C5-C6-N1	-7.07	117.46	121.00
36	5	2739	A	C8-N9-C4	7.07	108.63	105.80
1	2	1456	C	C6-N1-C2	-7.07	117.47	120.30
36	1	878	G	C5-C6-O6	7.07	132.84	128.60
36	1	3092	C	O5'-P-OP1	-7.07	99.34	105.70
1	6	158	U	P-O3'-C3'	7.07	128.18	119.70
1	2	1458	G	C6-C5-N7	-7.06	126.16	130.40
36	1	809	G	N1-C6-O6	7.06	124.14	119.90
1	6	901	G	C4-C5-N7	7.06	113.62	110.80
36	5	2724	U	C6-N1-C2	-7.06	116.76	121.00
36	1	2860	U	N1-C2-O2	7.06	127.74	122.80
36	1	3204	C	C6-N1-C2	-7.06	117.48	120.30
36	1	2287	C	N3-C4-C5	-7.06	119.08	121.90
38	8	26	U	N1-C2-O2	7.06	127.74	122.80
36	1	2400	G	C4-C5-N7	7.06	113.62	110.80
36	5	3107	U	N3-C4-O4	7.05	124.34	119.40
36	1	870	G	C8-N9-C4	-7.05	103.58	106.40
36	5	197	G	C6-C5-N7	-7.05	126.17	130.40
36	5	1592	G	N9-C4-C5	7.05	108.22	105.40
1	2	1128	C	O5'-P-OP1	-7.05	99.36	105.70
36	1	2393	G	C5-C6-O6	-7.05	124.37	128.60
36	1	953	G	N1-C6-O6	7.05	124.13	119.90
36	5	842	G	C4-C5-N7	7.05	113.62	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	910	G	C5-C6-N1	-7.04	107.98	111.50
36	1	3085	G	N3-C2-N2	-7.04	114.97	119.90
36	5	2359	C	C6-N1-C2	7.04	123.12	120.30
36	1	2983	C	O5'-P-OP1	-7.04	99.36	105.70
36	5	2157	G	N3-C4-C5	7.04	132.12	128.60
36	5	2346	C	N3-C4-N4	7.04	122.92	118.00
36	1	727	G	C8-N9-C4	-7.03	103.59	106.40
36	5	412	G	C8-N9-C4	-7.03	103.59	106.40
36	1	2689	A	N1-C6-N6	-7.03	114.38	118.60
36	5	1179	A	N1-C2-N3	7.03	132.82	129.30
36	5	1194	G	C8-N9-C4	-7.03	103.59	106.40
36	5	2169	G	N1-C6-O6	-7.03	115.68	119.90
36	1	2606	G	N3-C4-C5	-7.03	125.09	128.60
1	2	354	C	N3-C4-C5	-7.03	119.09	121.90
36	1	1834	U	N3-C4-C5	-7.03	110.38	114.60
36	1	2636	A	N7-C8-N9	7.02	117.31	113.80
1	6	1537	C	C6-N1-C1'	7.02	129.23	120.80
36	5	1147	G	C8-N9-C4	-7.02	103.59	106.40
36	1	1165	A	C8-N9-C4	7.02	108.61	105.80
36	1	1878	G	O4'-C1'-N9	-7.02	102.58	108.20
1	6	25	C	P-O3'-C3'	7.02	128.12	119.70
36	5	1370	G	N1-C2-N3	7.02	128.11	123.90
15	C3	22	ALA	C-N-CD	-7.01	105.17	120.60
36	1	1149	G	N1-C2-N3	7.01	128.11	123.90
36	1	1307	G	C8-N9-C4	-7.01	103.59	106.40
36	1	1329	U	C6-N1-C2	-7.01	116.79	121.00
1	6	53	G	N1-C2-N3	7.01	128.11	123.90
36	1	358	G	C6-C5-N7	-7.01	126.19	130.40
1	6	553	G	C5-C6-O6	-7.01	124.39	128.60
36	5	423	A	C8-N9-C4	7.01	108.60	105.80
36	5	651	G	OP2-P-O3'	7.01	120.62	105.20
36	5	874	U	C6-N1-C2	7.01	125.21	121.00
36	5	934	G	N3-C4-N9	7.01	130.21	126.00
36	5	1321	G	C5-C6-O6	-7.01	124.40	128.60
36	1	2356	A	C5-C6-N6	-7.00	118.10	123.70
36	5	1199	C	O5'-P-OP2	-7.00	99.40	105.70
36	5	2849	C	N3-C4-N4	7.00	122.90	118.00
36	1	2764	C	N3-C4-C5	-7.00	119.10	121.90
1	6	1634	C	C2-N1-C1'	7.00	126.50	118.80
36	5	519	A	C6-C5-N7	-7.00	127.40	132.30
36	5	2323	G	C8-N9-C4	-7.00	103.60	106.40
36	1	1595	U	C6-N1-C2	7.00	125.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2916	U	N1-C2-O2	7.00	127.70	122.80
36	1	1904	C	N3-C4-N4	6.99	122.89	118.00
36	5	1206	G	N3-C4-C5	-6.99	125.10	128.60
36	5	87	U	N3-C2-O2	-6.99	117.31	122.20
36	1	229	G	N1-C6-O6	6.99	124.09	119.90
36	1	2684	C	N3-C4-C5	-6.99	119.10	121.90
1	2	16	G	N3-C4-N9	6.99	130.19	126.00
1	6	610	G	C8-N9-C1'	-6.99	117.92	127.00
45	L8	189	LEU	CA-CB-CG	6.98	131.36	115.30
18	C6	40	GLU	C-N-CD	-6.98	105.24	120.60
36	5	661	G	N7-C8-N9	6.98	116.59	113.10
36	5	638	C	C6-N1-C2	-6.98	117.51	120.30
36	1	1365	G	N3-C4-C5	-6.98	125.11	128.60
1	6	173	A	N1-C6-N6	6.98	122.79	118.60
36	5	2695	A	C6-N1-C2	-6.98	114.42	118.60
36	5	2620	G	N3-C2-N2	6.97	124.78	119.90
36	5	2993	G	C4-C5-N7	6.97	113.59	110.80
36	1	3311	C	C6-N1-C2	6.97	123.09	120.30
1	6	426	G	N3-C4-C5	-6.97	125.11	128.60
36	5	2160	G	N1-C6-O6	6.97	124.08	119.90
36	1	3050	U	N1-C2-O2	6.97	127.68	122.80
36	1	59	G	N1-C6-O6	6.96	124.08	119.90
1	6	343	C	N1-C2-O2	-6.96	114.72	118.90
36	5	728	G	N3-C4-N9	6.96	130.18	126.00
36	1	1820	U	P-O3'-C3'	6.96	128.05	119.70
36	1	2374	C	N3-C4-C5	-6.96	119.12	121.90
36	5	2936	A	N9-C4-C5	6.96	108.58	105.80
36	1	424	G	C5-C6-N1	6.96	114.98	111.50
1	2	1568	C	P-O3'-C3'	6.96	128.05	119.70
1	2	1657	U	O4'-C1'-N1	6.96	113.77	108.20
36	5	2405	C	C6-N1-C2	-6.96	117.52	120.30
36	1	884	A	N1-C6-N6	6.96	122.77	118.60
36	1	3085	G	N1-C6-O6	6.96	124.07	119.90
1	6	47	A	O5'-P-OP1	-6.96	99.44	105.70
36	5	1556	C	N1-C2-O2	6.96	123.07	118.90
36	5	2976	A	N1-C6-N6	-6.96	114.43	118.60
1	2	1773	C	N3-C4-C5	-6.95	119.12	121.90
36	1	1522	U	C5-C4-O4	-6.95	121.73	125.90
36	1	785	G	C2-N3-C4	6.95	115.38	111.90
36	5	2783	U	N1-C2-O2	6.95	127.67	122.80
36	1	1157	G	C8-N9-C4	-6.95	103.62	106.40
37	3	80	G	C8-N9-C4	-6.95	103.62	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	140	G	C8-N9-C4	-6.95	103.62	106.40
36	5	36	C	C2-N3-C4	-6.95	116.43	119.90
36	5	2817	A	C5-C6-N6	-6.95	118.14	123.70
36	5	972	A	C4-C5-C6	6.95	120.47	117.00
1	2	1180	C	N1-C2-O2	6.94	123.07	118.90
1	2	553	G	C6-C5-N7	-6.94	126.24	130.40
36	1	2986	U	N1-C2-O2	-6.94	117.94	122.80
36	5	2653	C	N1-C2-O2	-6.94	114.74	118.90
36	5	567	G	C5-C6-O6	-6.94	124.44	128.60
56	n0	113	ARG	NE-CZ-NH1	-6.93	116.83	120.30
36	1	1433	A	N1-C6-N6	-6.93	114.44	118.60
36	1	1556	C	C2-N1-C1'	6.93	126.42	118.80
36	5	2858	U	N3-C4-O4	6.93	124.25	119.40
1	2	73	U	OP1-P-O3'	6.93	120.44	105.20
36	5	2950	G	C6-C5-N7	-6.93	126.24	130.40
36	5	2992	U	C5-C6-N1	6.93	126.16	122.70
36	1	2917	G	C5-C6-N1	6.92	114.96	111.50
36	5	2943	G	C6-C5-N7	-6.92	126.25	130.40
36	5	1319	G	N7-C8-N9	-6.92	109.64	113.10
1	6	1629	G	N3-C4-C5	-6.92	125.14	128.60
36	5	2281	A	N1-C6-N6	6.92	122.75	118.60
36	1	1899	G	C8-N9-C4	-6.92	103.63	106.40
52	m6	78	ARG	NE-CZ-NH2	-6.92	116.84	120.30
36	1	1450	G	C5-N7-C8	-6.91	100.84	104.30
36	5	2966	G	C8-N9-C4	-6.91	103.63	106.40
38	8	14	C	O5'-P-OP2	-6.91	99.48	105.70
36	1	2385	G	N3-C4-C5	6.91	132.06	128.60
36	5	3374	U	C6-N1-C2	6.91	125.15	121.00
36	1	2726	C	N3-C4-N4	-6.91	113.16	118.00
36	5	2723	U	C5-C6-N1	6.91	126.15	122.70
36	1	640	U	C6-N1-C2	-6.91	116.86	121.00
36	1	640	U	C5-C6-N1	6.91	126.15	122.70
36	5	3035	A	C8-N9-C4	6.91	108.56	105.80
36	5	2629	U	N3-C2-O2	6.90	127.03	122.20
37	3	82	G	N3-C4-C5	-6.90	125.15	128.60
36	5	1124	U	C5-C4-O4	6.90	130.04	125.90
36	1	713	U	C5-C6-N1	-6.90	119.25	122.70
36	1	2311	G	C8-N9-C4	-6.90	103.64	106.40
36	1	895	A	C6-C5-N7	-6.89	127.47	132.30
1	6	103	A	O4'-C1'-N9	6.89	113.71	108.20
36	5	940	G	N1-C6-O6	-6.89	115.77	119.90
38	8	100	U	C5-C6-N1	6.89	126.15	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1077	U	C2-N1-C1'	-6.89	109.43	117.70
36	1	2938	G	N1-C2-N3	6.89	128.03	123.90
36	5	640	U	N3-C4-O4	6.89	124.22	119.40
37	3	105	C	OP2-P-O3'	6.88	120.34	105.20
36	5	3378	C	O5'-P-OP2	-6.88	99.50	105.70
36	1	1303	A	N9-C4-C5	-6.88	103.05	105.80
36	1	3210	A	O5'-P-OP2	-6.88	99.51	105.70
1	6	619	A	N1-C6-N6	-6.88	114.47	118.60
36	1	1897	G	C5-C6-O6	-6.88	124.47	128.60
36	5	1152	G	N7-C8-N9	6.88	116.54	113.10
36	5	2885	C	C5-C4-N4	-6.88	115.39	120.20
1	2	1274	C	C6-N1-C2	-6.88	117.55	120.30
38	4	29	U	N3-C4-O4	6.87	124.21	119.40
36	5	1604	G	N3-C4-C5	-6.87	125.16	128.60
36	5	2160	G	C6-C5-N7	-6.87	126.28	130.40
36	5	360	G	C5-C6-O6	6.87	132.72	128.60
36	5	2801	A	C8-N9-C4	6.87	108.55	105.80
36	5	36	C	N3-C4-C5	6.87	124.65	121.90
36	5	1513	G	N3-C4-C5	-6.87	125.17	128.60
36	5	2239	G	N1-C6-O6	6.87	124.02	119.90
36	5	2620	G	N9-C4-C5	-6.87	102.65	105.40
36	5	1115	G	N1-C6-O6	6.86	124.02	119.90
36	5	1367	G	C4-C5-C6	6.86	122.92	118.80
36	1	3054	U	N1-C2-N3	6.86	119.01	114.90
1	6	605	A	O5'-P-OP2	-6.86	99.53	105.70
52	M6	110	PRO	C-N-CD	-6.86	105.52	120.60
36	5	1192	C	C6-N1-C1'	-6.86	112.57	120.80
36	5	1604	G	C6-C5-N7	-6.86	126.29	130.40
36	5	2249	G	C8-N9-C4	-6.86	103.66	106.40
36	5	3326	G	C8-N9-C4	6.86	109.14	106.40
36	1	2688	U	C6-N1-C1'	-6.85	111.60	121.20
36	5	2842	U	O5'-P-OP2	6.85	118.92	110.70
36	5	1182	A	C5-N7-C8	-6.85	100.47	103.90
36	1	283	G	C5-N7-C8	-6.85	100.88	104.30
36	1	988	U	C5-C6-N1	-6.85	119.28	122.70
36	1	1312	C	O5'-P-OP1	-6.85	99.54	105.70
36	1	1437	C	N3-C4-C5	-6.85	119.16	121.90
36	1	3219	G	C5-C6-O6	-6.85	124.49	128.60
36	5	2531	C	N1-C2-O2	6.85	123.01	118.90
37	7	9	C	C6-N1-C2	-6.84	117.56	120.30
36	1	2606	G	C4-C5-C6	6.84	122.90	118.80
36	5	2620	G	C4-C5-N7	6.84	113.54	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2385	G	N3-C4-N9	-6.84	121.90	126.00
36	5	410	U	C5-C6-N1	6.84	126.12	122.70
36	5	3172	A	C5-C6-N6	-6.84	118.23	123.70
36	1	2392	C	C6-N1-C2	6.84	123.03	120.30
36	1	2283	G	N1-C6-O6	6.84	124.00	119.90
1	6	310	C	C6-N1-C2	-6.84	117.57	120.30
1	2	1560	U	N3-C2-O2	-6.83	117.42	122.20
1	6	160	C	N3-C2-O2	-6.83	117.11	121.90
36	5	666	A	N1-C6-N6	-6.83	114.50	118.60
36	5	2364	G	N9-C4-C5	6.83	108.13	105.40
36	5	104	G	C8-N9-C4	6.83	109.13	106.40
36	1	1191	U	O5'-P-OP1	-6.83	99.55	105.70
36	1	2699	G	N1-C6-O6	6.83	124.00	119.90
36	5	1370	G	C4-C5-N7	-6.82	108.07	110.80
36	5	1897	G	C6-C5-N7	-6.82	126.31	130.40
36	5	2331	C	O5'-P-OP1	-6.82	99.56	105.70
1	2	90	C	C6-N1-C2	-6.82	117.57	120.30
36	1	2853	A	C2-N3-C4	-6.82	107.19	110.60
36	5	934	G	C5-C6-N1	6.82	114.91	111.50
36	5	1434	G	O5'-P-OP2	-6.82	99.56	105.70
1	2	992	A	C5-N7-C8	-6.82	100.49	103.90
36	1	1428	A	N1-C2-N3	6.81	132.71	129.30
36	1	1175	C	C5-C6-N1	-6.81	117.59	121.00
1	6	176	C	N3-C2-O2	-6.81	117.14	121.90
36	5	2893	C	C6-N1-C2	-6.81	117.58	120.30
37	7	45	A	N1-C6-N6	-6.81	114.52	118.60
36	5	942	U	C4-C5-C6	6.80	123.78	119.70
36	5	2552	C	C2-N1-C1'	6.80	126.28	118.80
36	5	2856	G	N3-C2-N2	-6.80	115.14	119.90
36	5	3154	C	N3-C2-O2	-6.80	117.14	121.90
36	1	2846	U	N3-C2-O2	-6.80	117.44	122.20
36	1	608	A	C4-C5-C6	6.80	120.40	117.00
36	1	3278	C	N3-C4-C5	-6.80	119.18	121.90
36	5	2907	G	C5-N7-C8	-6.80	100.90	104.30
36	5	204	A	C8-N9-C4	-6.79	103.08	105.80
36	1	1115	G	N7-C8-N9	6.79	116.50	113.10
36	1	3344	A	N1-C6-N6	6.79	122.67	118.60
36	5	1449	A	N1-C6-N6	6.79	122.67	118.60
36	5	3225	C	C6-N1-C2	-6.79	117.58	120.30
36	1	332	C	C6-N1-C2	6.79	123.02	120.30
56	n0	144	LEU	CA-CB-CG	-6.79	99.69	115.30
36	5	339	C	N1-C2-O2	-6.79	114.83	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2915	U	N3-C2-O2	6.79	126.95	122.20
36	1	2622	C	C6-N1-C2	-6.78	117.59	120.30
38	8	25	G	N3-C4-N9	6.78	130.07	126.00
36	1	1838	G	N1-C6-O6	6.78	123.97	119.90
1	6	250	C	C5-C6-N1	6.78	124.39	121.00
36	1	291	C	C6-N1-C2	-6.78	117.59	120.30
36	5	1550	C	C6-N1-C2	-6.78	117.59	120.30
36	5	1416	C	N3-C2-O2	-6.78	117.16	121.90
36	1	2237	C	C6-N1-C2	6.77	123.01	120.30
36	1	2688	U	C2-N1-C1'	6.77	125.83	117.70
36	1	3319	U	N3-C2-O2	-6.77	117.46	122.20
36	5	970	A	N9-C4-C5	-6.77	103.09	105.80
36	5	1710	C	C6-N1-C2	6.77	123.01	120.30
36	1	2326	A	N1-C6-N6	-6.77	114.54	118.60
36	1	2617	U	N1-C2-N3	6.77	118.96	114.90
36	1	3142	A	N1-C2-N3	6.77	132.68	129.30
36	5	2880	U	N3-C2-O2	-6.77	117.46	122.20
1	2	959	U	N3-C2-O2	-6.77	117.46	122.20
1	6	536	C	C6-N1-C2	-6.77	117.59	120.30
36	1	2662	G	N9-C4-C5	-6.76	102.69	105.40
36	5	2726	C	N1-C2-N3	6.76	123.94	119.20
36	5	715	A	C8-N9-C4	-6.76	103.09	105.80
36	5	1885	U	C6-N1-C2	6.76	125.06	121.00
1	2	1241	G	C4-N9-C1'	6.76	135.29	126.50
36	1	905	U	N1-C2-N3	6.76	118.96	114.90
1	6	1028	C	C6-N1-C2	6.76	123.00	120.30
36	5	1161	G	O5'-P-OP2	6.76	118.81	110.70
36	5	1348	U	N3-C2-O2	-6.76	117.47	122.20
38	4	53	A	C5-C6-N1	6.76	121.08	117.70
36	5	3382	U	N3-C2-O2	-6.76	117.47	122.20
36	5	907	G	N3-C4-N9	6.76	130.06	126.00
36	1	1366	A	N1-C6-N6	-6.76	114.55	118.60
38	8	99	C	C6-N1-C2	6.76	123.00	120.30
36	5	656	A	N1-C6-N6	6.75	122.65	118.60
36	5	1841	A	O5'-P-OP1	-6.75	99.62	105.70
36	5	1433	A	N7-C8-N9	6.75	117.18	113.80
38	8	17	A	C5-C6-N6	-6.75	118.30	123.70
1	6	543	C	N3-C2-O2	-6.75	117.17	121.90
1	6	1550	A	C8-N9-C4	-6.75	103.10	105.80
36	5	644	G	C8-N9-C4	-6.75	103.70	106.40
36	1	1885	U	C6-N1-C2	6.74	125.05	121.00
36	5	2865	U	C4-C5-C6	-6.74	115.65	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	970	A	C5-N7-C8	-6.74	100.53	103.90
36	5	917	A	C8-N9-C4	-6.74	103.10	105.80
36	1	519	A	C4-C5-C6	6.74	120.37	117.00
36	1	2860	U	C4-C5-C6	-6.74	115.66	119.70
36	5	718	G	O4'-C1'-N9	6.74	113.59	108.20
1	2	1200	G	C6-C5-N7	-6.74	126.36	130.40
36	5	2964	G	C5-C6-O6	6.74	132.64	128.60
12	C0	88	PRO	N-CA-CB	6.74	111.38	103.30
36	1	397	A	N1-C6-N6	-6.74	114.56	118.60
36	1	1846	C	N1-C2-O2	-6.74	114.86	118.90
1	6	1725	U	N3-C2-O2	-6.74	117.49	122.20
36	1	677	A	OP1-P-OP2	-6.73	109.50	119.60
36	5	1752	A	N1-C6-N6	6.73	122.64	118.60
36	5	3108	G	C2-N3-C4	-6.73	108.53	111.90
36	1	1306	G	N1-C6-O6	6.73	123.94	119.90
24	d2	93	LEU	CA-CB-CG	6.73	130.77	115.30
36	1	1292	C	C6-N1-C2	6.72	122.99	120.30
36	1	2836	C	C5-C4-N4	6.72	124.91	120.20
36	1	108	A	N1-C6-N6	6.72	122.63	118.60
36	1	1077	U	C5-C6-N1	-6.72	119.34	122.70
36	1	1340	G	C5-C6-O6	-6.72	124.57	128.60
36	1	2549	G	N1-C2-N2	-6.72	110.15	116.20
1	6	1782	A	C8-N9-C4	-6.72	103.11	105.80
36	5	1339	C	O5'-P-OP1	-6.72	99.65	105.70
36	1	1899	G	N9-C4-C5	6.72	108.09	105.40
36	1	864	G	O5'-P-OP1	-6.72	99.66	105.70
36	1	905	U	N1-C2-O2	-6.72	118.10	122.80
36	1	2787	G	C6-C5-N7	-6.72	126.37	130.40
36	1	921	A	C4-C5-N7	-6.71	107.34	110.70
36	1	514	G	N1-C6-O6	6.71	123.93	119.90
36	1	1165	A	C2-N3-C4	-6.71	107.24	110.60
36	1	2875	U	N1-C2-O2	6.71	127.50	122.80
36	5	46	U	N1-C2-O2	-6.71	118.10	122.80
36	5	725	G	C5-C6-N1	-6.71	108.14	111.50
36	1	709	A	N9-C4-C5	-6.71	103.12	105.80
37	7	49	G	N3-C4-N9	-6.71	121.97	126.00
36	1	212	G	N1-C6-O6	6.71	123.92	119.90
36	5	1900	A	C5-C6-N6	-6.71	118.33	123.70
36	1	421	G	N3-C4-C5	-6.70	125.25	128.60
36	5	2953	U	N3-C4-O4	6.70	124.09	119.40
36	1	1371	G	C8-N9-C4	6.70	109.08	106.40
36	1	1835	A	C8-N9-C4	6.70	108.48	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1452	A	C4-C5-N7	6.70	114.05	110.70
37	7	1	G	N1-C2-N2	-6.70	110.17	116.20
36	5	788	C	OP2-P-O3'	6.70	119.94	105.20
1	2	453	U	N3-C2-O2	-6.70	117.51	122.20
36	1	39	A	C5-C6-N6	6.70	129.06	123.70
36	5	2966	G	C4-C5-C6	6.70	122.82	118.80
36	5	2552	C	N3-C2-O2	-6.69	117.22	121.90
1	2	1194	A	C8-N9-C4	-6.69	103.12	105.80
36	5	3326	G	N9-C4-C5	-6.69	102.72	105.40
36	1	906	A	C4-C5-C6	6.69	120.34	117.00
36	1	3278	C	N3-C2-O2	-6.69	117.22	121.90
36	1	591	G	O5'-P-OP1	6.68	118.72	110.70
36	1	3306	U	N3-C4-O4	-6.68	114.72	119.40
36	1	96	G	C2-N3-C4	-6.68	108.56	111.90
36	1	643	U	N1-C2-O2	6.68	127.48	122.80
36	1	1198	C	C6-N1-C2	-6.68	117.63	120.30
36	5	1152	G	N9-C4-C5	6.68	108.07	105.40
1	6	1285	U	C2-N1-C1'	6.68	125.71	117.70
1	2	577	G	C6-C5-N7	-6.68	126.39	130.40
36	1	1065	A	O5'-P-OP1	-6.67	99.69	105.70
36	1	864	G	N1-C6-O6	-6.67	115.90	119.90
36	1	3134	A	C8-N9-C4	6.67	108.47	105.80
36	5	3245	A	C4-C5-C6	6.67	120.33	117.00
36	1	2400	G	C5-C6-O6	-6.67	124.60	128.60
36	5	40	A	N1-C6-N6	6.67	122.60	118.60
36	5	798	G	N7-C8-N9	6.67	116.43	113.10
36	5	3024	A	C2-N3-C4	-6.66	107.27	110.60
36	1	2606	G	N3-C4-N9	6.66	130.00	126.00
1	2	16	G	C6-C5-N7	-6.66	126.41	130.40
1	6	1481	C	N3-C2-O2	-6.66	117.24	121.90
1	6	1751	C	C5-C6-N1	-6.66	117.67	121.00
36	5	3144	G	N3-C4-C5	-6.66	125.27	128.60
36	1	2647	A	C8-N9-C4	-6.66	103.14	105.80
1	2	1654	G	N3-C4-C5	-6.66	125.27	128.60
36	1	983	A	C6-N1-C2	-6.66	114.61	118.60
36	5	2645	G	C5-C6-O6	6.66	132.59	128.60
36	1	803	C	C6-N1-C1'	-6.65	112.82	120.80
36	1	969	C	N1-C2-O2	-6.65	114.91	118.90
36	1	1450	G	C4-C5-N7	6.65	113.46	110.80
36	5	371	G	N1-C6-O6	-6.65	115.91	119.90
36	1	913	A	O5'-P-OP1	-6.65	99.72	105.70
36	5	2698	G	C8-N9-C4	6.65	109.06	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	36	C	C6-N1-C2	6.65	122.96	120.30
1	2	75	U	N1-C2-O2	6.65	127.45	122.80
36	5	2372	A	P-O3'-C3'	6.65	127.68	119.70
36	1	638	C	N1-C2-O2	6.64	122.89	118.90
36	1	2615	G	C5-C6-O6	-6.64	124.61	128.60
36	5	523	A	N1-C6-N6	-6.64	114.61	118.60
1	2	1458	G	C4-C5-N7	6.64	113.46	110.80
1	6	473	A	N1-C6-N6	-6.64	114.62	118.60
36	1	2329	C	O5'-P-OP2	-6.64	99.73	105.70
1	6	619	A	N9-C4-C5	6.64	108.45	105.80
36	5	410	U	N3-C4-O4	6.64	124.05	119.40
36	5	803	C	C5-C6-N1	6.64	124.32	121.00
36	5	709	A	C8-N9-C4	6.63	108.45	105.80
36	1	300	G	N1-C6-O6	-6.63	115.92	119.90
36	1	2708	C	C6-N1-C2	6.63	122.95	120.30
36	5	414	U	N3-C2-O2	6.63	126.84	122.20
36	5	2758	A	C8-N9-C4	-6.63	103.15	105.80
36	1	2279	A	C4-C5-N7	6.63	114.01	110.70
37	3	91	G	C5-C6-O6	-6.63	124.62	128.60
36	5	2827	U	N3-C2-O2	-6.63	117.56	122.20
36	1	2921	U	O5'-P-OP1	6.63	118.65	110.70
37	7	82	G	C5-C6-O6	-6.63	124.62	128.60
38	4	93	U	N3-C4-O4	-6.62	114.76	119.40
36	5	822	G	O5'-P-OP1	-6.62	99.74	105.70
36	5	2620	G	C5-C6-N1	6.62	114.81	111.50
36	5	2966	G	N3-C4-C5	-6.62	125.29	128.60
36	5	3295	A	C5-C6-N1	6.62	121.01	117.70
1	6	1074	G	N1-C6-O6	6.62	123.87	119.90
36	1	2884	C	C6-N1-C2	6.61	122.94	120.30
36	1	2621	G	N3-C2-N2	-6.61	115.27	119.90
36	5	1588	A	N1-C6-N6	-6.61	114.63	118.60
36	1	3275	U	C6-N1-C2	-6.61	117.03	121.00
36	1	65	A	P-O3'-C3'	6.61	127.63	119.70
36	1	1307	G	N1-C6-O6	-6.61	115.94	119.90
36	5	2412	G	N3-C4-C5	-6.61	125.30	128.60
36	5	2783	U	N3-C2-O2	-6.60	117.58	122.20
36	1	424	G	C4-C5-N7	6.60	113.44	110.80
36	1	2434	U	N3-C2-O2	-6.60	117.58	122.20
1	6	904	G	N3-C4-C5	-6.60	125.30	128.60
36	5	1149	G	C6-C5-N7	-6.60	126.44	130.40
36	5	1416	C	N1-C2-O2	6.60	122.86	118.90
36	5	2423	U	N3-C2-O2	-6.60	117.58	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1103	A	C8-N9-C4	6.60	108.44	105.80
36	5	2167	A	C8-N9-C4	-6.60	103.16	105.80
36	5	2639	G	C6-C5-N7	-6.60	126.44	130.40
36	1	2174	G	C8-N9-C4	-6.59	103.76	106.40
1	2	623	A	O5'-P-OP1	-6.59	99.77	105.70
1	6	359	A	N3-C4-C5	6.59	131.41	126.80
1	6	1773	C	N3-C4-N4	6.59	122.61	118.00
36	1	3275	U	C5-C6-N1	6.59	126.00	122.70
36	5	424	G	C4-C5-N7	6.59	113.44	110.80
36	1	2416	U	C5-C6-N1	6.59	126.00	122.70
36	1	2310	U	O5'-P-OP1	-6.59	99.77	105.70
36	5	728	G	C6-C5-N7	-6.59	126.45	130.40
36	5	931	C	N3-C4-C5	6.58	124.53	121.90
36	5	2849	C	O5'-P-OP2	-6.58	99.78	105.70
36	5	2966	G	C6-C5-N7	-6.58	126.45	130.40
38	8	46	G	O5'-P-OP1	-6.58	99.77	105.70
36	1	663	C	N3-C4-C5	-6.58	119.27	121.90
36	5	1379	G	C6-C5-N7	-6.58	126.45	130.40
36	1	1400	G	C4-N9-C1'	6.58	135.05	126.50
36	1	3092	C	C5-C6-N1	-6.58	117.71	121.00
62	N6	126	LEU	CA-CB-CG	6.58	130.43	115.30
36	5	91	G	N9-C4-C5	-6.58	102.77	105.40
1	2	1490	C	O5'-P-OP1	-6.58	99.78	105.70
36	1	685	G	C8-N9-C4	6.58	109.03	106.40
36	1	2395	G	C4-C5-N7	6.58	113.43	110.80
36	1	2525	G	C6-C5-N7	-6.58	126.45	130.40
36	5	2403	G	N1-C6-O6	6.58	123.85	119.90
36	5	2434	U	O5'-P-OP2	-6.58	99.78	105.70
36	1	1429	G	N1-C2-N3	6.58	127.85	123.90
1	2	402	C	C6-N1-C2	6.57	122.93	120.30
36	1	1139	G	O5'-P-OP1	-6.57	99.78	105.70
36	1	3278	C	C6-N1-C2	-6.57	117.67	120.30
36	5	1370	G	N3-C4-C5	-6.57	125.31	128.60
36	1	1054	A	O5'-P-OP1	6.57	118.58	110.70
36	1	1906	G	N1-C6-O6	6.57	123.84	119.90
36	1	2821	C	O5'-P-OP1	-6.57	99.79	105.70
36	1	358	G	C5-C6-O6	-6.57	124.66	128.60
36	5	2947	G	C5-C6-O6	-6.57	124.66	128.60
1	2	830	U	C2-N1-C1'	6.56	125.58	117.70
36	1	1389	G	C6-C5-N7	-6.56	126.46	130.40
36	5	2832	C	C6-N1-C2	6.56	122.92	120.30
36	5	2763	U	OP2-P-O3'	6.56	119.63	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	553	G	C6-C5-N7	-6.56	126.46	130.40
36	5	1589	A	C8-N9-C4	-6.56	103.18	105.80
36	1	685	G	N1-C6-O6	6.56	123.83	119.90
36	1	1495	U	C4-C5-C6	6.56	123.63	119.70
36	1	2556	C	N1-C2-O2	6.56	122.83	118.90
36	5	424	G	O5'-P-OP1	6.56	118.57	110.70
36	5	1440	G	C5-C6-O6	6.56	132.53	128.60
1	6	272	U	N3-C2-O2	-6.56	117.61	122.20
36	1	3278	C	C2-N3-C4	6.55	123.18	119.90
36	5	586	C	N1-C2-O2	-6.55	114.97	118.90
36	1	608	A	C6-C5-N7	-6.55	127.71	132.30
36	5	970	A	N1-C6-N6	6.55	122.53	118.60
36	1	49	A	N1-C6-N6	6.55	122.53	118.60
36	5	641	C	O5'-P-OP1	-6.55	99.81	105.70
38	4	113	U	N1-C2-N3	6.55	118.83	114.90
1	6	272	U	C2-N1-C1'	6.55	125.56	117.70
1	6	1031	U	N1-C2-O2	-6.55	118.22	122.80
36	1	784	A	N1-C6-N6	6.54	122.53	118.60
36	1	1849	C	N3-C4-C5	6.54	124.52	121.90
36	5	1379	G	N1-C6-O6	6.54	123.83	119.90
36	1	1544	G	C5-C6-O6	-6.54	124.67	128.60
36	1	221	A	O5'-P-OP2	-6.54	99.81	105.70
36	5	633	C	N3-C4-C5	-6.54	119.28	121.90
36	5	2832	C	O5'-P-OP1	-6.54	99.81	105.70
36	5	3103	A	O5'-P-OP2	-6.54	99.81	105.70
36	5	1148	G	N9-C4-C5	-6.54	102.78	105.40
36	5	3195	U	OP1-P-O3'	6.54	119.59	105.20
36	1	39	A	N9-C4-C5	6.54	108.41	105.80
36	1	29	C	N3-C4-N4	6.53	122.57	118.00
36	1	1848	G	N3-C2-N2	6.53	124.47	119.90
46	L9	176	LEU	CA-CB-CG	-6.53	100.28	115.30
36	5	1417	G	N7-C8-N9	6.53	116.37	113.10
1	2	407	A	N1-C6-N6	-6.53	114.68	118.60
36	1	2755	C	O5'-P-OP1	-6.53	99.82	105.70
37	3	104	A	N1-C6-N6	-6.53	114.68	118.60
36	5	1012	G	C8-N9-C1'	6.53	135.49	127.00
36	5	1317	A	C4-C5-N7	6.53	113.97	110.70
37	7	51	A	N1-C6-N6	6.53	122.52	118.60
36	1	612	U	N1-C2-N3	6.53	118.82	114.90
1	6	325	G	C8-N9-C4	-6.53	103.79	106.40
1	2	1467	C	C6-N1-C2	-6.53	117.69	120.30
36	1	922	U	N1-C2-O2	6.53	127.37	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1857	C	C6-N1-C2	6.53	122.91	120.30
1	6	144	U	N3-C2-O2	-6.52	117.63	122.20
1	6	431	C	C2-N1-C1'	-6.52	111.63	118.80
36	5	3245	A	C4-C5-N7	6.52	113.96	110.70
36	1	993	G	N3-C4-C5	-6.52	125.34	128.60
36	1	2247	G	C4-N9-C1'	6.52	134.98	126.50
36	5	808	A	C8-N9-C4	-6.52	103.19	105.80
36	5	1133	A	N1-C6-N6	6.52	122.51	118.60
36	5	2933	A	N1-C6-N6	6.52	122.51	118.60
36	5	304	G	N9-C4-C5	6.52	108.01	105.40
36	5	800	G	N3-C4-N9	6.52	129.91	126.00
36	5	2282	U	C6-N1-C2	6.52	124.91	121.00
36	1	410	U	C6-N1-C2	-6.52	117.09	121.00
36	5	3015	G	N1-C6-O6	6.52	123.81	119.90
38	4	46	G	C5-C6-O6	6.51	132.51	128.60
36	1	3191	G	O5'-P-OP2	-6.51	99.84	105.70
36	1	197	G	C5-C6-O6	-6.51	124.69	128.60
36	5	587	U	C5-C4-O4	-6.51	121.99	125.90
36	5	942	U	N1-C2-O2	-6.51	118.24	122.80
36	5	2419	A	O5'-P-OP2	6.51	118.51	110.70
1	2	426	G	C6-C5-N7	-6.51	126.49	130.40
36	1	131	C	C6-N1-C2	-6.51	117.70	120.30
36	1	1400	G	N3-C4-C5	-6.51	125.34	128.60
36	5	3269	U	P-O3'-C3'	6.51	127.51	119.70
36	1	2136	C	N3-C4-C5	-6.51	119.30	121.90
36	5	3108	G	N1-C2-N3	6.50	127.80	123.90
36	1	339	C	N3-C4-C5	6.50	124.50	121.90
36	5	1159	A	C2-N3-C4	-6.50	107.35	110.60
36	5	1160	C	C6-N1-C1'	6.50	128.60	120.80
36	5	2892	A	N1-C6-N6	6.50	122.50	118.60
36	1	3212	C	C2-N1-C1'	-6.50	111.65	118.80
36	5	87	U	C6-N1-C2	-6.50	117.10	121.00
1	2	1082	C	N1-C2-O2	6.50	122.80	118.90
36	1	1518	U	C4-C5-C6	6.50	123.60	119.70
36	5	1130	A	C5-C6-N1	6.50	120.95	117.70
36	1	895	A	C5-N7-C8	-6.49	100.65	103.90
36	1	2422	C	N3-C2-O2	-6.49	117.36	121.90
36	5	720	A	N9-C4-C5	-6.49	103.20	105.80
36	5	2662	G	C8-N9-C1'	-6.49	118.56	127.00
36	1	2760	C	N1-C2-O2	-6.49	115.01	118.90
36	5	2875	U	N1-C1'-C2'	-6.49	104.86	112.00
36	1	1604	G	C4-N9-C1'	6.49	134.94	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2899	C	N3-C4-N4	6.49	122.54	118.00
36	5	1303	A	C8-N9-C4	6.49	108.39	105.80
1	6	965	U	N1-C2-O2	6.48	127.34	122.80
1	6	1747	G	O5'-P-OP2	-6.48	99.87	105.70
36	5	718	G	C8-N9-C1'	-6.48	118.57	127.00
36	5	2709	C	N3-C4-C5	6.48	124.49	121.90
36	1	225	C	N3-C4-C5	-6.48	119.31	121.90
36	1	1846	C	N3-C4-C5	-6.48	119.31	121.90
36	1	3214	U	N3-C2-O2	-6.48	117.66	122.20
1	6	542	A	N7-C8-N9	6.48	117.04	113.80
36	5	1135	A	N1-C6-N6	-6.48	114.71	118.60
38	4	29	U	C5-C4-O4	-6.48	122.01	125.90
36	5	1075	A	C8-N9-C4	6.48	108.39	105.80
36	5	2285	C	C6-N1-C1'	6.48	128.57	120.80
36	1	1279	C	C6-N1-C2	-6.48	117.71	120.30
36	5	2699	G	C5-C6-O6	-6.47	124.72	128.60
36	1	1332	A	O5'-P-OP1	-6.47	99.88	105.70
36	5	319	A	C8-N9-C4	6.47	108.39	105.80
1	2	334	G	N3-C4-N9	-6.47	122.12	126.00
36	1	651	G	N3-C4-N9	6.47	129.88	126.00
1	6	65	A	C2-N3-C4	-6.47	107.36	110.60
36	5	2585	G	N3-C4-N9	6.47	129.88	126.00
1	2	396	G	N3-C4-C5	6.47	131.83	128.60
36	5	793	C	C6-N1-C2	-6.47	117.71	120.30
36	1	421	G	C2-N3-C4	6.46	115.13	111.90
36	1	1367	G	N1-C6-O6	6.46	123.78	119.90
1	6	334	G	N3-C2-N2	-6.46	115.38	119.90
36	5	2307	G	N1-C6-O6	-6.46	116.02	119.90
36	1	1008	U	C5-C6-N1	-6.46	119.47	122.70
38	4	16	G	C8-N9-C4	6.46	108.98	106.40
1	6	334	G	N3-C4-N9	-6.46	122.12	126.00
36	5	2316	G	C4-C5-N7	-6.46	108.22	110.80
36	5	3214	U	N3-C2-O2	-6.46	117.68	122.20
1	2	323	A	O5'-P-OP2	-6.46	99.89	105.70
37	3	58	C	C6-N1-C2	-6.46	117.72	120.30
37	7	51	A	N1-C2-N3	6.46	132.53	129.30
36	1	369	A	N7-C8-N9	6.46	117.03	113.80
36	1	1886	A	N9-C4-C5	6.46	108.38	105.80
1	6	1564	U	C6-N1-C2	6.46	124.87	121.00
36	5	3313	U	O5'-P-OP2	-6.46	99.89	105.70
36	1	1005	G	C8-N9-C4	6.45	108.98	106.40
36	1	1404	G	C4-C5-N7	-6.45	108.22	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3387	U	C5-C6-N1	-6.45	119.47	122.70
36	1	940	G	C5-C6-N1	6.45	114.73	111.50
36	5	720	A	C4-C5-N7	6.45	113.93	110.70
37	7	92	A	N1-C6-N6	6.45	122.47	118.60
36	1	145	G	C5-C6-O6	-6.45	124.73	128.60
36	1	1901	A	C2-N3-C4	6.45	113.83	110.60
36	1	2772	C	O4'-C1'-N1	6.45	113.36	108.20
36	5	1301	A	C4-C5-C6	6.45	120.22	117.00
36	1	39	A	N3-C4-N9	-6.45	122.24	127.40
36	1	645	A	C6-N1-C2	-6.45	114.73	118.60
36	5	781	G	N3-C4-C5	-6.45	125.38	128.60
36	1	218	G	N1-C6-O6	6.45	123.77	119.90
36	1	809	G	C8-N9-C4	6.45	108.98	106.40
36	5	976	U	O5'-P-OP2	-6.45	99.90	105.70
1	2	543	C	N1-C2-O2	6.44	122.77	118.90
36	1	1429	G	C4-C5-N7	-6.44	108.22	110.80
1	6	1751	C	C6-N1-C2	6.44	122.88	120.30
36	5	421	G	C4-N9-C1'	6.44	134.87	126.50
1	2	577	G	C5-N7-C8	-6.44	101.08	104.30
36	1	658	G	C8-N9-C1'	-6.44	118.63	127.00
36	5	1126	G	C4-C5-C6	6.44	122.66	118.80
36	5	2392	C	C5-C6-N1	-6.44	117.78	121.00
37	7	75	G	C6-C5-N7	-6.44	126.54	130.40
1	2	1761	U	N1-C2-N3	6.44	118.76	114.90
1	6	1629	G	C8-N9-C4	-6.44	103.83	106.40
1	2	1280	C	N3-C4-C5	-6.43	119.33	121.90
36	1	676	G	N3-C2-N2	6.43	124.40	119.90
36	1	924	G	O5'-P-OP1	-6.43	99.91	105.70
36	1	1807	G	C4-N9-C1'	6.43	134.86	126.50
36	1	2875	U	P-O3'-C3'	-6.43	111.98	119.70
1	6	1645	G	N1-C6-O6	-6.43	116.04	119.90
36	5	1851	G	C5-C6-N1	-6.43	108.28	111.50
36	5	3303	G	O5'-P-OP2	-6.43	99.91	105.70
36	5	1369	A	C5-C6-N1	-6.43	114.48	117.70
36	5	2624	G	C6-C5-N7	-6.43	126.54	130.40
36	5	2805	G	N1-C6-O6	6.43	123.76	119.90
36	5	2647	A	N1-C6-N6	-6.43	114.74	118.60
36	5	1443	G	C4-C5-N7	6.43	113.37	110.80
36	5	2278	C	N1-C2-O2	6.42	122.75	118.90
36	5	3244	A	O4'-C1'-N9	-6.42	103.06	108.20
36	5	800	G	N9-C4-C5	-6.42	102.83	105.40
36	5	220	G	O5'-P-OP2	-6.42	99.92	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1452	A	C5-C6-N6	-6.42	118.56	123.70
36	5	2334	U	C6-N1-C2	-6.42	117.15	121.00
36	1	3379	C	O5'-P-OP2	-6.42	99.92	105.70
36	5	2420	C	N3-C2-O2	6.42	126.39	121.90
1	2	1539	G	C6-C5-N7	-6.42	126.55	130.40
36	1	2353	G	N1-C6-O6	6.42	123.75	119.90
1	6	272	U	C6-N1-C2	-6.42	117.15	121.00
36	5	936	A	O4'-C1'-N9	6.42	113.33	108.20
36	1	727	G	N1-C6-O6	-6.42	116.05	119.90
36	1	857	G	N1-C6-O6	6.41	123.75	119.90
36	1	2355	G	C4-C5-N7	6.41	113.36	110.80
36	5	2942	C	N3-C4-N4	6.41	122.49	118.00
36	5	3107	U	OP2-P-O3'	6.41	119.31	105.20
36	1	2889	C	N3-C2-O2	-6.41	117.41	121.90
36	1	2987	A	N1-C6-N6	6.41	122.45	118.60
36	1	890	C	N3-C4-C5	6.41	124.46	121.90
38	4	81	U	N1-C2-O2	6.41	127.29	122.80
36	5	1434	G	C8-N9-C4	-6.41	103.84	106.40
36	1	895	A	C4-C5-N7	6.41	113.91	110.70
1	6	1790	A	C8-N9-C4	6.41	108.36	105.80
36	5	1851	G	N1-C6-O6	6.41	123.75	119.90
36	1	2699	G	C6-C5-N7	-6.41	126.56	130.40
36	5	1481	A	C8-N9-C4	-6.41	103.24	105.80
36	5	3153	U	N1-C2-O2	6.40	127.28	122.80
36	1	1054	A	O5'-P-OP2	-6.40	99.94	105.70
36	5	916	G	O5'-P-OP1	-6.40	99.94	105.70
36	1	809	G	N9-C4-C5	-6.40	102.84	105.40
36	1	2860	U	C2-N1-C1'	6.40	125.38	117.70
36	5	2695	A	C5-C6-N1	6.40	120.90	117.70
36	5	3218	A	N1-C6-N6	6.40	122.44	118.60
1	6	298	C	C6-N1-C2	-6.40	117.74	120.30
36	5	84	U	N1-C2-O2	6.40	127.28	122.80
1	2	1116	A	N1-C6-N6	6.40	122.44	118.60
36	1	1536	G	N3-C2-N2	-6.40	115.42	119.90
36	5	345	G	C5-C6-O6	-6.39	124.76	128.60
36	5	968	G	C6-C5-N7	-6.39	126.56	130.40
36	5	3362	A	O4'-C1'-N9	6.39	113.32	108.20
36	5	874	U	C5-C6-N1	-6.39	119.50	122.70
36	5	2158	A	C5-C6-N1	6.39	120.90	117.70
36	1	2844	C	C6-N1-C2	6.39	122.86	120.30
36	5	2129	U	C5-C4-O4	6.39	129.74	125.90
36	1	39	A	C6-C5-N7	6.39	136.77	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	109	A	OP1-P-O3'	6.39	119.26	105.20
35	sM	167	PRO	N-CA-CB	6.39	110.97	103.30
36	5	3209	A	O4'-C1'-N9	6.39	113.31	108.20
36	1	720	A	N1-C6-N6	6.39	122.43	118.60
36	1	1001	G	C8-N9-C4	6.39	108.95	106.40
36	1	632	G	C6-C5-N7	-6.39	126.57	130.40
36	1	937	G	C8-N9-C4	6.39	108.95	106.40
36	1	3003	G	C8-N9-C4	6.39	108.95	106.40
36	5	1514	G	N3-C4-N9	6.39	129.83	126.00
36	1	2383	C	C5-C6-N1	6.38	124.19	121.00
36	5	429	U	C5-C6-N1	-6.38	119.51	122.70
36	5	867	G	N1-C6-O6	6.38	123.73	119.90
1	6	18	C	C6-N1-C2	-6.38	117.75	120.30
36	5	1161	G	N3-C4-N9	6.38	129.83	126.00
1	2	1297	G	N9-C4-C5	-6.38	102.85	105.40
36	1	933	A	C5-C6-N6	-6.38	118.60	123.70
36	1	1329	U	C5-C6-N1	6.38	125.89	122.70
36	1	2606	G	C6-C5-N7	-6.38	126.57	130.40
36	5	414	U	N1-C2-O2	-6.38	118.34	122.80
36	5	799	G	N1-C6-O6	-6.38	116.07	119.90
1	6	1169	G	C8-N9-C4	-6.38	103.85	106.40
36	5	1161	G	C5-C6-N1	6.38	114.69	111.50
37	7	51	A	C4-C5-C6	6.38	120.19	117.00
36	1	968	G	C6-C5-N7	-6.37	126.58	130.40
36	1	1792	C	N1-C2-O2	-6.37	115.08	118.90
36	5	2736	A	C6-C5-N7	-6.37	127.84	132.30
36	5	2308	C	N3-C2-O2	-6.37	117.44	121.90
36	1	111	C	N3-C2-O2	6.37	126.36	121.90
1	6	478	A	N1-C6-N6	6.37	122.42	118.60
1	2	351	C	N3-C2-O2	-6.37	117.44	121.90
36	1	2620	G	N1-C2-N3	-6.37	120.08	123.90
36	5	1599	G	C8-N9-C4	6.37	108.95	106.40
36	5	2968	G	O4'-C1'-N9	-6.37	103.11	108.20
36	5	3107	U	C6-N1-C2	-6.37	117.18	121.00
36	5	1497	C	N3-C2-O2	6.37	126.36	121.90
36	1	86	G	C4-N9-C1'	-6.36	118.23	126.50
36	5	2890	A	C8-N9-C4	-6.36	103.25	105.80
50	m4	72	LEU	CA-CB-CG	6.36	129.94	115.30
36	1	283	G	N7-C8-N9	6.36	116.28	113.10
36	1	906	A	C5-C6-N6	-6.36	118.61	123.70
36	5	3208	G	C6-C5-N7	-6.36	126.58	130.40
1	2	1170	G	C4-N9-C1'	6.36	134.77	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3192	U	N3-C4-O4	6.36	123.85	119.40
1	2	553	G	C4-C5-N7	6.36	113.34	110.80
36	1	2937	G	C8-N9-C4	6.35	108.94	106.40
1	6	553	G	C4-C5-N7	6.35	113.34	110.80
36	5	2421	U	C6-N1-C2	-6.35	117.19	121.00
36	1	2662	G	C5-C6-O6	-6.35	124.79	128.60
36	1	1349	G	N3-C4-N9	6.35	129.81	126.00
36	5	2856	G	N1-C6-O6	6.35	123.71	119.90
1	2	16	G	N3-C4-C5	-6.35	125.43	128.60
36	1	2190	U	C4-C5-C6	6.35	123.51	119.70
36	1	66	A	O5'-P-OP2	6.34	118.31	110.70
1	2	1657	U	C4-C5-C6	6.34	123.51	119.70
36	1	2620	G	N1-C2-N2	6.34	121.91	116.20
1	6	1606	C	O5'-P-OP2	-6.34	99.99	105.70
36	5	358	G	N3-C4-C5	6.34	131.77	128.60
36	1	2549	G	N3-C2-N2	6.34	124.34	119.90
36	1	2877	G	N9-C4-C5	6.34	107.94	105.40
1	6	1560	U	N3-C2-O2	-6.34	117.76	122.20
1	2	1458	G	C4-N9-C1'	6.34	134.74	126.50
36	1	2923	U	C6-N1-C2	6.34	124.80	121.00
28	d6	42	ARG	NE-CZ-NH2	6.34	123.47	120.30
36	5	1408	G	OP2-P-O3'	6.34	119.14	105.20
45	l8	69	LEU	CA-CB-CG	6.34	129.88	115.30
36	1	3140	G	C4-C5-N7	6.34	113.33	110.80
36	1	3214	U	O4'-C1'-N1	6.34	113.27	108.20
1	6	410	A	N1-C6-N6	6.34	122.40	118.60
1	6	467	G	C8-N9-C4	6.34	108.94	106.40
36	5	170	G	C4-N9-C1'	6.34	134.74	126.50
1	6	943	C	O5'-P-OP1	-6.33	100.00	105.70
36	1	1305	U	C5-C4-O4	6.33	129.70	125.90
36	1	2167	A	O5'-P-OP1	-6.33	100.00	105.70
36	5	595	G	C8-N9-C4	-6.33	103.87	106.40
36	5	3295	A	N1-C6-N6	-6.33	114.80	118.60
36	5	1158	A	N1-C6-N6	6.33	122.40	118.60
36	5	2129	U	N3-C2-O2	-6.33	117.77	122.20
36	5	2531	C	N3-C2-O2	-6.33	117.47	121.90
35	SM	167	PRO	N-CA-CB	6.33	110.89	103.30
36	1	2355	G	C5-C6-O6	-6.33	124.80	128.60
36	5	2377	G	N1-C6-O6	-6.33	116.10	119.90
36	5	2899	C	N3-C2-O2	-6.33	117.47	121.90
36	5	3315	G	C4-C5-C6	6.33	122.60	118.80
36	1	878	G	C4-C5-N7	-6.32	108.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1363	U	N1-C2-O2	6.32	127.23	122.80
36	1	961	C	C6-N1-C2	6.32	122.83	120.30
36	1	1428	A	C6-N1-C2	-6.32	114.81	118.60
36	5	2976	A	C5-C6-N6	6.32	128.76	123.70
1	2	992	A	N1-C6-N6	6.32	122.39	118.60
36	1	3269	U	C6-N1-C2	-6.32	117.21	121.00
36	1	230	U	N1-C2-N3	6.32	118.69	114.90
36	1	2373	A	O5'-P-OP1	-6.32	100.01	105.70
1	6	1428	G	C8-N9-C4	-6.32	103.87	106.40
36	5	204	A	N9-C4-C5	6.32	108.33	105.80
36	5	869	G	C5-C6-O6	-6.32	124.81	128.60
36	5	2692	A	C8-N9-C4	-6.32	103.27	105.80
36	1	1166	G	C5-N7-C8	-6.31	101.14	104.30
52	m6	84	LEU	CA-CB-CG	-6.31	100.78	115.30
37	7	35	C	N1-C2-O2	6.31	122.69	118.90
36	1	840	C	C5-C4-N4	-6.31	115.78	120.20
36	1	1851	G	C4-C5-N7	6.31	113.32	110.80
36	1	833	G	N1-C6-O6	-6.31	116.11	119.90
36	1	1891	A	C8-N9-C4	6.31	108.32	105.80
36	5	2403	G	C5-N7-C8	6.31	107.45	104.30
36	5	2945	G	N3-C4-N9	6.31	129.79	126.00
36	1	364	G	C5-C6-O6	-6.31	124.82	128.60
36	1	639	G	N1-C6-O6	6.31	123.69	119.90
36	1	3319	U	N1-C2-O2	6.31	127.22	122.80
36	5	718	G	N3-C4-C5	-6.31	125.45	128.60
36	1	2828	G	N3-C2-N2	6.31	124.31	119.90
1	6	1672	G	N3-C4-N9	6.30	129.78	126.00
36	5	514	G	C5-C6-O6	-6.30	124.82	128.60
36	5	2868	U	N1-C2-O2	6.30	127.21	122.80
36	1	232	G	N3-C4-N9	6.30	129.78	126.00
36	1	776	U	C5-C4-O4	6.30	129.68	125.90
36	5	2354	C	N1-C2-O2	-6.30	115.12	118.90
36	5	2938	G	C5-C6-O6	-6.30	124.82	128.60
36	5	1152	G	C4-C5-N7	6.29	113.32	110.80
36	1	3209	A	N1-C6-N6	6.29	122.38	118.60
39	L2	237	LEU	CA-CB-CG	-6.29	100.82	115.30
36	5	400	G	O5'-P-OP1	-6.29	100.04	105.70
36	5	1012	G	C6-C5-N7	6.29	134.18	130.40
36	5	1474	A	C8-N9-C4	6.29	108.32	105.80
36	1	73	C	N1-C2-O2	-6.29	115.12	118.90
36	5	2279	A	O4'-C1'-N9	6.29	113.23	108.20
36	5	2907	G	N3-C4-N9	-6.29	122.22	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	189	G	N1-C6-O6	-6.29	116.13	119.90
36	5	1126	G	C6-C5-N7	-6.29	126.63	130.40
36	5	2531	C	C2-N1-C1'	6.29	125.72	118.80
36	1	2261	G	N3-C4-N9	6.29	129.77	126.00
36	1	3242	G	C4-N9-C1'	-6.29	118.33	126.50
36	1	3306	U	N3-C2-O2	-6.29	117.80	122.20
37	7	6	C	C6-N1-C2	6.29	122.81	120.30
1	2	507	U	N1-C2-O2	6.29	127.20	122.80
1	2	863	A	C8-N9-C4	6.29	108.31	105.80
36	1	2930	A	C8-N9-C4	6.29	108.31	105.80
36	1	1349	G	N3-C4-C5	-6.28	125.46	128.60
36	1	2307	G	OP2-P-O3'	6.28	119.02	105.20
36	5	197	G	N3-C4-N9	6.28	129.77	126.00
36	1	1433	A	N7-C8-N9	6.28	116.94	113.80
36	5	718	G	C8-N9-C4	-6.28	103.89	106.40
36	1	650	C	O5'-P-OP1	-6.28	100.05	105.70
36	5	1744	G	C4-N9-C1'	6.28	134.66	126.50
36	5	2748	A	N1-C6-N6	6.28	122.37	118.60
1	2	1124	A	C2-N3-C4	-6.28	107.46	110.60
36	1	648	C	C5-C4-N4	-6.28	115.81	120.20
36	1	698	U	O4'-C1'-N1	6.28	113.22	108.20
36	1	1362	G	C8-N9-C4	6.28	108.91	106.40
1	6	360	A	N1-C6-N6	6.28	122.37	118.60
1	2	1340	U	N3-C2-O2	-6.28	117.81	122.20
1	2	1600	A	N1-C6-N6	6.28	122.36	118.60
36	1	2661	G	N1-C6-O6	6.28	123.67	119.90
36	5	1116	G	N3-C4-C5	-6.28	125.46	128.60
36	5	2160	G	C5-C6-O6	-6.28	124.83	128.60
36	1	2601	A	C8-N9-C4	6.27	108.31	105.80
36	1	1209	G	C4-C5-N7	-6.27	108.29	110.80
1	6	325	G	N9-C4-C5	6.27	107.91	105.40
36	5	2156	C	C2-N1-C1'	-6.27	111.90	118.80
36	1	1371	G	C5-C6-N1	-6.27	108.36	111.50
1	2	305	C	C6-N1-C2	-6.27	117.79	120.30
36	1	1377	G	C5-C6-O6	-6.27	124.84	128.60
36	5	648	C	N1-C2-O2	-6.27	115.14	118.90
36	5	2246	G	C8-N9-C4	-6.27	103.89	106.40
36	1	1381	A	N1-C6-N6	6.27	122.36	118.60
36	1	3362	A	C4-N9-C1'	6.27	137.58	126.30
36	5	2950	G	C4-C5-N7	6.27	113.31	110.80
36	5	1370	G	C5-C6-O6	6.27	132.36	128.60
1	6	542	A	C4-N9-C1'	6.26	137.57	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1798	U	C2-N1-C1'	6.26	125.22	117.70
36	5	1443	G	C5-C6-O6	-6.26	124.84	128.60
36	5	2376	G	C8-N9-C4	-6.26	103.89	106.40
36	1	2812	C	C2-N3-C4	-6.26	116.77	119.90
36	5	1171	G	N3-C4-N9	-6.26	122.24	126.00
36	1	999	G	C5-C6-O6	-6.26	124.84	128.60
1	2	970	A	N9-C4-C5	-6.26	103.30	105.80
36	1	1581	C	C6-N1-C2	-6.26	117.80	120.30
36	1	2306	C	N1-C2-O2	6.26	122.65	118.90
1	6	558	U	N1-C2-O2	6.26	127.18	122.80
36	1	2376	G	C4-C5-N7	6.25	113.30	110.80
38	4	143	U	O5'-P-OP1	-6.25	100.07	105.70
36	5	1370	G	C4-C5-C6	6.25	122.55	118.80
1	6	861	U	O5'-P-OP2	-6.25	100.07	105.70
36	5	922	U	C5-C6-N1	-6.25	119.57	122.70
36	5	2385	G	N3-C4-C5	6.25	131.73	128.60
36	1	2616	C	N3-C2-O2	-6.25	117.53	121.90
36	5	562	C	C2-N1-C1'	6.25	125.67	118.80
36	1	2725	U	C6-N1-C2	6.25	124.75	121.00
36	5	1793	C	N1-C2-O2	-6.25	115.15	118.90
36	5	2145	A	O5'-P-OP1	-6.25	100.08	105.70
36	5	2991	A	C6-N1-C2	-6.25	114.85	118.60
37	3	75	G	O5'-P-OP1	-6.25	100.08	105.70
36	5	2727	A	N1-C6-N6	-6.25	114.85	118.60
1	2	416	A	C8-N9-C4	6.24	108.30	105.80
36	1	810	A	C5-C6-N1	6.24	120.82	117.70
36	1	2245	C	C6-N1-C2	-6.24	117.80	120.30
36	5	739	G	O5'-P-OP1	-6.24	100.08	105.70
36	1	62	A	O5'-P-OP2	-6.24	100.08	105.70
36	1	1886	A	N1-C6-N6	-6.24	114.86	118.60
1	6	337	G	O4'-C1'-N9	-6.24	103.21	108.20
1	6	904	G	N3-C4-N9	6.24	129.74	126.00
36	5	2626	A	C2-N3-C4	-6.24	107.48	110.60
1	2	16	G	C4-N9-C1'	6.24	134.61	126.50
36	5	2957	G	N3-C4-N9	-6.24	122.26	126.00
1	2	1170	G	C8-N9-C1'	-6.24	118.89	127.00
36	1	3099	C	O5'-P-OP1	-6.24	100.09	105.70
1	2	1739	C	C6-N1-C2	6.23	122.79	120.30
36	1	983	A	N1-C2-N3	6.23	132.42	129.30
1	2	6	G	C8-N9-C4	-6.23	103.91	106.40
36	1	3181	C	N3-C2-O2	-6.23	117.54	121.90
36	1	3362	A	C4-C5-C6	6.23	120.11	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2370	G	C8-N9-C4	-6.23	103.91	106.40
1	6	779	U	N3-C2-O2	-6.23	117.84	122.20
36	1	1512	U	O5'-P-OP2	-6.22	100.10	105.70
36	1	2620	G	C4-N9-C1'	-6.22	118.41	126.50
1	6	1130	G	N7-C8-N9	-6.22	109.99	113.10
36	5	2662	G	C4-N9-C1'	6.22	134.59	126.50
36	1	924	G	N3-C2-N2	6.22	124.25	119.90
1	6	427	C	N1-C2-O2	-6.22	115.17	118.90
36	1	366	A	N1-C6-N6	-6.22	114.87	118.60
36	1	2385	G	C4-N9-C1'	-6.22	118.41	126.50
1	6	1634	C	N1-C2-O2	6.22	122.63	118.90
36	1	676	G	C4-C5-C6	6.22	122.53	118.80
36	1	718	G	C4-N9-C1'	6.22	134.59	126.50
36	1	933	A	C6-C5-N7	-6.22	127.95	132.30
36	1	1585	C	C5-C4-N4	-6.22	115.85	120.20
36	5	3144	G	N3-C4-N9	6.22	129.73	126.00
36	5	2947	G	C4-C5-N7	6.22	113.29	110.80
36	1	620	U	N3-C2-O2	-6.21	117.85	122.20
38	4	53	A	C6-C5-N7	6.21	136.65	132.30
36	1	1149	G	C5-C6-N1	-6.21	108.39	111.50
36	1	2283	G	C4-C5-N7	6.21	113.28	110.80
36	1	3182	G	C6-C5-N7	-6.21	126.67	130.40
36	5	1661	G	N1-C6-O6	6.21	123.63	119.90
1	2	1082	C	N3-C2-O2	-6.21	117.55	121.90
36	1	369	A	N9-C4-C5	6.21	108.28	105.80
36	1	3375	A	N9-C4-C5	6.21	108.28	105.80
36	1	24	G	C4-C5-C6	6.21	122.52	118.80
36	1	2342	U	C5-C6-N1	-6.21	119.60	122.70
36	1	714	G	N1-C6-O6	6.20	123.62	119.90
1	6	444	C	C6-N1-C2	6.20	122.78	120.30
36	5	1294	A	N1-C6-N6	-6.20	114.88	118.60
36	1	2194	G	C6-C5-N7	-6.20	126.68	130.40
36	5	1915	A	C8-N9-C4	6.20	108.28	105.80
36	1	698	U	C5-C4-O4	6.20	129.62	125.90
36	1	1118	C	C6-N1-C2	-6.20	117.82	120.30
36	1	1145	G	O5'-P-OP2	-6.20	100.12	105.70
36	1	1377	G	C4-C5-N7	6.20	113.28	110.80
36	1	3302	U	C5-C6-N1	-6.20	119.60	122.70
37	3	111	U	O5'-P-OP1	-6.20	100.12	105.70
1	6	542	A	C4-C5-C6	6.20	120.10	117.00
1	6	1137	A	C8-N9-C4	6.20	108.28	105.80
36	5	46	U	N3-C2-O2	6.20	126.54	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	715	A	C4-C5-N7	-6.20	107.60	110.70
36	5	1133	A	C5-C6-N6	-6.20	118.74	123.70
36	5	1376	C	C6-N1-C2	-6.20	117.82	120.30
36	1	341	G	C8-N9-C4	-6.20	103.92	106.40
36	1	1899	G	C5-C6-O6	6.20	132.32	128.60
36	1	2409	G	N3-C4-N9	6.20	129.72	126.00
1	6	619	A	C8-N9-C4	-6.20	103.32	105.80
36	5	888	A	C5-C6-N6	-6.20	118.74	123.70
36	1	2662	G	C4-C5-N7	6.20	113.28	110.80
1	6	425	A	C8-N9-C4	-6.20	103.32	105.80
36	5	2400	G	C5-C6-N1	-6.20	108.40	111.50
36	1	1125	U	O5'-P-OP1	-6.19	100.12	105.70
36	1	1178	G	N1-C2-N2	-6.19	110.62	116.20
36	5	1381	A	C2-N3-C4	-6.19	107.50	110.60
36	1	2416	U	C6-N1-C2	-6.19	117.28	121.00
36	5	904	A	C5-C6-N1	6.19	120.80	117.70
36	5	1317	A	C5-N7-C8	-6.19	100.80	103.90
36	5	1370	G	N9-C4-C5	6.19	107.88	105.40
36	5	2954	U	C2-N1-C1'	6.19	125.13	117.70
1	2	453	U	N1-C2-O2	6.19	127.13	122.80
36	1	1429	G	N3-C4-C5	-6.19	125.50	128.60
1	6	512	A	N1-C6-N6	6.19	122.31	118.60
36	5	610	G	N3-C4-C5	-6.19	125.50	128.60
36	5	706	A	C8-N9-C4	6.19	108.28	105.80
36	5	1879	A	O5'-P-OP1	6.19	118.13	110.70
36	5	2617	U	N3-C4-C5	-6.19	110.89	114.60
36	5	3028	G	N3-C2-N2	6.19	124.23	119.90
37	7	79	A	N1-C6-N6	6.19	122.31	118.60
36	5	410	U	N1-C2-O2	-6.19	118.47	122.80
36	1	645	A	C5-C6-N1	6.19	120.79	117.70
36	1	2675	C	N1-C2-O2	6.19	122.61	118.90
36	1	1901	A	N1-C6-N6	-6.18	114.89	118.60
1	6	402	C	N1-C2-O2	6.18	122.61	118.90
36	5	2727	A	O5'-P-OP2	-6.18	100.13	105.70
36	5	3294	A	N9-C4-C5	6.18	108.27	105.80
1	2	354	C	C6-N1-C2	-6.18	117.83	120.30
36	5	2283	G	N3-C4-C5	6.18	131.69	128.60
36	5	3143	C	N1-C2-O2	-6.18	115.19	118.90
1	2	55	A	C8-N9-C4	-6.18	103.33	105.80
1	2	1297	G	C8-N9-C4	6.18	108.87	106.40
36	1	1852	G	N1-C6-O6	6.18	123.61	119.90
1	6	1672	G	N1-C2-N2	-6.18	110.64	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2978	U	C4-C5-C6	6.18	123.41	119.70
37	7	88	G	N3-C4-C5	-6.18	125.51	128.60
1	6	158	U	OP1-P-O3'	6.18	118.79	105.20
36	5	2891	U	N3-C4-C5	6.18	118.31	114.60
36	1	2151	C	C6-N1-C2	6.18	122.77	120.30
36	1	2662	G	C6-C5-N7	-6.18	126.69	130.40
36	5	1208	U	C5-C4-O4	6.18	129.60	125.90
37	7	5	G	N7-C8-N9	-6.18	110.01	113.10
36	1	3074	G	N3-C4-C5	6.17	131.69	128.60
1	6	467	G	N3-C4-N9	6.17	129.70	126.00
1	6	1085	G	N3-C4-N9	-6.17	122.30	126.00
36	1	590	G	C4-C5-N7	6.17	113.27	110.80
1	2	992	A	C2-N3-C4	-6.17	107.51	110.60
36	5	2702	A	N1-C2-N3	6.17	132.38	129.30
36	5	2817	A	N1-C6-N6	6.17	122.30	118.60
36	5	3154	C	C6-N1-C2	-6.17	117.83	120.30
36	1	2758	A	C8-N9-C4	6.17	108.27	105.80
36	5	3053	G	N1-C6-O6	6.17	123.60	119.90
1	6	435	C	C6-N1-C2	6.17	122.77	120.30
36	5	1377	G	N1-C6-O6	-6.17	116.20	119.90
36	5	3108	G	C4-C5-C6	6.17	122.50	118.80
1	6	337	G	C8-N9-C1'	-6.17	118.98	127.00
36	5	929	A	O5'-P-OP2	-6.17	100.15	105.70
36	5	1517	G	N3-C4-N9	-6.17	122.30	126.00
36	5	2690	G	C4-N9-C1'	6.17	134.52	126.50
1	2	765	G	O4'-C1'-N9	-6.16	103.27	108.20
36	1	2788	C	N3-C2-O2	6.16	126.21	121.90
36	1	2968	G	C5-C6-O6	-6.16	124.90	128.60
36	5	973	A	N1-C6-N6	6.16	122.30	118.60
37	7	100	C	C6-N1-C2	6.16	122.77	120.30
36	5	804	C	N3-C2-O2	6.16	126.21	121.90
36	5	1519	G	N1-C6-O6	6.16	123.60	119.90
36	5	1347	U	O5'-P-OP2	-6.16	100.16	105.70
36	5	1373	A	C5-C6-N6	-6.16	118.77	123.70
36	5	3094	A	C8-N9-C4	6.16	108.26	105.80
1	2	1600	A	C2-N3-C4	-6.16	107.52	110.60
36	1	360	G	C4-C5-N7	6.16	113.26	110.80
36	5	2693	C	C6-N1-C2	6.16	122.76	120.30
36	5	2812	C	N3-C4-C5	6.16	124.36	121.90
36	5	360	G	C4-C5-C6	6.16	122.49	118.80
39	12	237	LEU	CA-CB-CG	-6.16	101.14	115.30
1	2	1489	U	N1-C2-O2	6.16	127.11	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	360	G	C6-C5-N7	-6.16	126.71	130.40
36	1	1660	C	C6-N1-C2	-6.16	117.84	120.30
36	5	1001	G	O5'-P-OP1	-6.16	100.16	105.70
36	5	2754	G	N1-C2-N2	-6.16	110.66	116.20
1	2	1560	U	C5-C4-O4	6.15	129.59	125.90
36	1	2787	G	C4-C5-N7	6.15	113.26	110.80
1	2	1004	U	N3-C2-O2	-6.15	117.89	122.20
36	1	1736	G	N1-C6-O6	6.15	123.59	119.90
36	1	2341	A	O5'-P-OP2	-6.15	100.16	105.70
36	5	965	A	N9-C4-C5	6.15	108.26	105.80
36	1	1507	G	C6-C5-N7	-6.15	126.71	130.40
36	1	1904	C	C2-N1-C1'	6.15	125.57	118.80
36	1	1079	A	C8-N9-C4	6.15	108.26	105.80
36	1	56	G	C5-C6-N1	6.15	114.57	111.50
36	1	229	G	O5'-P-OP2	6.15	118.08	110.70
36	1	1365	G	C8-N9-C4	-6.15	103.94	106.40
36	1	2166	A	N1-C6-N6	6.15	122.29	118.60
36	1	2306	C	C2-N1-C1'	6.15	125.56	118.80
36	1	2608	G	N1-C6-O6	6.15	123.59	119.90
36	1	3133	C	C6-N1-C2	-6.15	117.84	120.30
1	6	1700	C	C2-N1-C1'	6.15	125.56	118.80
36	5	92	G	C4-C5-N7	-6.15	108.34	110.80
36	5	1894	U	C5-C6-N1	-6.15	119.63	122.70
36	1	1807	G	N3-C4-C5	-6.14	125.53	128.60
36	1	2276	G	C6-C5-N7	-6.14	126.71	130.40
1	6	1600	A	N9-C1'-C2'	6.14	121.99	114.00
36	1	51	A	C4-C5-N7	6.14	113.77	110.70
36	5	2849	C	N3-C2-O2	6.14	126.20	121.90
36	5	2954	U	O4'-C1'-N1	6.14	113.11	108.20
36	1	968	G	C4-N9-C1'	6.14	134.48	126.50
36	5	1321	G	C5-N7-C8	-6.14	101.23	104.30
1	2	553	G	N9-C4-C5	-6.14	102.94	105.40
1	2	554	C	N3-C4-C5	-6.14	119.44	121.90
36	1	229	G	N1-C2-N2	6.14	121.72	116.20
36	1	1224	C	C6-N1-C2	-6.14	117.84	120.30
36	5	2961	G	O5'-P-OP2	-6.14	100.17	105.70
36	5	3180	A	N1-C2-N3	6.14	132.37	129.30
36	5	2624	G	N7-C8-N9	6.14	116.17	113.10
36	5	2772	C	P-O3'-C3'	6.14	127.07	119.70
36	5	3362	A	C2-N3-C4	-6.14	107.53	110.60
36	1	2870	C	N3-C4-C5	6.14	124.35	121.90
36	5	1889	G	C4-C5-N7	6.14	113.25	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	e1	100	LEU	CA-CB-CG	6.13	129.41	115.30
36	1	1929	G	N9-C4-C5	-6.13	102.95	105.40
1	6	1031	U	N3-C2-O2	6.13	126.49	122.20
36	1	1412	G	C6-C5-N7	-6.13	126.72	130.40
1	6	453	U	N3-C2-O2	-6.13	117.91	122.20
36	1	2836	C	N3-C4-C5	-6.13	119.45	121.90
36	5	424	G	C6-C5-N7	-6.13	126.72	130.40
36	5	1016	C	O5'-P-OP1	-6.13	100.19	105.70
36	1	716	A	C4-C5-N7	6.12	113.76	110.70
36	1	1601	U	C5-C4-O4	6.12	129.57	125.90
36	1	1793	C	C6-N1-C2	6.12	122.75	120.30
36	1	3172	A	N9-C4-C5	6.12	108.25	105.80
1	6	1119	G	C8-N9-C4	-6.12	103.95	106.40
1	6	1631	A	O5'-P-OP2	-6.12	100.19	105.70
36	5	522	A	C6-C5-N7	-6.12	128.01	132.30
36	5	826	G	C5-C6-O6	-6.12	124.92	128.60
36	5	1386	A	C5-C6-N1	-6.12	114.64	117.70
36	1	642	U	N3-C4-C5	-6.12	110.93	114.60
36	1	679	U	N3-C4-O4	-6.12	115.11	119.40
1	6	1600	A	N1-C2-N3	6.12	132.36	129.30
36	5	681	U	C2-N1-C1'	6.12	125.05	117.70
36	5	2623	G	C8-N9-C4	6.12	108.85	106.40
36	5	3080	G	N1-C6-O6	6.12	123.57	119.90
36	1	633	C	C4-C5-C6	6.12	120.46	117.40
36	5	511	G	N3-C2-N2	-6.12	115.62	119.90
36	1	3057	U	N3-C2-O2	-6.12	117.92	122.20
36	5	30	G	O5'-P-OP2	6.12	118.04	110.70
36	5	1435	A	C6-N1-C2	-6.12	114.93	118.60
36	5	2142	A	C5-C6-N1	6.12	120.76	117.70
38	8	84	C	C6-N1-C2	-6.12	117.85	120.30
36	5	2661	G	N3-C4-N9	6.12	129.67	126.00
36	1	953	G	N9-C4-C5	-6.12	102.95	105.40
36	1	2374	C	C4-C5-C6	6.12	120.46	117.40
1	6	1130	G	N3-C4-C5	6.11	131.66	128.60
36	5	883	A	N9-C4-C5	6.11	108.25	105.80
1	2	1198	G	C8-N9-C4	-6.11	103.95	106.40
36	5	907	G	C5-C6-N1	6.11	114.56	111.50
36	5	3245	A	N1-C2-N3	6.11	132.36	129.30
36	1	1792	C	C6-N1-C1'	6.11	128.13	120.80
1	6	402	C	O5'-P-OP2	-6.11	100.20	105.70
36	5	2968	G	O5'-P-OP1	-6.11	100.20	105.70
1	2	1137	A	C2-N3-C4	-6.11	107.55	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1297	G	N1-C6-O6	6.11	123.56	119.90
36	1	3089	C	C6-N1-C2	-6.11	117.86	120.30
36	5	1384	U	C6-N1-C2	-6.11	117.34	121.00
36	1	28	C	N3-C4-C5	6.11	124.34	121.90
36	1	519	A	N1-C6-N6	6.11	122.26	118.60
36	1	1171	G	N9-C4-C5	6.11	107.84	105.40
36	1	3098	G	O5'-P-OP1	-6.11	100.20	105.70
36	5	2968	G	C8-N9-C1'	-6.11	119.06	127.00
36	1	3133	C	C5-C6-N1	6.10	124.05	121.00
36	5	1790	G	N1-C6-O6	6.10	123.56	119.90
36	5	967	A	N7-C8-N9	6.10	116.85	113.80
36	5	1117	G	N1-C6-O6	6.10	123.56	119.90
36	1	1116	G	N9-C4-C5	6.10	107.84	105.40
36	1	3217	C	C6-N1-C1'	-6.10	113.48	120.80
1	6	603	U	N3-C2-O2	6.10	126.47	122.20
36	1	1141	C	C5-C6-N1	-6.10	117.95	121.00
36	1	2143	A	C5-N7-C8	-6.10	100.85	103.90
1	6	171	A	O5'-P-OP2	-6.10	100.21	105.70
1	6	553	G	C5-N7-C8	-6.10	101.25	104.30
36	5	1193	A	N1-C2-N3	6.10	132.35	129.30
36	5	2413	A	N9-C4-C5	-6.10	103.36	105.80
36	5	3298	C	O5'-P-OP1	-6.10	100.21	105.70
36	1	648	C	C6-N1-C2	-6.09	117.86	120.30
1	6	1128	C	O5'-P-OP1	-6.09	100.22	105.70
38	8	26	U	C6-N1-C2	-6.09	117.34	121.00
1	2	425	A	C4-C5-N7	6.09	113.75	110.70
36	1	1100	U	N3-C4-C5	6.09	118.26	114.60
36	5	2411	U	N3-C4-O4	-6.09	115.14	119.40
36	1	625	G	N1-C6-O6	6.09	123.56	119.90
37	7	13	A	C5-C6-N1	6.09	120.75	117.70
1	2	144	U	N3-C2-O2	-6.09	117.94	122.20
36	1	699	A	N3-C4-N9	-6.09	122.53	127.40
36	1	2625	C	N1-C2-O2	-6.09	115.25	118.90
36	5	3095	U	N1-C2-N3	6.09	118.55	114.90
36	1	2177	G	N3-C4-N9	6.09	129.65	126.00
36	5	25	U	C5-C6-N1	-6.09	119.66	122.70
36	5	2282	U	N1-C2-O2	-6.09	118.54	122.80
36	1	876	A	N1-C2-N3	-6.09	126.26	129.30
36	1	1362	G	OP2-P-O3'	6.09	118.59	105.20
36	1	1445	U	N1-C2-N3	6.09	118.55	114.90
1	2	545	A	OP1-P-O3'	6.08	118.59	105.20
36	1	3128	G	N3-C4-N9	6.08	129.65	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1130	G	C4-N9-C1'	-6.08	118.59	126.50
36	5	3208	G	N9-C4-C5	-6.08	102.97	105.40
36	1	1371	G	N1-C6-O6	6.08	123.55	119.90
36	1	2774	C	C2-N1-C1'	6.08	125.49	118.80
1	6	117	U	C6-N1-C2	-6.08	117.35	121.00
1	2	1212	G	C4-C5-N7	6.08	113.23	110.80
36	5	1909	A	C2-N3-C4	-6.08	107.56	110.60
11	S9	93	LEU	CA-CB-CG	6.08	129.28	115.30
36	1	2273	G	C4-N9-C1'	-6.08	118.60	126.50
36	1	2860	U	C6-N1-C1'	-6.08	112.69	121.20
1	6	610	G	C4-N9-C1'	6.08	134.40	126.50
36	5	197	G	C4-N9-C1'	6.08	134.40	126.50
36	5	1379	G	N9-C4-C5	-6.08	102.97	105.40
37	7	1	G	C8-N9-C1'	-6.08	119.10	127.00
1	2	1539	G	C8-N9-C1'	-6.08	119.10	127.00
36	1	2415	C	OP1-P-O3'	6.08	118.57	105.20
36	5	650	C	OP2-P-O3'	6.08	118.57	105.20
36	5	1208	U	N1-C2-O2	6.08	127.05	122.80
36	5	2818	U	N3-C2-O2	6.08	126.45	122.20
1	6	408	C	C6-N1-C2	-6.08	117.87	120.30
36	5	2167	A	C2-N3-C4	6.08	113.64	110.60
36	5	3362	A	C5-N7-C8	-6.08	100.86	103.90
1	2	380	U	N1-C2-O2	6.07	127.05	122.80
36	1	2648	G	N9-C1'-C2'	-6.07	105.32	112.00
36	5	1551	C	C6-N1-C2	-6.07	117.87	120.30
36	5	425	G	O5'-P-OP1	6.07	117.99	110.70
36	1	335	G	O5'-P-OP2	6.07	117.99	110.70
1	6	1698	G	P-O3'-C3'	6.07	126.98	119.70
36	1	2372	A	N1-C6-N6	6.07	122.24	118.60
36	1	2978	U	C5-C6-N1	-6.07	119.67	122.70
1	6	1765	A	N1-C6-N6	-6.07	114.96	118.60
36	5	709	A	N9-C4-C5	-6.07	103.37	105.80
41	14	20	LEU	CA-CB-CG	-6.07	101.34	115.30
36	1	2852	C	C5-C4-N4	-6.07	115.95	120.20
1	2	137	U	O5'-P-OP1	-6.06	100.24	105.70
36	5	360	G	C5-C6-N1	-6.06	108.47	111.50
36	5	2295	A	C5-C6-N1	6.06	120.73	117.70
36	1	953	G	OP1-P-O3'	6.06	118.54	105.20
36	5	2964	G	N1-C6-O6	-6.06	116.26	119.90
1	2	1212	G	C6-C5-N7	-6.06	126.76	130.40
36	1	1325	U	C6-N1-C2	6.06	124.64	121.00
1	6	1620	C	C6-N1-C2	-6.06	117.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	725	G	C4-N9-C1'	6.06	134.38	126.50
36	5	887	G	N1-C6-O6	6.06	123.53	119.90
36	1	1074	U	O5'-P-OP1	-6.06	100.25	105.70
36	5	998	A	O5'-P-OP1	-6.06	100.25	105.70
36	5	2145	A	C4-C5-C6	6.06	120.03	117.00
36	1	965	A	C5-N7-C8	-6.06	100.87	103.90
1	6	176	C	N1-C2-O2	6.05	122.53	118.90
36	5	3084	C	C6-N1-C2	6.05	122.72	120.30
36	5	3252	G	C8-N9-C4	6.05	108.82	106.40
36	1	2610	G	C2-N3-C4	-6.05	108.87	111.90
36	5	2843	U	N1-C2-O2	6.05	127.04	122.80
36	1	947	G	C4-C5-C6	6.05	122.43	118.80
36	1	1419	A	O5'-P-OP2	-6.05	100.25	105.70
38	4	13	A	OP1-P-OP2	6.05	128.68	119.60
38	4	26	U	N1-C2-O2	6.05	127.04	122.80
36	1	283	G	C8-N9-C4	-6.05	103.98	106.40
1	6	85	A	C8-N9-C4	-6.05	103.38	105.80
36	5	2182	A	OP1-P-O3'	6.05	118.50	105.20
36	5	2794	G	C8-N9-C4	6.05	108.82	106.40
1	2	346	G	N9-C4-C5	-6.04	102.98	105.40
36	1	2609	A	O5'-P-OP1	6.04	117.95	110.70
36	5	1744	G	N3-C4-N9	6.04	129.63	126.00
36	5	2295	A	N1-C6-N6	6.04	122.23	118.60
36	1	2409	G	C6-N1-C2	-6.04	121.47	125.10
36	1	2513	U	P-O3'-C3'	6.04	126.95	119.70
36	1	3277	U	N3-C2-O2	-6.04	117.97	122.20
36	5	2391	G	C2-N3-C4	6.04	114.92	111.90
36	5	2943	G	C4-C5-C6	6.04	122.42	118.80
37	7	1	G	N3-C2-N2	6.04	124.13	119.90
36	1	3093	C	N3-C4-C5	6.04	124.32	121.90
36	1	2695	A	O4'-C1'-N9	6.04	113.03	108.20
36	5	419	G	O5'-P-OP1	6.04	117.95	110.70
36	5	637	C	O5'-P-OP1	-6.04	100.27	105.70
36	5	1443	G	N9-C4-C5	-6.04	102.98	105.40
36	5	2775	U	C2-N1-C1'	-6.04	110.45	117.70
36	1	2836	C	N3-C2-O2	-6.04	117.67	121.90
36	5	1182	A	N1-C6-N6	6.04	122.22	118.60
36	5	1450	G	N1-C6-O6	6.04	123.52	119.90
36	1	1129	A	C5-C6-N6	-6.04	118.87	123.70
36	1	2991	A	C2-N3-C4	-6.04	107.58	110.60
36	1	1406	A	N1-C6-N6	6.03	122.22	118.60
36	1	2279	A	N9-C4-C5	-6.03	103.39	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1004	U	C6-N1-C2	-6.03	117.38	121.00
36	1	2774	C	N3-C4-N4	6.03	122.22	118.00
1	6	1672	G	N3-C4-C5	-6.03	125.58	128.60
36	5	809	G	C8-N9-C4	6.03	108.81	106.40
36	5	3309	G	C8-N9-C1'	-6.03	119.16	127.00
1	2	1541	G	C4-N9-C1'	6.03	134.34	126.50
36	1	2949	U	C6-N1-C2	6.03	124.62	121.00
36	1	1545	A	N1-C2-N3	6.03	132.31	129.30
36	1	29	C	C5-C4-N4	-6.03	115.98	120.20
36	5	43	A	O4'-C1'-N9	6.03	113.02	108.20
36	5	71	A	O5'-P-OP1	-6.03	100.28	105.70
36	1	3344	A	C4-N9-C1'	6.02	137.14	126.30
36	5	718	G	N3-C4-N9	6.02	129.61	126.00
36	5	2940	A	N1-C6-N6	-6.02	114.99	118.60
36	1	716	A	C8-N9-C4	6.02	108.21	105.80
36	1	718	G	C6-C5-N7	-6.02	126.79	130.40
36	1	3312	U	C5-C6-N1	-6.02	119.69	122.70
1	6	1619	C	C6-N1-C2	-6.02	117.89	120.30
1	6	1774	G	N1-C6-O6	-6.02	116.29	119.90
36	5	2160	G	N3-C4-N9	6.02	129.61	126.00
36	5	1857	C	C2-N1-C1'	6.02	125.42	118.80
36	5	3116	G	C4-C5-N7	6.02	113.21	110.80
37	7	26	C	C4-C5-C6	6.02	120.41	117.40
36	1	1451	C	N3-C4-C5	6.02	124.31	121.90
36	5	2403	G	N7-C8-N9	-6.02	110.09	113.10
36	5	3116	G	N9-C4-C5	-6.02	102.99	105.40
1	2	704	C	O4'-C1'-N1	6.02	113.01	108.20
36	1	921	A	C6-N1-C2	-6.02	114.99	118.60
36	5	1497	C	C5-C4-N4	-6.02	115.99	120.20
36	5	1592	G	C4-C5-N7	-6.02	108.39	110.80
36	1	25	U	N1-C2-O2	-6.02	118.59	122.80
36	1	2414	G	C5-C6-N1	-6.02	108.49	111.50
1	6	557	G	N3-C4-C5	-6.02	125.59	128.60
1	2	1539	G	N3-C4-N9	6.01	129.61	126.00
36	1	99	A	O4'-C1'-N9	6.01	113.01	108.20
36	1	658	G	C4-N9-C1'	6.01	134.32	126.50
36	1	1076	C	C6-N1-C2	6.01	122.71	120.30
36	5	1882	G	C4-C5-N7	6.01	113.20	110.80
1	2	1363	U	N3-C2-O2	-6.01	117.99	122.20
36	1	2787	G	C5-C6-O6	-6.01	124.99	128.60
36	5	578	A	O5'-P-OP2	6.01	117.92	110.70
1	2	1241	G	C4-C5-N7	6.01	113.20	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2411	U	C5-C6-N1	-6.01	119.69	122.70
36	1	197	G	C4-C5-N7	6.01	113.20	110.80
36	1	651	G	N9-C4-C5	-6.01	103.00	105.40
36	5	1582	C	C6-N1-C2	-6.01	117.90	120.30
36	5	2680	A	N1-C6-N6	-6.01	114.99	118.60
36	5	1081	U	N1-C2-O2	6.01	127.01	122.80
36	5	2145	A	C6-C5-N7	-6.01	128.09	132.30
36	5	2818	U	C4-C5-C6	-6.01	116.09	119.70
36	1	1522	U	C6-N1-C2	6.01	124.60	121.00
1	2	507	U	N3-C2-O2	-6.00	118.00	122.20
1	6	901	G	N1-C6-O6	6.00	123.50	119.90
36	1	342	A	O5'-P-OP2	-6.00	100.30	105.70
36	1	816	A	C5-C6-N1	6.00	120.70	117.70
36	1	1863	G	C4-C5-N7	6.00	113.20	110.80
36	5	2351	U	N1-C2-N3	6.00	118.50	114.90
36	1	3370	A	O5'-P-OP2	-6.00	100.30	105.70
1	6	1389	C	N3-C2-O2	-6.00	117.70	121.90
1	6	163	G	N3-C4-N9	-6.00	122.40	126.00
1	2	1541	G	N3-C4-N9	6.00	129.60	126.00
36	1	2993	G	OP1-P-OP2	6.00	128.59	119.60
1	6	1389	C	N1-C2-O2	6.00	122.50	118.90
36	5	437	G	N3-C4-N9	-6.00	122.40	126.00
36	5	3080	G	C5-C6-O6	-6.00	125.00	128.60
36	5	1374	G	O5'-P-OP2	-6.00	100.30	105.70
36	1	75	G	N1-C6-O6	5.99	123.50	119.90
36	1	285	A	C8-N9-C4	5.99	108.20	105.80
36	1	2639	G	N1-C6-O6	5.99	123.50	119.90
1	6	937	C	N3-C2-O2	-5.99	117.70	121.90
1	6	1606	C	N1-C2-O2	5.99	122.50	118.90
36	5	816	A	C2-N3-C4	5.99	113.60	110.60
36	5	2400	G	C2-N3-C4	-5.99	108.90	111.90
36	5	2615	G	C2-N3-C4	-5.99	108.90	111.90
36	1	1416	C	C5-C6-N1	-5.99	118.00	121.00
36	1	2802	A	N9-C4-C5	5.99	108.20	105.80
1	2	1600	A	C5-C6-N1	-5.99	114.70	117.70
36	1	342	A	N9-C4-C5	5.99	108.20	105.80
36	1	2658	G	C4-C5-N7	-5.99	108.41	110.80
36	5	651	G	N3-C4-C5	-5.99	125.61	128.60
36	5	1897	G	C2-N3-C4	-5.99	108.91	111.90
36	5	2968	G	C4-N9-C1'	5.99	134.29	126.50
36	1	189	G	N1-C6-O6	-5.99	116.31	119.90
36	1	1323	G	C5-N7-C8	-5.99	101.31	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2261	G	N3-C4-C5	-5.99	125.61	128.60
36	1	2283	G	C5-N7-C8	-5.99	101.31	104.30
36	1	2643	A	C2-N3-C4	-5.99	107.61	110.60
36	1	2647	A	C6-N1-C2	-5.99	115.01	118.60
36	5	660	A	N1-C6-N6	-5.99	115.01	118.60
36	5	1182	A	C4-C5-N7	5.99	113.69	110.70
36	5	1897	G	N3-C2-N2	-5.99	115.71	119.90
36	1	1020	G	C5-C6-O6	-5.98	125.01	128.60
36	1	1429	G	N1-C2-N2	-5.98	110.81	116.20
36	1	965	A	C2-N3-C4	-5.98	107.61	110.60
36	1	1186	G	N3-C4-N9	5.98	129.59	126.00
1	6	54	C	C6-N1-C2	-5.98	117.91	120.30
36	5	330	G	N1-C6-O6	5.98	123.49	119.90
36	5	1128	U	C5-C6-N1	-5.98	119.71	122.70
36	5	2403	G	C8-N9-C1'	-5.98	119.22	127.00
36	1	1369	A	C2-N3-C4	-5.98	107.61	110.60
36	5	725	G	C8-N9-C1'	-5.98	119.23	127.00
36	5	931	C	N3-C4-N4	-5.98	113.81	118.00
38	8	32	C	C6-N1-C2	5.98	122.69	120.30
1	2	1733	C	N3-C4-N4	5.98	122.19	118.00
1	2	348	U	O5'-P-OP2	-5.98	100.32	105.70
36	1	2647	A	N3-C4-C5	-5.98	122.62	126.80
1	6	781	U	C2-N1-C1'	5.98	124.87	117.70
36	5	2368	A	C8-N9-C4	-5.98	103.41	105.80
36	1	3312	U	C6-N1-C2	5.98	124.59	121.00
36	1	1851	G	C5-N7-C8	-5.97	101.31	104.30
36	1	1906	G	N3-C2-N2	-5.97	115.72	119.90
36	1	1908	A	N1-C6-N6	5.97	122.19	118.60
36	1	2126	A	C8-N9-C4	5.97	108.19	105.80
36	5	1885	U	C2-N1-C1'	-5.97	110.53	117.70
36	5	1917	C	C5-C6-N1	-5.97	118.01	121.00
36	1	1890	U	N3-C2-O2	5.97	126.38	122.20
36	1	2688	U	N1-C2-N3	-5.97	111.32	114.90
36	5	659	G	N3-C2-N2	5.97	124.08	119.90
36	5	923	C	C5-C4-N4	-5.97	116.02	120.20
36	5	2255	A	O5'-P-OP1	-5.97	100.33	105.70
36	5	1148	G	C8-N9-C4	5.97	108.79	106.40
36	1	558	U	N1-C2-O2	5.97	126.98	122.80
36	1	3266	G	N9-C4-C5	5.97	107.79	105.40
1	6	1731	A	N1-C6-N6	-5.96	115.02	118.60
36	5	1923	C	O5'-P-OP1	-5.96	100.33	105.70
36	5	2661	G	C5-C6-O6	-5.96	125.02	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2943	G	C5-C6-N1	-5.96	108.52	111.50
36	5	1404	G	N1-C6-O6	5.96	123.48	119.90
1	6	426	G	C4-N9-C1'	5.96	134.25	126.50
36	5	1406	A	C6-N1-C2	-5.96	115.02	118.60
1	2	1539	G	N3-C4-C5	-5.96	125.62	128.60
36	5	1212	A	N1-C6-N6	5.96	122.18	118.60
36	5	1347	U	N3-C2-O2	5.96	126.37	122.20
1	2	704	C	N1-C2-O2	5.96	122.47	118.90
36	1	2148	U	O5'-P-OP1	-5.96	100.34	105.70
36	5	672	A	N1-C6-N6	-5.96	115.02	118.60
36	1	1442	U	N3-C4-O4	5.96	123.57	119.40
36	1	1716	U	P-O3'-C3'	5.96	126.85	119.70
36	5	1592	G	C5-C6-N1	-5.96	108.52	111.50
36	5	3245	A	O4'-C1'-N9	5.96	112.97	108.20
36	1	123	A	C4-C5-N7	5.96	113.68	110.70
36	1	2836	C	N1-C2-N3	5.96	123.37	119.20
1	6	51	A	C8-N9-C4	5.95	108.18	105.80
1	6	938	G	N3-C4-C5	-5.95	125.62	128.60
1	6	1058	U	OP1-P-O3'	5.95	118.30	105.20
36	5	210	U	C5-C4-O4	5.95	129.47	125.90
36	5	2955	U	OP2-P-O3'	5.95	118.30	105.20
38	4	20	U	C5-C6-N1	-5.95	119.72	122.70
36	5	2608	G	OP2-P-O3'	5.95	118.29	105.20
36	5	2726	C	N3-C4-N4	-5.95	113.83	118.00
36	1	1393	A	N1-C6-N6	-5.95	115.03	118.60
36	1	3277	U	C5-C4-O4	5.95	129.47	125.90
36	1	936	A	C8-N9-C4	5.95	108.18	105.80
36	1	1522	U	C5-C6-N1	-5.95	119.73	122.70
1	6	1097	U	P-O3'-C3'	5.95	126.84	119.70
36	5	2914	G	N3-C4-C5	-5.95	125.63	128.60
1	2	1733	C	N3-C2-O2	5.95	126.06	121.90
1	2	87	C	C6-N1-C2	-5.95	117.92	120.30
36	1	2200	U	C4-C5-C6	5.95	123.27	119.70
36	5	119	U	N3-C4-O4	-5.95	115.24	119.40
36	5	197	G	C8-N9-C1'	-5.95	119.27	127.00
36	5	438	A	C8-N9-C4	5.95	108.18	105.80
37	3	80	G	C6-C5-N7	-5.94	126.83	130.40
36	5	2760	C	C5-C4-N4	-5.94	116.04	120.20
1	2	1761	U	P-O3'-C3'	5.94	126.83	119.70
36	1	693	A	N1-C6-N6	5.94	122.17	118.60
36	1	1851	G	C5-C6-O6	-5.94	125.03	128.60
36	5	2863	G	N1-C6-O6	-5.94	116.33	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2888	U	C5-C4-O4	-5.94	122.33	125.90
36	1	895	A	N1-C6-N6	5.94	122.16	118.60
36	1	1306	G	C2-N3-C4	-5.94	108.93	111.90
36	1	3310	A	C8-N9-C4	5.94	108.18	105.80
37	3	94	C	N3-C2-O2	5.94	126.06	121.90
36	5	1166	G	N3-C4-C5	5.94	131.57	128.60
36	5	1179	A	C2-N3-C4	-5.94	107.63	110.60
36	5	2757	U	C6-N1-C2	-5.94	117.44	121.00
36	5	1124	U	C6-N1-C2	-5.94	117.44	121.00
36	1	2991	A	N1-C2-N3	5.94	132.27	129.30
1	6	20	G	C2-N3-C4	-5.94	108.93	111.90
1	6	1058	U	P-O3'-C3'	5.94	126.83	119.70
36	5	2416	U	N3-C2-O2	-5.94	118.04	122.20
38	8	17	A	C4-C5-N7	5.94	113.67	110.70
36	1	1323	G	N3-C4-N9	5.94	129.56	126.00
1	6	194	U	C2-N1-C1'	5.93	124.82	117.70
36	5	922	U	N3-C2-O2	-5.93	118.05	122.20
36	5	1065	A	C8-N9-C4	5.93	108.17	105.80
36	5	1611	G	N1-C6-O6	5.93	123.46	119.90
36	1	2830	G	N1-C6-O6	5.93	123.46	119.90
36	1	2942	C	C2-N1-C1'	-5.93	112.28	118.80
36	5	974	G	C8-N9-C4	-5.93	104.03	106.40
37	7	44	C	C4-C5-C6	5.93	120.37	117.40
1	2	51	A	C8-N9-C4	5.93	108.17	105.80
50	M4	30	GLY	N-CA-C	-5.93	98.27	113.10
36	5	632	G	N3-C4-N9	5.93	129.56	126.00
36	5	709	A	N1-C6-N6	5.93	122.16	118.60
36	1	1536	G	N1-C2-N2	5.93	121.54	116.20
1	2	499	U	P-O3'-C3'	5.93	126.81	119.70
36	5	1179	A	OP1-P-OP2	-5.93	110.71	119.60
36	1	691	A	N1-C6-N6	5.93	122.16	118.60
36	1	1416	C	N3-C4-C5	5.93	124.27	121.90
36	1	1437	C	C5-C6-N1	5.93	123.96	121.00
1	6	443	C	N3-C4-N4	5.93	122.15	118.00
37	7	82	G	N1-C6-O6	5.93	123.46	119.90
1	2	1052	U	C2-N1-C1'	5.92	124.81	117.70
36	1	2683	U	C6-N1-C2	5.92	124.56	121.00
1	6	542	A	P-O3'-C3'	5.92	126.81	119.70
36	1	2621	G	N1-C6-O6	5.92	123.45	119.90
36	5	2818	U	N1-C2-N3	-5.92	111.35	114.90
36	5	2944	U	N3-C4-O4	-5.92	115.25	119.40
1	2	1560	U	C6-N1-C2	-5.92	117.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	968	G	N3-C4-N9	5.92	129.55	126.00
36	1	2300	G	O5'-P-OP1	-5.92	100.37	105.70
1	6	1568	C	P-O3'-C3'	5.92	126.81	119.70
36	5	2705	A	C8-N9-C4	5.92	108.17	105.80
1	2	425	A	N1-C6-N6	5.92	122.15	118.60
36	5	86	G	N3-C4-C5	-5.92	125.64	128.60
36	1	833	G	C5-N7-C8	5.92	107.26	104.30
36	1	2112	U	P-O3'-C3'	5.92	126.80	119.70
36	1	2408	U	O5'-P-OP1	-5.92	100.37	105.70
36	5	814	U	C6-N1-C2	-5.92	117.45	121.00
36	5	3200	G	N1-C6-O6	5.92	123.45	119.90
36	1	2725	U	C5-C6-N1	-5.92	119.74	122.70
1	6	1614	A	C5-C6-N1	-5.92	114.74	117.70
1	2	1241	G	C8-N9-C4	-5.91	104.03	106.40
36	5	1181	U	N3-C4-C5	-5.91	111.05	114.60
36	5	1335	C	C5-C4-N4	-5.91	116.06	120.20
1	6	412	A	C8-N9-C4	-5.91	103.44	105.80
36	5	2128	C	C6-N1-C2	-5.91	117.94	120.30
36	1	2175	U	C4-C5-C6	5.91	123.25	119.70
36	1	3344	A	C4-C5-N7	5.91	113.65	110.70
36	5	1316	C	N3-C4-N4	5.91	122.14	118.00
1	2	1100	G	C4-N9-C1'	5.91	134.18	126.50
1	2	1768	G	N9-C4-C5	5.91	107.76	105.40
36	1	1179	A	C2-N3-C4	-5.91	107.65	110.60
1	6	66	U	P-O3'-C3'	5.91	126.79	119.70
36	5	2846	U	N3-C2-O2	-5.91	118.06	122.20
36	1	300	G	C5-C6-O6	5.91	132.14	128.60
36	1	1419	A	C6-N1-C2	-5.91	115.06	118.60
36	1	2333	C	N3-C4-N4	-5.91	113.87	118.00
36	1	2336	U	N3-C2-O2	-5.91	118.07	122.20
1	6	1306	C	C5-C6-N1	5.91	123.95	121.00
36	5	991	G	N1-C6-O6	-5.91	116.36	119.90
36	5	1845	G	N3-C4-N9	5.91	129.54	126.00
36	5	2361	A	C8-N9-C4	-5.91	103.44	105.80
36	5	2888	U	O5'-P-OP1	-5.91	100.39	105.70
36	1	787	G	N3-C4-C5	-5.90	125.65	128.60
36	1	789	A	N1-C6-N6	-5.90	115.06	118.60
36	1	2370	G	C5-C6-N1	-5.90	108.55	111.50
1	6	1132	A	O5'-P-OP2	-5.90	100.39	105.70
36	5	522	A	C5-C6-N6	-5.90	118.98	123.70
36	5	994	G	N3-C4-C5	-5.90	125.65	128.60
36	1	2917	G	C2-N3-C4	5.90	114.85	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1306	G	C6-C5-N7	-5.90	126.86	130.40
36	5	2802	A	N1-C2-N3	-5.90	126.35	129.30
36	5	3362	A	N1-C6-N6	5.90	122.14	118.60
1	2	610	G	C8-N9-C1'	-5.90	119.33	127.00
1	6	1010	C	N3-C4-C5	-5.90	119.54	121.90
36	5	2111	G	N3-C4-N9	-5.90	122.46	126.00
36	1	1269	U	N1-C2-O2	5.90	126.93	122.80
36	1	2777	G	C8-N9-C4	-5.90	104.04	106.40
1	2	377	G	C8-N9-C4	5.89	108.76	106.40
36	5	1466	G	C5-C6-O6	-5.89	125.06	128.60
36	1	3344	A	C4-C5-C6	5.89	119.95	117.00
36	5	431	U	C6-N1-C2	5.89	124.53	121.00
36	5	3131	U	C6-N1-C2	5.89	124.54	121.00
42	15	110	LEU	CA-CB-CG	5.89	128.85	115.30
1	2	971	A	N1-C2-N3	5.89	132.25	129.30
36	1	1802	C	C5-C6-N1	5.89	123.94	121.00
36	1	2915	U	N3-C4-O4	5.89	123.52	119.40
37	3	40	C	C6-N1-C2	-5.89	117.94	120.30
1	6	1208	A	O4'-C1'-N9	5.89	112.91	108.20
36	1	335	G	N3-C4-N9	-5.89	122.47	126.00
36	1	2393	G	C4-C5-N7	5.89	113.16	110.80
1	6	1730	A	N9-C4-C5	5.89	108.16	105.80
1	6	448	C	C6-N1-C2	-5.89	117.94	120.30
1	6	455	C	C5-C6-N1	5.89	123.94	121.00
36	5	3303	G	C8-N9-C4	5.89	108.75	106.40
36	5	656	A	C5-C6-N6	-5.88	118.99	123.70
36	5	887	G	C5-N7-C8	-5.88	101.36	104.30
36	5	2715	A	OP2-P-O3'	5.88	118.15	105.20
36	5	2942	C	C6-N1-C2	-5.88	117.95	120.30
36	1	1745	C	O5'-P-OP2	-5.88	100.41	105.70
1	6	1533	C	C6-N1-C2	-5.88	117.95	120.30
36	5	968	G	N1-C6-O6	5.88	123.43	119.90
36	5	1149	G	C2-N3-C4	-5.88	108.96	111.90
36	5	2231	C	O4'-C1'-N1	5.88	112.91	108.20
36	5	3285	C	N1-C2-O2	5.88	122.43	118.90
36	1	212	G	C8-N9-C1'	-5.88	119.36	127.00
36	1	344	A	N1-C6-N6	-5.88	115.07	118.60
36	1	1694	U	N1-C2-O2	5.88	126.91	122.80
36	1	2890	A	N9-C4-C5	5.88	108.15	105.80
36	1	3214	U	C6-N1-C2	-5.88	117.47	121.00
36	5	2585	G	N3-C4-C5	-5.88	125.66	128.60
36	5	3299	A	N9-C4-C5	5.88	108.15	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	927	C	O5'-P-OP1	-5.88	100.41	105.70
36	1	348	A	C8-N9-C4	5.88	108.15	105.80
36	1	350	C	C2-N1-C1'	5.88	125.26	118.80
36	1	364	G	C4-C5-N7	5.88	113.15	110.80
36	1	682	U	N3-C4-O4	-5.88	115.29	119.40
36	1	857	G	C5-C6-N1	-5.88	108.56	111.50
1	6	1174	C	N1-C2-O2	5.88	122.43	118.90
36	5	2385	G	C5-C6-N1	-5.88	108.56	111.50
36	5	2992	U	C2-N1-C1'	5.88	124.75	117.70
36	1	1836	C	N1-C2-O2	5.88	122.42	118.90
36	1	188	U	N1-C2-O2	-5.87	118.69	122.80
36	1	214	G	C5-C6-O6	-5.87	125.08	128.60
36	1	648	C	N3-C2-O2	-5.87	117.79	121.90
36	1	937	G	C5-C6-O6	-5.87	125.08	128.60
36	1	2860	U	N1-C2-N3	-5.87	111.38	114.90
36	1	2876	C	N1-C2-O2	-5.87	115.38	118.90
1	6	334	G	C8-N9-C1'	5.87	134.63	127.00
36	5	356	C	C6-N1-C2	-5.87	117.95	120.30
1	6	1791	A	N1-C6-N6	5.87	122.12	118.60
36	5	36	C	C5-C4-N4	-5.87	116.09	120.20
36	5	2211	U	N3-C2-O2	-5.87	118.09	122.20
36	1	435	C	C6-N1-C2	5.87	122.65	120.30
36	1	2309	A	C5-C6-N6	-5.87	119.00	123.70
36	1	2356	A	C6-C5-N7	-5.87	128.19	132.30
1	6	1118	G	C8-N9-C4	5.87	108.75	106.40
36	1	86	G	C8-N9-C1'	5.87	134.63	127.00
36	5	397	A	N1-C6-N6	-5.87	115.08	118.60
36	5	2907	G	N3-C4-C5	5.87	131.53	128.60
36	5	3036	G	C5-C6-O6	5.87	132.12	128.60
36	1	2877	G	C8-N9-C4	-5.86	104.06	106.40
47	M0	167	LEU	CA-CB-CG	5.86	128.79	115.30
36	1	335	G	N3-C4-C5	5.86	131.53	128.60
36	5	1481	A	P-O3'-C3'	5.86	126.73	119.70
36	5	2904	U	C6-N1-C1'	-5.86	113.00	121.20
1	2	1110	G	C8-N9-C4	5.86	108.74	106.40
36	1	1366	A	N9-C4-C5	5.86	108.14	105.80
36	1	2356	A	C4-C5-N7	5.86	113.63	110.70
36	1	3303	G	C5-C6-O6	-5.86	125.09	128.60
36	5	1514	G	C6-C5-N7	-5.86	126.89	130.40
36	5	2281	A	C5-C6-N6	-5.86	119.02	123.70
1	2	793	A	C8-N9-C4	-5.85	103.46	105.80
1	2	1003	A	O4'-C1'-N9	5.85	112.88	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	817	A	N9-C1'-C2'	5.85	121.61	114.00
36	1	2860	U	C5-C6-N1	5.85	125.63	122.70
36	1	1733	G	N3-C4-N9	5.85	129.51	126.00
36	1	2688	U	C5-C4-O4	-5.85	122.39	125.90
36	1	3270	U	O5'-P-OP1	-5.85	100.43	105.70
36	5	3303	G	N3-C4-C5	5.85	131.52	128.60
36	5	658	G	C6-C5-N7	-5.85	126.89	130.40
36	5	2706	G	O5'-P-OP2	-5.85	100.44	105.70
38	8	42	G	N1-C6-O6	5.85	123.41	119.90
36	1	2828	G	N3-C4-N9	5.85	129.51	126.00
36	5	2337	C	N1-C2-O2	5.85	122.41	118.90
1	2	734	A	OP1-P-O3'	5.84	118.06	105.20
36	1	864	G	C5-C6-O6	5.84	132.11	128.60
1	6	1421	A	C8-N9-C4	5.84	108.14	105.80
36	5	328	U	C5-C4-O4	5.84	129.41	125.90
36	5	2411	U	C6-N1-C2	5.84	124.51	121.00
36	5	2817	A	N3-C4-N9	5.84	132.08	127.40
36	5	3049	A	C8-N9-C4	5.84	108.14	105.80
38	8	10	A	C2-N3-C4	-5.84	107.68	110.60
36	1	1124	U	C5-C4-O4	5.84	129.41	125.90
36	1	1126	G	N1-C6-O6	5.84	123.41	119.90
36	5	2345	A	C6-C5-N7	-5.84	128.21	132.30
36	5	2629	U	N1-C2-O2	-5.84	118.71	122.80
36	5	40	A	C6-C5-N7	-5.84	128.21	132.30
36	5	644	G	N3-C4-C5	-5.84	125.68	128.60
1	2	1745	G	N3-C4-N9	5.84	129.50	126.00
36	1	36	C	N3-C4-C5	5.84	124.23	121.90
36	1	394	G	N3-C4-N9	-5.84	122.50	126.00
36	1	1536	G	C5-C6-O6	-5.84	125.10	128.60
36	1	1855	U	C2-N1-C1'	5.84	124.70	117.70
36	5	1394	A	N1-C6-N6	-5.84	115.10	118.60
1	6	1614	A	N1-C6-N6	5.83	122.10	118.60
36	5	2572	C	C2-N1-C1'	5.83	125.22	118.80
47	M0	176	LEU	CA-CB-CG	5.83	128.71	115.30
36	5	959	C	N1-C2-O2	-5.83	115.40	118.90
36	5	1379	G	C5-C6-O6	-5.83	125.10	128.60
36	5	1855	U	N3-C2-O2	-5.83	118.12	122.20
36	5	2700	G	C8-N9-C4	5.83	108.73	106.40
36	1	1311	G	N1-C6-O6	5.83	123.40	119.90
36	5	1855	U	C6-N1-C2	-5.83	117.50	121.00
37	7	96	U	N1-C2-O2	-5.83	118.72	122.80
36	1	1313	G	C5-C6-O6	-5.83	125.10	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	65	A	C8-N9-C4	5.83	108.13	105.80
1	6	421	A	C8-N9-C4	5.83	108.13	105.80
1	6	886	U	N3-C2-O2	-5.83	118.12	122.20
36	5	2632	G	N1-C6-O6	5.83	123.40	119.90
54	M8	166	LEU	CA-CB-CG	-5.83	101.90	115.30
36	5	3315	G	N1-C6-O6	5.83	123.40	119.90
1	2	959	U	N1-C2-O2	5.83	126.88	122.80
36	1	974	G	N3-C4-C5	-5.83	125.69	128.60
36	1	1411	C	N3-C2-O2	-5.83	117.82	121.90
36	5	2820	A	C8-N9-C4	-5.83	103.47	105.80
36	1	690	A	N1-C2-N3	5.82	132.21	129.30
36	1	1923	C	C6-N1-C2	5.82	122.63	120.30
36	5	1301	A	N3-C4-N9	5.82	132.06	127.40
36	1	422	A	C8-N9-C4	-5.82	103.47	105.80
38	8	12	A	N1-C6-N6	5.82	122.09	118.60
1	2	447	U	N3-C4-O4	5.82	123.47	119.40
1	2	1100	G	C8-N9-C1'	-5.82	119.43	127.00
36	1	933	A	N1-C2-N3	5.82	132.21	129.30
36	1	2572	C	N1-C2-O2	5.82	122.39	118.90
36	5	519	A	C5-N7-C8	-5.82	100.99	103.90
36	1	1369	A	C4-C5-C6	5.82	119.91	117.00
1	6	1285	U	N3-C2-O2	-5.82	118.13	122.20
36	5	2190	U	N1-C2-N3	5.82	118.39	114.90
36	1	339	C	C2-N3-C4	-5.82	116.99	119.90
36	1	2975	U	N1-C2-O2	5.82	126.87	122.80
36	5	2137	U	N3-C4-C5	5.82	118.09	114.60
1	2	1590	G	N1-C6-O6	-5.82	116.41	119.90
36	1	908	G	C8-N9-C1'	-5.82	119.44	127.00
36	5	826	G	C4-C5-N7	5.82	113.13	110.80
36	1	3362	A	C5-N7-C8	-5.81	100.99	103.90
36	5	720	A	C5-C6-N6	-5.81	119.05	123.70
36	1	2935	U	C2-N3-C4	5.81	130.49	127.00
1	6	13	C	C6-N1-C2	-5.81	117.98	120.30
36	5	969	C	N1-C2-O2	-5.81	115.41	118.90
36	5	1458	U	O5'-P-OP1	-5.81	100.47	105.70
36	5	2388	U	N1-C2-N3	5.81	118.39	114.90
36	1	1179	A	OP2-P-O3'	5.81	117.98	105.20
36	1	2273	G	N7-C8-N9	-5.81	110.19	113.10
36	1	3204	C	N1-C2-O2	5.81	122.39	118.90
36	5	1878	G	P-O3'-C3'	5.81	126.67	119.70
36	5	2929	C	C5-C4-N4	-5.81	116.13	120.20
36	5	3107	U	N3-C4-C5	-5.81	111.11	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1105	C	C6-N1-C2	-5.81	117.98	120.30
36	1	809	G	C4-C5-N7	5.81	113.12	110.80
36	5	511	G	N3-C4-N9	-5.81	122.52	126.00
36	5	531	G	O5'-P-OP1	-5.81	100.47	105.70
36	5	896	A	O5'-P-OP2	-5.81	100.47	105.70
54	m8	127	LEU	CA-CB-CG	5.81	128.66	115.30
1	2	73	U	P-O3'-C3'	5.81	126.67	119.70
36	1	213	A	N1-C6-N6	5.81	122.08	118.60
36	1	2555	G	O5'-P-OP2	-5.81	100.47	105.70
1	6	117	U	N3-C2-O2	-5.81	118.14	122.20
1	6	368	U	O5'-P-OP2	-5.81	100.47	105.70
1	2	521	A	C8-N9-C4	-5.80	103.48	105.80
36	1	2397	A	C5-N7-C8	-5.80	101.00	103.90
36	1	2954	U	OP1-P-O3'	5.80	117.97	105.20
36	1	3000	A	C8-N9-C4	5.80	108.12	105.80
36	5	676	G	N3-C4-C5	-5.80	125.70	128.60
36	5	2231	C	C2-N1-C1'	5.80	125.19	118.80
36	5	2801	A	N7-C8-N9	-5.80	110.90	113.80
36	1	1733	G	C8-N9-C4	-5.80	104.08	106.40
36	5	2911	A	O5'-P-OP2	-5.80	100.48	105.70
36	1	1492	G	N3-C4-N9	5.80	129.48	126.00
36	5	366	A	N1-C6-N6	5.80	122.08	118.60
36	5	2392	C	C2-N1-C1'	-5.80	112.42	118.80
36	5	3150	A	N1-C6-N6	5.80	122.08	118.60
1	2	331	A	N1-C6-N6	-5.80	115.12	118.60
1	2	1077	C	C5-C6-N1	5.80	123.90	121.00
36	1	609	G	N1-C6-O6	5.80	123.38	119.90
1	6	901	G	C5-C6-O6	-5.80	125.12	128.60
36	1	776	U	N1-C2-N3	5.80	118.38	114.90
36	1	2434	U	C4-C5-C6	5.80	123.18	119.70
36	5	3108	G	N1-C6-O6	5.80	123.38	119.90
37	7	115	G	C5-C6-O6	-5.80	125.12	128.60
36	5	2800	G	C8-N9-C4	-5.79	104.08	106.40
36	1	339	C	N3-C4-N4	-5.79	113.94	118.00
36	1	2554	A	C8-N9-C4	5.79	108.12	105.80
36	1	2836	C	C6-N1-C2	-5.79	117.98	120.30
1	6	782	U	N1-C2-O2	5.79	126.86	122.80
36	5	804	C	N1-C2-O2	-5.79	115.42	118.90
37	7	3	U	C5-C6-N1	-5.79	119.80	122.70
36	1	343	U	N3-C2-O2	-5.79	118.15	122.20
36	1	682	U	C5-C4-O4	5.79	129.38	125.90
1	6	402	C	O4'-C1'-N1	5.79	112.83	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1115	U	C5-C6-N1	-5.79	119.80	122.70
36	5	1704	A	C8-N9-C4	5.79	108.12	105.80
36	5	2354	C	N3-C4-C5	-5.79	119.58	121.90
70	O4	51	LEU	CA-CB-CG	5.79	128.62	115.30
36	1	1365	G	N3-C4-N9	5.79	129.47	126.00
36	1	3002	C	C6-N1-C2	5.79	122.61	120.30
36	5	2412	G	N3-C4-N9	5.79	129.47	126.00
36	5	2760	C	C2-N3-C4	-5.79	117.00	119.90
36	1	1154	A	C4-C5-C6	5.79	119.89	117.00
36	1	2896	A	N1-C2-N3	5.79	132.19	129.30
36	1	906	A	O4'-C1'-N9	-5.79	103.57	108.20
36	5	567	G	C5-N7-C8	-5.79	101.41	104.30
36	5	2112	U	N1-C2-O2	-5.79	118.75	122.80
36	5	2185	G	C2-N3-C4	-5.79	109.01	111.90
36	5	2364	G	C4-C5-N7	-5.79	108.49	110.80
36	5	2627	C	C4-C5-C6	5.79	120.29	117.40
36	5	3180	A	C6-N1-C2	-5.79	115.13	118.60
36	5	2515	A	N1-C6-N6	-5.78	115.13	118.60
36	5	3010	U	C5-C4-O4	5.78	129.37	125.90
1	2	325	G	N1-C6-O6	5.78	123.37	119.90
1	2	590	C	C6-N1-C2	-5.78	117.99	120.30
36	1	1129	A	N1-C6-N6	5.78	122.07	118.60
36	5	400	G	N9-C4-C5	5.78	107.71	105.40
36	1	1131	G	C6-C5-N7	-5.78	126.93	130.40
36	1	1839	A	O5'-P-OP1	-5.78	100.50	105.70
36	1	2949	U	N3-C2-O2	5.78	126.25	122.20
36	5	647	A	C8-N9-C4	-5.78	103.49	105.80
1	2	93	A	N9-C4-C5	5.78	108.11	105.80
36	1	1303	A	C6-C5-N7	-5.78	128.25	132.30
36	1	1422	G	C6-C5-N7	-5.78	126.93	130.40
36	1	2200	U	N1-C2-O2	-5.78	118.76	122.80
1	6	976	G	C4-C5-N7	5.78	113.11	110.80
36	5	1317	A	N7-C8-N9	5.78	116.69	113.80
36	1	688	G	N3-C4-C5	-5.78	125.71	128.60
36	1	803	C	C5-C4-N4	-5.78	116.16	120.20
36	1	1190	A	C4-C5-C6	5.78	119.89	117.00
36	1	1321	G	N9-C4-C5	5.78	107.71	105.40
36	5	725	G	C4-C5-C6	5.77	122.26	118.80
36	5	2271	A	C2-N3-C4	5.77	113.49	110.60
36	5	2700	G	N9-C4-C5	-5.77	103.09	105.40
36	1	1446	A	C8-N9-C4	-5.77	103.49	105.80
36	1	86	G	O5'-P-OP2	-5.77	100.51	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	345	G	C6-C5-N7	-5.77	126.94	130.40
36	5	2724	U	N3-C4-C5	-5.77	111.14	114.60
36	5	3181	C	N3-C4-C5	-5.77	119.59	121.90
36	1	633	C	N3-C4-C5	-5.77	119.59	121.90
36	1	2688	U	N1-C2-O2	5.77	126.84	122.80
36	1	2919	A	C2-N3-C4	-5.77	107.72	110.60
36	5	1417	G	N3-C4-C5	-5.77	125.72	128.60
1	2	51	A	O5'-P-OP1	-5.77	100.51	105.70
36	1	102	C	O5'-P-OP1	5.77	117.62	110.70
36	1	1905	G	OP2-P-O3'	5.77	117.89	105.20
1	2	465	G	O5'-P-OP1	-5.76	100.51	105.70
36	1	642	U	O5'-P-OP2	-5.76	100.51	105.70
36	1	1442	U	N1-C2-O2	-5.76	118.77	122.80
36	1	2324	A	N1-C6-N6	-5.76	115.14	118.60
36	1	2868	U	N3-C2-O2	-5.76	118.16	122.20
36	5	561	C	N1-C2-O2	-5.76	115.44	118.90
36	5	1062	A	O5'-P-OP2	-5.76	100.51	105.70
36	1	999	G	C5-C6-N1	5.76	114.38	111.50
36	1	2996	U	C5-C6-N1	5.76	125.58	122.70
1	6	334	G	C4-N9-C1'	-5.76	119.01	126.50
36	1	1939	G	C4-N9-C1'	5.76	133.99	126.50
36	1	2365	C	C6-N1-C2	5.76	122.60	120.30
36	5	643	U	N3-C4-O4	5.76	123.43	119.40
36	5	1142	G	C4-N9-C1'	5.76	133.99	126.50
36	1	123	A	C5-C6-N6	-5.76	119.09	123.70
36	1	335	G	C5-N7-C8	-5.76	101.42	104.30
36	1	2664	C	C6-N1-C2	-5.76	118.00	120.30
36	5	2142	A	C2-N3-C4	5.76	113.48	110.60
1	2	425	A	C5-N7-C8	-5.76	101.02	103.90
36	1	968	G	N3-C4-C5	-5.76	125.72	128.60
36	5	1208	U	N3-C2-O2	-5.76	118.17	122.20
36	5	1193	A	C2-N3-C4	-5.75	107.72	110.60
38	8	96	A	C5-C6-N6	-5.75	119.10	123.70
37	3	91	G	N1-C6-O6	5.75	123.35	119.90
36	5	938	C	OP1-P-O3'	5.75	117.86	105.20
36	5	1886	A	C8-N9-C4	-5.75	103.50	105.80
36	5	2411	U	C2-N1-C1'	-5.75	110.80	117.70
1	2	28	A	C5-C6-N1	5.75	120.58	117.70
36	1	1296	C	C6-N1-C2	-5.75	118.00	120.30
36	1	2403	G	C4-C5-C6	5.75	122.25	118.80
36	5	1142	G	N3-C4-N9	5.75	129.45	126.00
36	5	2112	U	P-O3'-C3'	5.75	126.60	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	84	C	N3-C4-C5	-5.75	119.60	121.90
1	2	610	G	C4-N9-C1'	5.75	133.97	126.50
1	6	957	G	N1-C6-O6	5.75	123.35	119.90
37	7	73	C	OP1-P-O3'	5.75	117.85	105.20
36	1	1084	A	N1-C6-N6	5.75	122.05	118.60
36	1	2774	C	C5-C4-N4	-5.75	116.17	120.20
36	5	2805	G	C5-C6-O6	-5.75	125.15	128.60
36	1	2697	A	N9-C4-C5	5.75	108.10	105.80
36	1	3028	G	C8-N9-C4	-5.75	104.10	106.40
36	5	1371	G	N7-C8-N9	-5.75	110.23	113.10
36	5	2621	G	N3-C2-N2	-5.75	115.88	119.90
36	1	570	A	N1-C6-N6	-5.74	115.15	118.60
36	1	716	A	N1-C6-N6	5.74	122.05	118.60
1	6	87	C	C6-N1-C2	-5.74	118.00	120.30
36	5	651	G	C6-C5-N7	-5.74	126.95	130.40
36	5	1124	U	N1-C2-N3	5.74	118.35	114.90
36	1	1001	G	C8-N9-C1'	-5.74	119.54	127.00
36	1	3214	U	C5-C4-O4	5.74	129.34	125.90
36	1	1171	G	N3-C4-N9	-5.74	122.56	126.00
1	6	1594	G	O5'-P-OP1	-5.74	100.53	105.70
37	7	48	U	C5-C4-O4	-5.74	122.46	125.90
1	2	555	A	C8-N9-C4	-5.74	103.50	105.80
36	1	2370	G	C5-C6-O6	5.74	132.04	128.60
36	1	3266	G	C5-C6-O6	5.74	132.04	128.60
36	5	1885	U	C5-C6-N1	-5.74	119.83	122.70
1	2	736	C	C6-N1-C2	-5.74	118.01	120.30
36	1	375	A	OP1-P-O3'	5.74	117.82	105.20
36	1	1330	A	C5-C6-N1	-5.74	114.83	117.70
36	1	2406	C	C5-C4-N4	-5.74	116.19	120.20
36	1	2647	A	C5-C6-N6	-5.74	119.11	123.70
1	6	1645	G	N9-C4-C5	5.74	107.69	105.40
36	5	994	G	C2-N3-C4	5.74	114.77	111.90
36	5	2234	G	C8-N9-C4	5.74	108.69	106.40
36	5	1048	A	N7-C8-N9	-5.73	110.93	113.80
36	1	3181	C	N3-C4-C5	-5.73	119.61	121.90
36	5	1793	C	N3-C2-O2	5.73	125.91	121.90
36	5	2818	U	C5-C4-O4	-5.73	122.46	125.90
1	2	1753	A	N1-C6-N6	5.73	122.04	118.60
36	1	2938	G	C6-N1-C2	-5.73	121.66	125.10
36	1	3112	G	N3-C4-N9	5.73	129.44	126.00
37	3	66	A	C8-N9-C4	5.73	108.09	105.80
1	6	815	G	C4-C5-N7	5.73	113.09	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1575	G	N1-C6-O6	-5.73	116.46	119.90
36	5	400	G	C5-C6-O6	5.73	132.04	128.60
36	1	1303	A	C4-C5-N7	5.73	113.56	110.70
36	1	2287	C	N1-C2-O2	-5.73	115.46	118.90
1	6	95	G	C2-N3-C4	5.73	114.76	111.90
1	6	187	G	P-O3'-C3'	5.73	126.57	119.70
36	5	508	U	C6-N1-C2	-5.73	117.56	121.00
36	5	1190	A	N1-C6-N6	-5.73	115.16	118.60
1	6	422	G	C8-N9-C4	-5.73	104.11	106.40
36	5	3270	U	O5'-P-OP1	-5.73	100.55	105.70
1	2	720	G	OP1-P-O3'	5.72	117.80	105.20
36	1	363	G	C8-N9-C4	-5.72	104.11	106.40
37	7	101	G	N1-C6-O6	5.72	123.33	119.90
36	1	1279	C	C5-C6-N1	5.72	123.86	121.00
36	1	1419	A	O5'-P-OP1	5.72	117.57	110.70
36	1	2829	U	N3-C4-O4	5.72	123.41	119.40
36	1	145	G	C6-C5-N7	-5.72	126.97	130.40
36	1	895	A	C2-N3-C4	-5.72	107.74	110.60
1	6	1340	U	C5-C4-O4	5.72	129.33	125.90
36	1	997	A	C8-N9-C4	-5.72	103.51	105.80
36	1	2180	G	C2-N3-C4	-5.72	109.04	111.90
36	1	2639	G	C8-N9-C1'	-5.72	119.56	127.00
36	1	3063	C	C2-N3-C4	-5.72	117.04	119.90
1	6	390	G	C5-C6-O6	-5.72	125.17	128.60
12	c0	83	PRO	N-CA-CB	5.72	110.16	103.30
36	1	342	A	C8-N9-C4	-5.72	103.51	105.80
36	1	2890	A	C8-N9-C4	-5.72	103.51	105.80
36	5	3129	A	O4'-C1'-N9	5.72	112.78	108.20
3	S1	181	LEU	CA-CB-CG	5.72	128.45	115.30
36	1	1445	U	C2-N3-C4	-5.72	123.57	127.00
36	1	3143	C	N3-C2-O2	5.72	125.90	121.90
37	7	37	G	C5-C6-O6	-5.72	125.17	128.60
1	2	730	G	C4-N9-C1'	5.71	133.93	126.50
36	1	2300	G	C5-C6-N1	-5.71	108.64	111.50
36	1	2903	A	N1-C6-N6	5.71	122.03	118.60
37	3	33	U	N1-C2-O2	5.71	126.80	122.80
8	s6	133	LEU	CA-CB-CG	5.71	128.44	115.30
36	5	2897	A	C6-N1-C2	-5.71	115.17	118.60
36	5	3150	A	C2-N3-C4	-5.71	107.74	110.60
36	1	974	G	N3-C4-N9	5.71	129.43	126.00
36	1	2924	U	O5'-P-OP1	-5.71	100.56	105.70
36	1	2237	C	N1-C2-O2	5.71	122.33	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1490	C	C6-N1-C2	-5.71	118.02	120.30
36	5	282	G	N1-C2-N2	-5.71	111.06	116.20
36	5	366	A	C8-N9-C4	5.71	108.08	105.80
38	8	87	G	O4'-C1'-N9	5.71	112.77	108.20
1	2	542	A	O4'-C1'-N9	5.71	112.77	108.20
1	6	67	A	N1-C6-N6	5.71	122.03	118.60
1	6	338	C	C5-C6-N1	5.71	123.86	121.00
1	2	1622	G	N3-C4-C5	5.71	131.45	128.60
36	1	1316	C	N3-C4-N4	5.71	122.00	118.00
36	1	1445	U	N1-C2-O2	-5.71	118.80	122.80
36	1	1952	G	N3-C4-C5	-5.71	125.75	128.60
36	1	2525	G	N3-C4-N9	5.71	129.43	126.00
36	5	934	G	C5-C6-O6	-5.71	125.17	128.60
36	5	1913	A	C4-C5-C6	5.71	119.85	117.00
36	5	2400	G	C5-C6-O6	-5.71	125.17	128.60
36	5	3029	A	C5-C6-N6	5.71	128.27	123.70
36	1	760	G	O4'-C1'-N9	5.71	112.77	108.20
36	1	918	C	C2-N1-C1'	-5.71	112.52	118.80
36	1	2827	U	C6-N1-C1'	5.71	129.19	121.20
1	6	65	A	N3-C4-C5	5.71	130.79	126.80
1	6	938	G	N3-C4-N9	5.71	129.42	126.00
36	5	2729	U	O5'-P-OP2	5.71	117.55	110.70
37	7	103	A	OP2-P-O3'	5.71	117.75	105.20
36	1	1010	G	C5-C6-O6	-5.71	125.18	128.60
36	1	1308	A	O5'-P-OP1	-5.70	100.57	105.70
36	5	1604	G	C4-C5-C6	5.70	122.22	118.80
36	1	2366	C	O5'-P-OP2	-5.70	100.57	105.70
36	1	2916	U	C5-C6-N1	5.70	125.55	122.70
36	1	3057	U	N1-C2-N3	5.70	118.32	114.90
36	5	1198	C	N3-C4-N4	-5.70	114.01	118.00
1	2	1455	G	C5-C6-N1	-5.70	108.65	111.50
36	1	773	G	N9-C4-C5	5.70	107.68	105.40
36	5	2419	A	N7-C8-N9	5.70	116.65	113.80
1	2	511	A	C8-N9-C4	-5.70	103.52	105.80
1	6	1637	C	C2-N1-C1'	5.70	125.07	118.80
36	5	808	A	N9-C4-C5	5.70	108.08	105.80
36	5	1332	A	C8-N9-C1'	-5.70	117.44	127.70
36	5	1404	G	C5-C6-N1	-5.70	108.65	111.50
1	6	1117	U	O5'-P-OP2	-5.70	100.57	105.70
36	1	924	G	C4-C5-N7	5.70	113.08	110.80
36	1	2329	C	N1-C2-O2	-5.70	115.48	118.90
36	5	2130	G	N9-C1'-C2'	-5.70	105.73	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	80	A	C8-N9-C4	-5.70	103.52	105.80
36	1	2632	G	C2-N3-C4	-5.69	109.05	111.90
36	1	3180	A	C8-N9-C4	5.69	108.08	105.80
73	O7	65	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	6	1133	A	N1-C6-N6	5.69	122.02	118.60
36	5	2849	C	N1-C2-O2	-5.69	115.48	118.90
36	5	3179	U	N3-C2-O2	-5.69	118.21	122.20
52	m6	78	ARG	NE-CZ-NH1	5.69	123.15	120.30
36	1	2869	U	O5'-P-OP2	5.69	117.53	110.70
36	5	694	C	N3-C2-O2	-5.69	117.92	121.90
36	1	2620	G	C2-N3-C4	5.69	114.75	111.90
36	1	3093	C	C6-N1-C2	5.69	122.58	120.30
1	6	1000	C	C2-N1-C1'	5.69	125.06	118.80
36	5	1417	G	OP1-P-OP2	-5.69	111.07	119.60
36	5	1744	G	C8-N9-C1'	-5.69	119.60	127.00
36	5	1868	G	N1-C6-O6	5.69	123.31	119.90
36	5	3028	G	N1-C2-N2	-5.69	111.08	116.20
38	4	9	A	O5'-P-OP2	-5.69	100.58	105.70
1	2	1749	A	N1-C2-N3	5.69	132.14	129.30
36	1	967	A	O5'-P-OP1	-5.69	100.58	105.70
36	1	1187	C	C4-C5-C6	-5.69	114.56	117.40
36	1	2554	A	P-O3'-C3'	5.69	126.52	119.70
1	6	517	U	C5-C4-O4	5.69	129.31	125.90
36	5	1319	G	C5-N7-C8	5.69	107.14	104.30
36	5	1556	C	C6-N1-C2	-5.69	118.03	120.30
36	5	2129	U	C6-N1-C2	-5.69	117.59	121.00
36	5	2687	G	N3-C4-N9	5.69	129.41	126.00
36	5	2923	U	C6-N1-C2	-5.69	117.59	121.00
36	5	3195	U	P-O3'-C3'	5.69	126.53	119.70
1	2	1241	G	O4'-C1'-N9	5.69	112.75	108.20
1	2	1145	U	N1-C2-O2	-5.68	118.82	122.80
36	1	780	A	N1-C2-N3	5.68	132.14	129.30
36	1	1294	A	O4'-C1'-N9	5.68	112.75	108.20
36	1	2403	G	N3-C4-N9	5.68	129.41	126.00
36	1	2403	G	C8-N9-C1'	-5.68	119.61	127.00
36	1	3015	G	C5-C6-O6	-5.68	125.19	128.60
36	5	883	A	N1-C6-N6	-5.68	115.19	118.60
36	5	1927	G	C8-N9-C1'	-5.68	119.61	127.00
36	5	2376	G	N7-C8-N9	5.68	115.94	113.10
36	5	3144	G	N1-C2-N2	-5.68	111.08	116.20
36	1	637	C	C6-N1-C1'	-5.68	113.98	120.80
36	5	1879	A	C6-C5-N7	-5.68	128.32	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	163	G	C4-N9-C1'	5.68	133.88	126.50
1	2	1773	C	C5-C6-N1	5.68	123.84	121.00
36	1	591	G	O5'-P-OP2	-5.68	100.59	105.70
36	1	776	U	N3-C2-O2	-5.68	118.22	122.20
36	1	953	G	C6-C5-N7	-5.68	126.99	130.40
36	1	2877	G	C4-C5-N7	-5.68	108.53	110.80
36	1	3269	U	N3-C2-O2	-5.68	118.22	122.20
1	6	1653	C	N3-C4-C5	-5.68	119.63	121.90
36	5	2875	U	C5-C6-N1	5.68	125.54	122.70
36	1	2976	A	N9-C4-C5	5.68	108.07	105.80
37	3	82	G	N3-C4-N9	5.68	129.41	126.00
36	5	1450	G	N3-C2-N2	-5.68	115.92	119.90
1	2	1747	G	C5-C6-N1	-5.68	108.66	111.50
36	1	54	C	O5'-P-OP2	5.68	117.51	110.70
36	5	888	A	C4-C5-N7	5.68	113.54	110.70
36	5	2113	A	N7-C8-N9	-5.68	110.96	113.80
36	1	1863	G	C6-C5-N7	-5.67	127.00	130.40
36	5	938	C	N3-C4-C5	5.67	124.17	121.90
1	6	997	G	C8-N9-C4	5.67	108.67	106.40
36	5	1205	A	C8-N9-C4	-5.67	103.53	105.80
36	5	2717	U	C2-N1-C1'	-5.67	110.89	117.70
36	1	948	C	C2-N1-C1'	-5.67	112.56	118.80
36	1	979	U	N1-C2-N3	5.67	118.30	114.90
36	1	3182	G	N1-C2-N2	-5.67	111.10	116.20
37	7	82	G	N9-C4-C5	-5.67	103.13	105.40
36	1	3022	G	C6-C5-N7	-5.67	127.00	130.40
36	5	116	A	O4'-C1'-N9	5.67	112.73	108.20
36	5	1184	A	N7-C8-N9	-5.67	110.97	113.80
36	5	2754	G	N3-C2-N2	5.67	123.87	119.90
36	1	1544	G	N3-C4-N9	5.67	129.40	126.00
36	1	358	G	N9-C4-C5	-5.66	103.14	105.40
36	1	2124	G	C5-C6-O6	-5.66	125.20	128.60
36	1	2905	U	N1-C2-O2	-5.66	118.84	122.80
36	1	3172	A	N1-C6-N6	-5.66	115.20	118.60
36	5	882	A	C6-N1-C2	-5.66	115.20	118.60
36	5	1927	G	C4-N9-C1'	5.66	133.86	126.50
36	5	2240	G	C8-N9-C4	-5.66	104.14	106.40
1	2	539	G	N7-C8-N9	5.66	115.93	113.10
36	1	997	A	O5'-P-OP2	-5.66	100.61	105.70
36	1	1604	G	N3-C4-C5	-5.66	125.77	128.60
36	1	2727	A	N1-C6-N6	-5.66	115.20	118.60
36	1	2728	G	N9-C4-C5	-5.66	103.14	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	L7	202	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	6	1115	U	C6-N1-C2	5.66	124.40	121.00
36	5	91	G	C8-N9-C4	5.66	108.66	106.40
36	5	400	G	N1-C6-O6	-5.66	116.50	119.90
36	5	914	A	C4-C5-C6	5.66	119.83	117.00
36	1	3139	A	C8-N9-C4	-5.66	103.54	105.80
1	6	530	C	C6-N1-C2	5.66	122.56	120.30
36	5	304	G	C4-C5-N7	-5.66	108.54	110.80
36	1	362	U	C5-C6-N1	-5.66	119.87	122.70
36	1	1124	U	N1-C2-O2	5.66	126.76	122.80
36	1	1796	G	N3-C4-C5	-5.66	125.77	128.60
36	1	1415	U	C5-C6-N1	-5.65	119.87	122.70
36	5	2806	U	O5'-P-OP2	-5.65	100.61	105.70
36	1	416	A	N1-C6-N6	5.65	121.99	118.60
36	1	769	G	N9-C4-C5	-5.65	103.14	105.40
36	1	1683	A	N1-C6-N6	5.65	121.99	118.60
36	1	2279	A	C5-N7-C8	-5.65	101.07	103.90
36	1	2342	U	N1-C2-O2	-5.65	118.84	122.80
36	1	2369	G	O5'-P-OP1	-5.65	100.61	105.70
36	5	397	A	N9-C4-C5	5.65	108.06	105.80
36	5	1212	A	N3-C4-N9	5.65	131.92	127.40
1	2	1241	G	C5-N7-C8	-5.65	101.47	104.30
36	1	328	U	N3-C2-O2	-5.65	118.24	122.20
36	1	684	G	C5-C6-O6	-5.65	125.21	128.60
36	1	1412	G	N1-C6-O6	5.65	123.29	119.90
56	N0	115	ARG	NE-CZ-NH2	-5.65	117.47	120.30
36	5	1592	G	C5-C6-O6	5.65	131.99	128.60
36	5	2380	U	O5'-P-OP2	-5.65	100.61	105.70
36	1	424	G	N1-C6-O6	5.65	123.29	119.90
36	1	691	A	C6-C5-N7	-5.65	128.35	132.30
36	5	423	A	N7-C8-N9	-5.65	110.97	113.80
36	1	1041	U	O5'-P-OP2	-5.65	100.62	105.70
1	6	543	C	N3-C4-N4	-5.65	114.05	118.00
1	6	575	C	N3-C4-C5	5.65	124.16	121.90
36	5	1147	G	N3-C4-C5	-5.65	125.78	128.60
36	5	2663	G	C5-C6-O6	-5.65	125.21	128.60
36	5	2690	G	C8-N9-C1'	-5.65	119.66	127.00
1	6	42	G	O4'-C1'-N9	5.65	112.72	108.20
36	5	644	G	C4-N9-C1'	5.64	133.84	126.50
36	5	971	G	OP2-P-O3'	5.64	117.62	105.20
36	1	320	G	O5'-P-OP2	-5.64	100.62	105.70
36	1	785	G	C8-N9-C4	-5.64	104.14	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1391	C	C5-C4-N4	-5.64	116.25	120.20
36	1	3382	U	N1-C2-O2	5.64	126.75	122.80
36	5	947	G	C5-C6-N1	-5.64	108.68	111.50
1	2	507	U	C2-N1-C1'	5.64	124.47	117.70
36	1	933	A	N7-C8-N9	5.64	116.62	113.80
36	1	953	G	C5-C6-O6	-5.64	125.22	128.60
36	5	794	U	O5'-P-OP2	-5.64	100.62	105.70
36	5	2662	G	N3-C4-C5	-5.64	125.78	128.60
36	5	3020	U	N3-C4-O4	5.64	123.35	119.40
46	19	166	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	2	407	A	N9-C4-C5	5.64	108.06	105.80
36	5	1496	C	C5-C6-N1	5.64	123.82	121.00
1	2	794	U	N3-C2-O2	-5.64	118.25	122.20
36	1	2395	G	C5-N7-C8	-5.64	101.48	104.30
36	1	2639	G	C4-N9-C1'	5.64	133.83	126.50
36	1	2899	C	O4'-C1'-N1	5.64	112.71	108.20
36	1	3150	A	N1-C6-N6	5.64	121.98	118.60
1	6	261	U	N1-C2-O2	5.64	126.75	122.80
36	5	2892	A	C4-C5-C6	5.64	119.82	117.00
36	5	3090	U	N3-C2-O2	-5.64	118.25	122.20
36	5	3218	A	C4-C5-N7	5.64	113.52	110.70
1	2	145	A	C8-N9-C4	-5.63	103.55	105.80
36	1	1883	A	C6-N1-C2	-5.63	115.22	118.60
36	5	1438	U	C2-N1-C1'	5.63	124.46	117.70
36	5	2231	C	C6-N1-C2	-5.63	118.05	120.30
36	5	2664	C	OP2-P-O3'	5.63	117.59	105.20
36	5	27	C	C6-N1-C2	-5.63	118.05	120.30
36	1	1445	U	C5-C6-N1	-5.63	119.88	122.70
36	1	3243	A	C4-C5-N7	5.63	113.52	110.70
36	5	660	A	C5-C6-N6	5.63	128.21	123.70
38	8	4	C	N1-C2-O2	5.63	122.28	118.90
36	1	102	C	OP2-P-O3'	5.63	117.59	105.20
38	4	103	G	N3-C4-C5	-5.63	125.78	128.60
1	6	1614	A	C4-C5-N7	5.63	113.51	110.70
36	5	1449	A	C5-C6-N6	-5.63	119.20	123.70
36	5	2304	C	N1-C2-O2	-5.63	115.52	118.90
36	1	666	A	C8-N9-C4	5.63	108.05	105.80
36	1	1845	G	OP2-P-O3'	5.63	117.58	105.20
1	6	606	A	N1-C6-N6	5.63	121.98	118.60
36	5	1117	G	C4-C5-N7	5.63	113.05	110.80
36	5	1312	C	N3-C4-C5	-5.63	119.65	121.90
36	5	1315	U	C6-N1-C2	5.63	124.38	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1369	A	N1-C2-N3	5.62	132.11	129.30
36	1	3243	A	C5-C6-N6	-5.62	119.20	123.70
36	5	1509	A	N1-C6-N6	5.62	121.97	118.60
36	5	2197	C	N3-C2-O2	5.62	125.84	121.90
36	1	558	U	C6-N1-C1'	-5.62	113.33	121.20
36	5	98	G	N3-C4-C5	-5.62	125.79	128.60
36	5	2385	G	N3-C2-N2	-5.62	115.96	119.90
36	5	2531	C	C6-N1-C2	-5.62	118.05	120.30
71	o5	69	LEU	CA-CB-CG	5.62	128.23	115.30
36	1	506	U	N1-C2-O2	-5.62	118.86	122.80
36	1	2658	G	O5'-P-OP2	-5.62	100.64	105.70
36	5	501	A	N1-C6-N6	-5.62	115.23	118.60
36	5	2320	A	C2-N3-C4	-5.62	107.79	110.60
36	5	2410	U	C2-N3-C4	-5.62	123.63	127.00
36	1	979	U	N1-C2-O2	5.62	126.73	122.80
36	5	2873	U	N3-C2-O2	-5.62	118.27	122.20
71	o5	89	ARG	NE-CZ-NH1	5.62	123.11	120.30
36	1	3375	A	C5-C6-N6	5.62	128.19	123.70
1	6	176	C	C2-N1-C1'	5.62	124.98	118.80
36	5	1296	C	C5-C4-N4	-5.62	116.27	120.20
36	5	1599	G	N1-C6-O6	5.62	123.27	119.90
36	1	262	U	N3-C2-O2	5.62	126.13	122.20
36	1	425	G	N1-C2-N2	-5.62	111.14	116.20
36	1	614	C	N3-C4-C5	5.62	124.15	121.90
36	5	2271	A	C6-C5-N7	5.62	136.23	132.30
36	5	2707	C	C5-C6-N1	-5.62	118.19	121.00
36	5	3088	G	N1-C6-O6	5.62	123.27	119.90
36	5	3374	U	C5-C6-N1	-5.62	119.89	122.70
36	1	212	G	N3-C4-N9	5.62	129.37	126.00
1	6	306	U	C5-C6-N1	-5.62	119.89	122.70
36	5	1475	A	O5'-P-OP2	-5.62	100.65	105.70
36	1	25	U	N3-C4-O4	5.61	123.33	119.40
36	1	285	A	N9-C4-C5	-5.61	103.56	105.80
36	1	1020	G	N9-C4-C5	-5.61	103.15	105.40
36	1	2899	C	C6-N1-C1'	-5.61	114.06	120.80
36	5	1421	G	O5'-P-OP1	-5.61	100.65	105.70
36	1	2247	G	C8-N9-C1'	-5.61	119.70	127.00
36	5	137	G	C6-C5-N7	-5.61	127.03	130.40
36	5	790	U	N1-C2-N3	5.61	118.27	114.90
1	6	273	G	O5'-P-OP1	-5.61	100.65	105.70
36	5	360	G	N3-C4-C5	-5.61	125.80	128.60
36	5	1046	A	N1-C2-N3	5.61	132.11	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1379	G	C8-N9-C1'	-5.61	119.71	127.00
36	5	2585	G	C2-N3-C4	5.61	114.70	111.90
36	5	2727	A	N9-C4-C5	5.61	108.04	105.80
36	5	2813	A	C4-C5-C6	5.61	119.81	117.00
36	1	2341	A	C8-N9-C4	5.61	108.04	105.80
36	1	2899	C	C4-C5-C6	5.61	120.20	117.40
38	4	22	U	N1-C2-N3	5.61	118.26	114.90
36	1	1890	U	C6-N1-C2	5.60	124.36	121.00
1	6	1789	G	C5-C6-O6	-5.60	125.24	128.60
36	1	1373	A	C8-N9-C4	-5.60	103.56	105.80
36	1	2730	G	C8-N9-C1'	5.60	134.28	127.00
1	6	390	G	O5'-P-OP1	-5.60	100.66	105.70
12	c0	88	PRO	N-CA-CB	5.60	110.02	103.30
36	5	1513	G	C8-N9-C4	-5.60	104.16	106.40
37	7	7	G	N1-C6-O6	-5.60	116.54	119.90
64	n8	73	LEU	CA-CB-CG	5.60	128.19	115.30
1	2	1733	C	C5-C4-N4	-5.60	116.28	120.20
36	1	1045	C	OP2-P-O3'	5.60	117.52	105.20
1	2	1456	C	O4'-C1'-N1	5.60	112.68	108.20
36	1	3269	U	C5-C4-O4	5.60	129.26	125.90
36	5	1178	G	C4-C5-C6	5.60	122.16	118.80
67	o1	20	LEU	CA-CB-CG	-5.60	102.42	115.30
36	1	1100	U	C2-N3-C4	-5.60	123.64	127.00
36	1	1139	G	C5-C6-O6	5.60	131.96	128.60
36	1	2130	G	C8-N9-C4	-5.60	104.16	106.40
36	1	3204	C	C2-N1-C1'	5.60	124.96	118.80
36	5	750	G	OP2-P-O3'	5.60	117.51	105.20
1	2	80	A	O5'-P-OP1	-5.60	100.66	105.70
1	6	160	C	N1-C2-O2	5.60	122.26	118.90
36	1	304	G	C4-C5-N7	-5.59	108.56	110.80
38	4	40	A	C5-C6-N6	-5.59	119.22	123.70
1	6	30	G	N3-C4-N9	-5.59	122.64	126.00
1	6	1280	C	C6-N1-C2	-5.59	118.06	120.30
36	5	644	G	C5-C6-O6	5.59	131.96	128.60
36	5	919	U	O5'-P-OP2	-5.59	100.67	105.70
36	5	2732	G	N1-C6-O6	5.59	123.26	119.90
38	8	84	C	O4'-C1'-N1	5.59	112.67	108.20
36	1	2747	A	C8-N9-C4	-5.59	103.56	105.80
36	5	633	C	C4-C5-C6	5.59	120.20	117.40
1	2	1180	C	N3-C2-O2	-5.59	117.99	121.90
36	1	648	C	C6-N1-C1'	-5.59	114.09	120.80
36	1	1807	G	C6-C5-N7	-5.59	127.05	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2935	U	N3-C4-C5	-5.59	111.25	114.60
1	6	144	U	C6-N1-C2	-5.59	117.65	121.00
1	6	453	U	N1-C2-O2	5.59	126.71	122.80
36	5	406	G	N1-C6-O6	-5.59	116.55	119.90
36	5	2818	U	C5-C6-N1	5.59	125.50	122.70
40	l3	178	LEU	CA-CB-CG	5.59	128.16	115.30
18	C6	40	GLU	C-N-CA	5.59	145.48	122.00
36	1	884	A	OP1-P-O3'	5.59	117.50	105.20
36	1	1122	U	N1-C2-N3	5.59	118.25	114.90
36	1	2606	G	N1-C2-N2	-5.59	111.17	116.20
36	1	2727	A	C4-C5-N7	-5.59	107.91	110.70
36	1	2948	C	N3-C4-C5	5.59	124.14	121.90
36	5	596	C	C6-N1-C2	-5.59	118.06	120.30
36	1	51	A	N7-C8-N9	5.59	116.59	113.80
36	1	880	G	N7-C8-N9	-5.59	110.31	113.10
36	5	780	A	O5'-P-OP1	-5.59	100.67	105.70
36	5	887	G	C6-C5-N7	-5.59	127.05	130.40
36	5	2946	A	OP2-P-O3'	5.59	117.49	105.20
36	1	1838	G	N9-C4-C5	-5.58	103.17	105.40
36	1	2276	G	C5-C6-O6	-5.58	125.25	128.60
1	6	1644	C	N3-C2-O2	-5.58	117.99	121.90
36	5	1468	A	N9-C4-C5	-5.58	103.57	105.80
1	2	275	C	C6-N1-C2	-5.58	118.07	120.30
1	2	1735	U	C5-C4-O4	5.58	129.25	125.90
36	1	3112	G	N3-C4-C5	-5.58	125.81	128.60
36	1	885	U	C6-N1-C2	5.58	124.35	121.00
36	1	1307	G	C6-C5-N7	5.58	133.75	130.40
36	1	3015	G	N1-C6-O6	5.58	123.25	119.90
1	6	163	G	C5-N7-C8	-5.58	101.51	104.30
1	2	1146	G	C8-N9-C4	-5.58	104.17	106.40
36	1	1709	C	N3-C4-C5	-5.58	119.67	121.90
1	6	1537	C	O4'-C1'-N1	5.58	112.66	108.20
36	5	2820	A	N7-C8-N9	5.58	116.59	113.80
36	5	3119	U	N3-C4-O4	5.58	123.31	119.40
1	2	389	G	C8-N9-C4	-5.58	104.17	106.40
36	1	857	G	C6-C5-N7	-5.58	127.05	130.40
36	5	1628	C	C6-N1-C2	-5.58	118.07	120.30
36	5	3013	U	N1-C2-O2	5.58	126.70	122.80
36	1	632	G	C4-C5-N7	5.58	113.03	110.80
36	5	1480	G	N1-C6-O6	5.58	123.25	119.90
36	5	2362	C	O5'-P-OP2	-5.58	100.68	105.70
36	5	2718	U	N1-C2-N3	5.58	118.25	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	704	C	C2-N1-C1'	5.57	124.93	118.80
36	1	86	G	O5'-P-OP1	5.57	117.39	110.70
36	1	1517	G	O5'-P-OP2	-5.57	100.68	105.70
36	1	1831	U	C5-C6-N1	5.57	125.49	122.70
1	6	91	G	N3-C4-C5	5.57	131.39	128.60
36	5	873	C	P-O3'-C3'	5.57	126.39	119.70
36	5	2993	G	N1-C6-O6	5.57	123.25	119.90
36	5	2891	U	N3-C2-O2	-5.57	118.30	122.20
36	1	22	G	C8-N9-C4	-5.57	104.17	106.40
1	6	1614	A	C5-N7-C8	-5.57	101.11	103.90
36	5	822	G	N3-C4-C5	5.57	131.38	128.60
36	5	841	A	C8-N9-C4	5.57	108.03	105.80
36	5	2199	G	C4-C5-N7	5.57	113.03	110.80
36	1	3140	G	N1-C6-O6	5.57	123.24	119.90
1	6	1560	U	N1-C2-O2	5.57	126.70	122.80
1	2	985	G	N3-C4-C5	-5.57	125.82	128.60
36	1	884	A	C6-C5-N7	-5.57	128.40	132.30
36	1	913	A	N7-C8-N9	5.57	116.58	113.80
36	5	574	U	C6-N1-C2	5.57	124.34	121.00
36	5	970	A	C8-N9-C4	5.57	108.03	105.80
36	5	1181	U	C4-C5-C6	5.57	123.04	119.70
36	5	2940	A	N9-C4-C5	5.57	108.03	105.80
36	1	123	A	C5-N7-C8	-5.57	101.12	103.90
36	1	2643	A	N9-C4-C5	-5.57	103.57	105.80
20	c8	18	LEU	CA-CB-CG	5.57	128.10	115.30
36	5	1331	U	N3-C2-O2	-5.57	118.30	122.20
36	5	2858	U	N3-C4-C5	-5.57	111.26	114.60
36	1	942	U	OP1-P-OP2	-5.56	111.25	119.60
36	1	655	C	N3-C4-C5	-5.56	119.67	121.90
36	1	1495	U	C2-N3-C4	-5.56	123.66	127.00
36	5	567	G	C4-N9-C1'	5.56	133.73	126.50
36	5	907	G	C8-N9-C4	5.56	108.62	106.40
36	5	1205	A	C4-C5-C6	5.56	119.78	117.00
36	5	1556	C	C2-N1-C1'	5.56	124.92	118.80
37	7	30	G	C4-N9-C1'	5.56	133.73	126.50
1	2	720	G	P-O3'-C3'	5.56	126.37	119.70
1	2	1240	U	O5'-P-OP2	-5.56	100.70	105.70
1	2	1541	G	C8-N9-C4	-5.56	104.18	106.40
36	1	898	U	N1-C2-N3	-5.56	111.56	114.90
1	6	1645	G	C6-C5-N7	5.56	133.74	130.40
1	6	1744	A	C5-N7-C8	-5.56	101.12	103.90
36	5	137	G	N1-C6-O6	5.56	123.24	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2274	U	C2-N1-C1'	5.56	124.37	117.70
36	5	2928	C	C5-C4-N4	-5.56	116.31	120.20
36	1	1851	G	C6-C5-N7	-5.56	127.07	130.40
36	5	3130	A	O5'-P-OP1	-5.56	100.70	105.70
19	C7	73	LEU	CA-CB-CG	5.55	128.07	115.30
1	6	1672	G	N3-C2-N2	5.55	123.79	119.90
1	6	1781	A	C8-N9-C4	-5.55	103.58	105.80
36	5	141	C	N1-C2-O2	-5.55	115.57	118.90
36	5	562	C	C6-N1-C2	-5.55	118.08	120.30
36	5	630	A	C8-N9-C4	5.55	108.02	105.80
36	5	1450	G	N3-C4-C5	5.55	131.38	128.60
36	1	27	C	C6-N1-C2	-5.55	118.08	120.30
36	1	612	U	C5-C6-N1	-5.55	119.92	122.70
36	1	1126	G	C6-C5-N7	-5.55	127.07	130.40
36	5	3215	A	N1-C6-N6	5.55	121.93	118.60
36	1	2192	C	O5'-P-OP2	-5.55	100.71	105.70
36	5	947	G	O5'-P-OP2	-5.55	100.70	105.70
36	5	1002	A	C2-N3-C4	-5.55	107.83	110.60
36	5	1911	A	C5-C6-N1	-5.55	114.92	117.70
36	5	2607	G	P-O3'-C3'	5.55	126.36	119.70
36	1	198	A	N1-C6-N6	5.55	121.93	118.60
36	5	1178	G	N7-C8-N9	5.55	115.87	113.10
36	1	345	G	C8-N9-C1'	-5.55	119.79	127.00
36	1	2288	G	C4-N9-C1'	5.55	133.71	126.50
37	3	91	G	N3-C2-N2	-5.55	116.02	119.90
36	5	1151	U	N3-C4-C5	-5.55	111.27	114.60
36	1	776	U	C4-C5-C6	5.54	123.03	119.70
36	1	2395	G	C6-C5-N7	-5.54	127.07	130.40
1	6	1653	C	N3-C4-N4	5.54	121.88	118.00
36	1	1366	A	OP2-P-O3'	5.54	117.39	105.20
36	1	2820	A	OP1-P-OP2	-5.54	111.29	119.60
38	4	85	G	C8-N9-C4	-5.54	104.18	106.40
36	5	2818	U	P-O3'-C3'	5.54	126.35	119.70
1	2	1611	A	C2-N3-C4	-5.54	107.83	110.60
36	1	1903	U	N3-C4-C5	-5.54	111.28	114.60
45	L8	158	ASP	C-N-CD	5.54	140.04	128.40
36	5	1310	G	N3-C4-N9	5.54	129.32	126.00
36	1	1049	C	N3-C4-C5	5.54	124.12	121.90
36	1	2134	G	C5-C6-O6	5.54	131.92	128.60
36	1	2276	G	C4-C5-N7	5.54	113.02	110.80
36	5	1485	G	C8-N9-C4	5.54	108.62	106.40
1	2	1059	U	O5'-P-OP1	-5.54	100.72	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	907	G	C5-C6-O6	-5.54	125.28	128.60
36	1	968	G	C8-N9-C1'	-5.54	119.80	127.00
36	5	1367	G	C6-C5-N7	-5.54	127.08	130.40
36	5	2826	U	N3-C2-O2	-5.54	118.32	122.20
36	1	649	A	C2-N3-C4	-5.54	107.83	110.60
36	1	1152	G	O5'-P-OP1	-5.54	100.72	105.70
36	5	1906	G	C6-C5-N7	-5.54	127.08	130.40
36	1	49	A	N9-C4-C5	-5.53	103.59	105.80
36	1	794	U	O5'-P-OP2	-5.53	100.72	105.70
36	1	1518	U	N3-C4-O4	5.53	123.27	119.40
36	1	59	G	C6-C5-N7	-5.53	127.08	130.40
36	1	1514	G	C4-N9-C1'	5.53	133.69	126.50
36	1	2699	G	C5-C6-O6	-5.53	125.28	128.60
36	5	412	G	N7-C8-N9	5.53	115.87	113.10
36	5	567	G	N9-C4-C5	-5.53	103.19	105.40
36	5	1590	G	O5'-P-OP1	-5.53	100.72	105.70
36	5	2904	U	C2-N1-C1'	5.53	124.34	117.70
36	5	3294	A	N1-C6-N6	-5.53	115.28	118.60
1	2	1156	C	C6-N1-C2	5.53	122.51	120.30
36	1	1331	U	C5-C6-N1	-5.53	119.94	122.70
36	1	2190	U	C6-N1-C2	-5.53	117.68	121.00
1	6	576	G	N1-C6-O6	5.53	123.22	119.90
36	5	924	G	C2-N3-C4	-5.53	109.14	111.90
36	5	2190	U	C6-N1-C2	-5.53	117.68	121.00
36	5	3202	G	N1-C6-O6	-5.53	116.58	119.90
36	5	3239	G	O5'-P-OP2	-5.53	100.72	105.70
36	1	716	A	C5-C6-N6	-5.53	119.28	123.70
36	1	773	G	C4-C5-N7	-5.53	108.59	110.80
36	1	1416	C	C2-N3-C4	-5.53	117.14	119.90
1	6	604	A	C8-N9-C4	-5.53	103.59	105.80
36	5	1889	G	N1-C6-O6	5.53	123.22	119.90
15	C3	22	ALA	C-N-CA	5.53	145.21	122.00
36	1	1329	U	N3-C4-O4	5.53	123.27	119.40
36	1	2174	G	N7-C8-N9	5.53	115.86	113.10
36	5	658	G	C8-N9-C4	-5.53	104.19	106.40
36	5	2816	G	O4'-C1'-N9	5.53	112.62	108.20
36	1	421	G	N3-C4-N9	5.52	129.31	126.00
36	1	816	A	C8-N9-C4	-5.52	103.59	105.80
36	1	2386	A	C4-C5-N7	5.52	113.46	110.70
1	6	1031	U	C2-N1-C1'	-5.52	111.07	117.70
36	1	22	G	N3-C4-C5	-5.52	125.84	128.60
36	1	423	A	OP2-P-O3'	5.52	117.35	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	682	U	C2-N1-C1'	-5.52	111.07	117.70
36	1	2277	C	C4-C5-C6	5.52	120.16	117.40
36	5	835	G	N1-C6-O6	-5.52	116.59	119.90
36	5	2912	G	OP1-P-OP2	5.52	127.89	119.60
36	1	3106	A	N1-C6-N6	5.52	121.91	118.60
36	1	229	G	C5-C6-O6	-5.52	125.29	128.60
36	1	1379	G	N1-C2-N3	5.52	127.21	123.90
36	1	1394	A	C4-C5-C6	-5.52	114.24	117.00
36	1	3046	A	C2-N3-C4	-5.52	107.84	110.60
1	6	1074	G	C5-C6-N1	-5.52	108.74	111.50
36	5	754	G	N1-C6-O6	-5.52	116.59	119.90
36	5	1405	U	C5-C4-O4	5.52	129.21	125.90
36	5	1444	G	OP2-P-O3'	5.52	117.34	105.20
36	5	2359	C	N3-C4-N4	5.52	121.86	118.00
36	5	2409	G	C5-C6-O6	-5.52	125.29	128.60
36	5	2552	C	C6-N1-C1'	-5.52	114.18	120.80
36	1	1057	A	C4-C5-C6	-5.52	114.24	117.00
36	1	1484	U	OP1-P-O3'	5.52	117.34	105.20
1	6	467	G	C8-N9-C1'	-5.52	119.83	127.00
36	5	607	A	N9-C4-C5	5.52	108.01	105.80
36	5	2123	G	N3-C4-C5	-5.52	125.84	128.60
36	5	3396	U	O4'-C1'-N1	5.52	112.61	108.20
37	7	28	C	O5'-P-OP1	-5.52	100.73	105.70
36	1	2408	U	N3-C2-O2	-5.52	118.34	122.20
36	5	1332	A	C4-N9-C1'	5.52	136.23	126.30
40	13	4	ARG	NE-CZ-NH1	5.52	123.06	120.30
36	1	866	A	N1-C6-N6	5.51	121.91	118.60
36	1	2837	A	N1-C6-N6	5.51	121.91	118.60
1	6	168	A	C8-N9-C4	-5.51	103.59	105.80
36	1	1352	A	OP1-P-O3'	5.51	117.33	105.20
36	1	1429	G	C6-N1-C2	-5.51	121.79	125.10
36	1	2680	A	N1-C6-N6	5.51	121.91	118.60
36	5	2947	G	N1-C6-O6	5.51	123.21	119.90
36	1	187	A	C8-N9-C4	-5.51	103.59	105.80
1	6	338	C	N3-C4-C5	-5.51	119.70	121.90
36	5	668	G	N1-C6-O6	-5.51	116.59	119.90
1	2	822	U	C6-N1-C2	-5.51	117.69	121.00
38	4	94	C	N3-C4-C5	5.51	124.10	121.90
36	5	3109	G	C4-C5-N7	5.51	113.00	110.80
36	1	345	G	C4-C5-C6	5.51	122.10	118.80
36	5	964	G	C5-C6-O6	-5.51	125.30	128.60
36	5	2629	U	N3-C4-O4	5.51	123.25	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2777	G	C6-C5-N7	5.51	133.70	130.40
1	2	1176	G	C6-C5-N7	-5.50	127.10	130.40
36	1	883	A	C6-N1-C2	-5.50	115.30	118.60
36	1	1441	G	N3-C4-N9	-5.50	122.70	126.00
36	1	1791	C	N3-C4-C5	-5.50	119.70	121.90
38	4	25	G	C4-C5-N7	-5.50	108.60	110.80
36	5	936	A	C4-C5-C6	5.50	119.75	117.00
36	1	53	G	N3-C4-C5	-5.50	125.85	128.60
1	6	1314	U	N1-C2-O2	5.50	126.65	122.80
36	5	1899	G	N9-C4-C5	5.50	107.60	105.40
36	5	2169	G	C2-N3-C4	5.50	114.65	111.90
36	1	1139	G	C4-C5-N7	-5.50	108.60	110.80
36	1	1148	G	C4-C5-C6	5.50	122.10	118.80
36	1	1307	G	C5-C6-O6	5.50	131.90	128.60
36	1	1417	G	N3-C4-N9	-5.50	122.70	126.00
36	1	2856	G	C5-C6-N1	-5.50	108.75	111.50
36	1	3201	C	N3-C4-C5	-5.50	119.70	121.90
36	5	658	G	C4-C5-N7	5.50	113.00	110.80
36	5	1367	G	C4-N9-C1'	5.50	133.65	126.50
36	5	1845	G	N3-C4-C5	-5.50	125.85	128.60
36	1	2412	G	C5-C6-N1	5.50	114.25	111.50
36	5	1331	U	N1-C2-N3	5.50	118.20	114.90
36	1	3390	G	N1-C6-O6	5.50	123.20	119.90
36	1	1868	G	N3-C4-N9	5.50	129.30	126.00
36	1	1940	G	N1-C2-N2	-5.50	111.25	116.20
1	6	1117	U	N3-C4-C5	-5.50	111.30	114.60
1	6	1648	A	C8-N9-C4	5.50	108.00	105.80
36	5	1409	G	N3-C4-C5	-5.50	125.85	128.60
1	6	1463	C	C6-N1-C2	5.50	122.50	120.30
36	5	2860	U	N1-C2-O2	5.50	126.65	122.80
37	7	32	U	C6-N1-C2	5.50	124.30	121.00
1	2	1645	G	N3-C4-N9	5.49	129.30	126.00
36	1	519	A	C6-C5-N7	-5.49	128.46	132.30
36	1	883	A	N1-C2-N3	5.49	132.05	129.30
38	4	52	A	N9-C4-C5	5.49	108.00	105.80
54	M8	49	LEU	CA-CB-CG	5.49	127.94	115.30
36	5	931	C	N3-C2-O2	-5.49	118.06	121.90
36	5	1384	U	C2-N1-C1'	5.49	124.29	117.70
36	5	1587	A	N9-C4-C5	-5.49	103.60	105.80
36	5	3181	C	N3-C2-O2	-5.49	118.06	121.90
36	1	818	C	N3-C4-C5	-5.49	119.70	121.90
36	1	954	U	C6-N1-C2	-5.49	117.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	210	A	N1-C6-N6	5.49	121.89	118.60
1	6	630	A	N7-C8-N9	-5.49	111.06	113.80
36	5	1354	G	C6-C5-N7	-5.49	127.11	130.40
36	5	3208	G	N1-C6-O6	5.49	123.19	119.90
36	1	1733	G	C4-N9-C1'	5.49	133.64	126.50
36	1	2376	G	C8-N9-C4	-5.49	104.20	106.40
36	5	3149	G	N3-C4-N9	-5.49	122.71	126.00
38	8	108	C	C6-N1-C2	-5.49	118.11	120.30
1	2	428	A	C8-N9-C4	-5.49	103.61	105.80
36	1	662	U	N3-C2-O2	-5.49	118.36	122.20
36	1	908	G	O4'-C1'-N9	-5.49	103.81	108.20
36	1	154	U	C2-N1-C1'	-5.49	111.12	117.70
36	1	636	C	C6-N1-C1'	-5.49	114.22	120.80
1	6	637	C	C6-N1-C2	-5.49	118.11	120.30
36	5	610	G	C2-N3-C4	5.49	114.64	111.90
38	8	42	G	C5-C6-O6	-5.49	125.31	128.60
1	2	1418	G	C4-N9-C1'	5.48	133.63	126.50
1	2	1109	G	C5-C6-N1	-5.48	108.76	111.50
36	1	3140	G	C6-C5-N7	-5.48	127.11	130.40
1	6	569	C	N3-C4-C5	-5.48	119.71	121.90
1	6	1742	U	C2-N1-C1'	5.48	124.28	117.70
36	5	942	U	N1-C2-N3	5.48	118.19	114.90
36	5	1900	A	C4-C5-N7	5.48	113.44	110.70
36	5	2624	G	N1-C6-O6	5.48	123.19	119.90
38	8	4	C	C2-N1-C1'	5.48	124.83	118.80
36	1	1375	G	N7-C8-N9	5.48	115.84	113.10
36	1	2624	G	C4-C5-N7	5.48	112.99	110.80
44	17	179	LEU	CA-CB-CG	5.48	127.91	115.30
36	1	787	G	C2-N3-C4	5.48	114.64	111.90
36	5	941	G	OP1-P-O3'	5.48	117.25	105.20
36	1	1844	C	C2-N1-C1'	-5.48	112.78	118.80
36	5	2894	C	N3-C4-C5	5.48	124.09	121.90
36	1	898	U	N1-C2-O2	5.48	126.63	122.80
36	1	1295	G	O5'-P-OP1	-5.48	100.77	105.70
36	1	85	A	C5-C6-N1	-5.47	114.96	117.70
36	1	964	G	N1-C2-N2	5.47	121.13	116.20
36	1	2134	G	N1-C6-O6	-5.47	116.61	119.90
36	1	2358	A	C5-C6-N6	-5.47	119.32	123.70
1	6	384	G	C2-N3-C4	-5.47	109.16	111.90
36	5	1332	A	C4-C5-C6	5.47	119.74	117.00
36	5	1384	U	N3-C2-O2	-5.47	118.37	122.20
36	5	2699	G	C8-N9-C4	5.47	108.59	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	345	G	C4-N9-C1'	5.47	133.61	126.50
36	1	648	C	N3-C4-N4	5.47	121.83	118.00
36	1	1201	C	N1-C2-O2	5.47	122.18	118.90
1	6	7	G	C8-N9-C4	-5.47	104.21	106.40
1	6	1764	C	N3-C4-C5	5.47	124.09	121.90
36	5	907	G	N1-C6-O6	5.47	123.18	119.90
36	5	3245	A	N7-C8-N9	5.47	116.54	113.80
36	5	2160	G	N9-C4-C5	-5.47	103.21	105.40
36	1	1855	U	C5-C6-N1	5.47	125.43	122.70
36	1	2201	G	O5'-P-OP2	-5.47	100.78	105.70
36	1	2643	A	OP2-P-O3'	5.47	117.23	105.20
1	6	272	U	N1-C2-O2	5.47	126.63	122.80
36	5	424	G	N9-C4-C5	-5.47	103.21	105.40
36	5	93	C	C6-N1-C2	5.47	122.49	120.30
36	5	1869	C	C2-N1-C1'	-5.47	112.78	118.80
36	5	2936	A	C5-C6-N1	5.47	120.43	117.70
36	1	938	C	C2-N1-C1'	5.47	124.81	118.80
36	1	3050	U	N3-C2-O2	-5.47	118.37	122.20
44	L7	163	LEU	CA-CB-CG	-5.47	102.73	115.30
36	5	917	A	N7-C8-N9	5.47	116.53	113.80
36	5	2398	A	N9-C4-C5	5.47	107.99	105.80
36	5	2711	C	C6-N1-C2	-5.47	118.11	120.30
36	5	2824	G	C2-N3-C4	-5.47	109.17	111.90
36	1	908	G	C4-N9-C1'	5.46	133.60	126.50
38	4	101	U	C2-N1-C1'	5.46	124.26	117.70
1	6	323	A	N1-C6-N6	-5.46	115.32	118.60
1	6	1340	U	N3-C2-O2	-5.46	118.38	122.20
36	5	1317	A	C5-C6-N6	-5.46	119.33	123.70
36	5	3149	G	C2-N3-C4	-5.46	109.17	111.90
44	17	83	LEU	CA-CB-CG	5.46	127.87	115.30
36	5	197	G	N9-C4-C5	-5.46	103.22	105.40
36	5	358	G	N3-C4-N9	-5.46	122.72	126.00
36	5	2884	C	N3-C4-N4	5.46	121.82	118.00
1	2	6	G	N3-C4-C5	-5.46	125.87	128.60
36	1	75	G	O5'-P-OP2	-5.46	100.78	105.70
36	1	1766	G	C4-N9-C1'	5.46	133.60	126.50
65	N9	20	GLY	N-CA-C	5.46	126.75	113.10
36	5	716	A	C8-N9-C4	5.46	107.98	105.80
1	2	1200	G	C5-C6-O6	-5.46	125.32	128.60
36	1	2380	U	C2-N3-C4	-5.46	123.72	127.00
36	5	2549	G	C6-C5-N7	-5.46	127.12	130.40
37	7	116	C	C6-N1-C2	-5.46	118.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1458	G	C8-N9-C1'	-5.46	119.90	127.00
1	2	1778	G	C5-N7-C8	-5.46	101.57	104.30
36	1	2639	G	C4-C5-N7	5.46	112.98	110.80
38	4	83	C	C2-N1-C1'	5.46	124.81	118.80
1	6	1742	U	C5-C6-N1	5.46	125.43	122.70
1	6	1791	A	C5-C6-N6	-5.46	119.33	123.70
25	d3	33	LEU	CB-CG-CD1	-5.46	101.72	111.00
36	5	3343	G	N3-C4-C5	-5.46	125.87	128.60
37	7	104	A	N1-C6-N6	5.46	121.88	118.60
36	5	208	C	C6-N1-C2	-5.46	118.12	120.30
36	5	3278	C	N3-C4-C5	5.46	124.08	121.90
36	1	96	G	N1-C2-N3	5.45	127.17	123.90
36	1	1162	U	N3-C2-O2	-5.45	118.38	122.20
36	1	1190	A	C4-N9-C1'	5.45	136.12	126.30
36	1	1917	C	C6-N1-C2	5.45	122.48	120.30
36	1	2625	C	O5'-P-OP1	-5.45	100.79	105.70
37	3	83	U	N1-C1'-C2'	-5.45	106.00	112.00
1	6	542	A	C6-C5-N7	-5.45	128.48	132.30
1	6	570	A	O5'-P-OP2	-5.45	100.79	105.70
36	5	776	U	N1-C2-N3	5.45	118.17	114.90
36	5	2360	C	C5-C6-N1	5.45	123.73	121.00
1	2	318	U	C2-N1-C1'	-5.45	111.16	117.70
1	6	1619	C	C5-C6-N1	5.45	123.73	121.00
36	5	1377	G	N3-C4-N9	5.45	129.27	126.00
1	2	554	C	C2-N3-C4	5.45	122.62	119.90
1	2	1194	A	N7-C8-N9	5.45	116.53	113.80
36	1	404	G	O5'-P-OP2	-5.45	100.79	105.70
36	1	512	U	C5-C6-N1	-5.45	119.97	122.70
36	1	2143	A	N1-C6-N6	5.45	121.87	118.60
1	6	403	G	N3-C4-N9	-5.45	122.73	126.00
1	6	1274	C	C2-N1-C1'	5.45	124.80	118.80
36	5	920	A	O5'-P-OP1	5.45	117.24	110.70
36	5	2132	C	C6-N1-C2	-5.45	118.12	120.30
36	5	2751	G	C8-N9-C4	-5.45	104.22	106.40
36	5	3116	G	C5-C6-O6	-5.45	125.33	128.60
36	1	2662	G	C2-N3-C4	-5.45	109.18	111.90
36	1	2687	G	N1-C6-O6	-5.45	116.63	119.90
38	4	40	A	N1-C6-N6	5.45	121.87	118.60
1	6	1560	U	C2-N1-C1'	5.45	124.24	117.70
36	5	816	A	N1-C6-N6	-5.45	115.33	118.60
36	5	2123	G	C2-N3-C4	5.45	114.62	111.90
36	1	580	C	N3-C2-O2	5.45	125.71	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1192	C	C2-N3-C4	5.45	122.62	119.90
36	5	61	A	C5-C6-N6	5.45	128.06	123.70
36	5	210	U	C5-C6-N1	-5.45	119.98	122.70
36	5	1048	A	C5-N7-C8	5.45	106.62	103.90
36	5	2992	U	N1-C2-O2	5.45	126.61	122.80
37	7	32	U	N3-C2-O2	5.45	126.01	122.20
1	6	1600	A	C5-N7-C8	-5.44	101.18	103.90
41	14	179	LEU	CA-CB-CG	5.44	127.82	115.30
1	2	992	A	C4-C5-N7	5.44	113.42	110.70
36	1	1389	G	N3-C2-N2	5.44	123.71	119.90
36	1	2342	U	C2-N1-C1'	-5.44	111.17	117.70
36	1	2976	A	N1-C6-N6	-5.44	115.33	118.60
36	5	698	U	C5-C4-O4	5.44	129.16	125.90
36	5	903	U	C5-C4-O4	5.44	129.17	125.90
36	5	1130	A	C2-N3-C4	5.44	113.32	110.60
37	7	41	G	N1-C6-O6	5.44	123.17	119.90
38	8	40	A	C8-N9-C4	-5.44	103.62	105.80
1	2	1014	G	N1-C6-O6	5.44	123.16	119.90
36	1	380	U	C6-N1-C2	-5.44	117.74	121.00
36	1	876	A	N9-C4-C5	-5.44	103.62	105.80
36	1	1473	G	C8-N9-C4	5.44	108.58	106.40
36	1	2273	G	C8-N9-C4	5.44	108.58	106.40
1	6	68	A	N1-C6-N6	5.44	121.86	118.60
1	6	1648	A	N1-C6-N6	5.44	121.86	118.60
20	c8	15	LEU	CA-CB-CG	5.44	127.81	115.30
36	5	1159	A	N3-C4-C5	5.44	130.61	126.80
36	1	22	G	C6-N1-C2	-5.44	121.84	125.10
36	1	1126	G	C5-C6-O6	-5.44	125.34	128.60
36	1	2808	A	C4-C5-N7	5.44	113.42	110.70
36	1	3364	C	O5'-P-OP1	-5.44	100.81	105.70
36	5	1373	A	OP2-P-O3'	5.44	117.17	105.20
36	1	717	C	C6-N1-C2	-5.44	118.12	120.30
36	1	816	A	C2-N3-C4	5.44	113.32	110.60
36	1	1547	G	N7-C8-N9	-5.44	110.38	113.10
36	1	2730	G	N3-C4-C5	5.44	131.32	128.60
1	6	100	A	N1-C6-N6	5.44	121.86	118.60
36	5	406	G	C5-C6-O6	5.44	131.86	128.60
36	5	3007	U	N3-C4-C5	5.44	117.86	114.60
36	5	3107	U	N1-C2-N3	5.44	118.16	114.90
36	5	3144	G	C4-N9-C1'	5.44	133.57	126.50
37	7	80	G	C4-N9-C1'	5.44	133.57	126.50
1	6	29	U	C4-C5-C6	5.44	122.96	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2878	G	C5-C6-N1	5.44	114.22	111.50
36	5	2918	G	C8-N9-C4	-5.44	104.22	106.40
36	1	1306	G	C5-C6-N1	-5.43	108.78	111.50
36	1	2650	U	N1-C2-O2	-5.43	119.00	122.80
36	5	61	A	C2-N3-C4	-5.43	107.88	110.60
36	5	1211	U	N3-C4-C5	5.43	117.86	114.60
36	5	1476	G	N3-C2-N2	5.43	123.70	119.90
36	5	2748	A	N9-C4-C5	-5.43	103.63	105.80
1	2	577	G	N9-C4-C5	-5.43	103.23	105.40
36	1	1492	G	N3-C2-N2	5.43	123.70	119.90
36	1	2606	G	N3-C2-N2	5.43	123.70	119.90
1	6	2	A	C8-N9-C4	5.43	107.97	105.80
1	6	103	A	P-O3'-C3'	5.43	126.22	119.70
1	6	1297	G	C5-C6-O6	5.43	131.86	128.60
36	5	1305	U	N3-C4-C5	-5.43	111.34	114.60
36	5	2346	C	C5-C4-N4	-5.43	116.40	120.20
36	5	3043	C	C6-N1-C2	5.43	122.47	120.30
36	1	1495	U	N1-C2-O2	-5.43	119.00	122.80
36	5	1203	A	C5-C6-N6	-5.43	119.36	123.70
36	5	1561	G	O4'-C1'-N9	5.43	112.55	108.20
36	5	1885	U	N3-C2-O2	5.43	126.00	122.20
1	2	305	C	C2-N1-C1'	5.43	124.77	118.80
1	2	399	A	C8-N9-C4	5.43	107.97	105.80
1	2	1559	A	O4'-C1'-N9	5.43	112.54	108.20
36	1	2772	C	C2-N1-C1'	5.43	124.77	118.80
38	4	40	A	C6-C5-N7	-5.43	128.50	132.30
38	4	51	G	N1-C6-O6	5.43	123.16	119.90
1	6	29	U	N3-C2-O2	-5.43	118.40	122.20
36	5	1012	G	C8-N9-C4	5.43	108.57	106.40
1	2	334	G	N3-C4-C5	5.43	131.31	128.60
36	1	145	G	N1-C6-O6	5.43	123.16	119.90
36	5	666	A	C4-C5-N7	-5.43	107.99	110.70
38	8	17	A	N9-C4-C5	-5.43	103.63	105.80
36	1	364	G	N1-C6-O6	5.42	123.15	119.90
37	3	80	G	N7-C8-N9	5.42	115.81	113.10
36	5	3116	G	N1-C6-O6	5.42	123.16	119.90
36	1	2898	G	O4'-C1'-N9	-5.42	103.86	108.20
1	6	1760	G	N1-C6-O6	5.42	123.15	119.90
36	5	968	G	C8-N9-C1'	-5.42	119.95	127.00
36	5	1452	A	C8-N9-C4	5.42	107.97	105.80
36	5	1919	G	C8-N9-C4	-5.42	104.23	106.40
36	5	2145	A	C6-N1-C2	-5.42	115.35	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1124	U	C6-N1-C2	-5.42	117.75	121.00
36	1	2376	G	N7-C8-N9	5.42	115.81	113.10
1	6	1614	A	O4'-C1'-N9	5.42	112.54	108.20
36	5	1056	U	OP2-P-O3'	5.42	117.12	105.20
36	5	2316	G	C5-C6-O6	5.42	131.85	128.60
1	6	163	G	N3-C4-C5	5.42	131.31	128.60
44	17	229	PHE	CB-CG-CD2	-5.42	117.01	120.80
36	1	169	U	OP1-P-O3'	5.42	117.12	105.20
36	1	558	U	N3-C2-O2	-5.42	118.41	122.20
36	1	1316	C	O5'-P-OP2	-5.42	100.82	105.70
1	6	17	C	C6-N1-C2	-5.42	118.13	120.30
1	6	778	G	C8-N9-C4	5.42	108.57	106.40
36	5	3309	G	C4-C5-C6	5.42	122.05	118.80
36	1	1205	A	C2-N3-C4	-5.42	107.89	110.60
36	1	2851	A	C5-C6-N1	-5.42	114.99	117.70
1	6	66	U	OP1-P-O3'	5.42	117.11	105.20
36	5	921	A	N9-C4-C5	5.42	107.97	105.80
36	5	934	G	C4-C5-N7	5.42	112.97	110.80
36	1	655	C	C6-N1-C2	-5.42	118.13	120.30
36	1	986	U	O5'-P-OP1	-5.42	100.83	105.70
36	1	1314	C	C4-C5-C6	-5.42	114.69	117.40
36	1	2763	U	O5'-P-OP2	-5.42	100.83	105.70
1	6	904	G	C4-N9-C1'	5.42	133.54	126.50
36	5	2804	A	N1-C2-N3	5.42	132.01	129.30
36	1	784	A	O4'-C1'-N9	5.41	112.53	108.20
36	1	988	U	C6-N1-C2	5.41	124.25	121.00
36	1	2983	C	C5-C6-N1	-5.41	118.29	121.00
36	5	388	G	N7-C8-N9	5.41	115.81	113.10
36	5	647	A	C4-C5-C6	5.41	119.71	117.00
36	5	1161	G	N3-C4-C5	-5.41	125.89	128.60
36	5	2941	A	C6-N1-C2	-5.41	115.35	118.60
36	1	2152	A	C5-C6-N1	5.41	120.41	117.70
36	5	351	A	N1-C6-N6	5.41	121.85	118.60
36	5	421	G	C6-C5-N7	-5.41	127.15	130.40
1	6	323	A	C8-N9-C4	-5.41	103.64	105.80
36	5	2801	A	C5-C6-N1	5.41	120.41	117.70
36	5	3315	G	C4-N9-C1'	5.41	133.53	126.50
1	2	973	A	N1-C2-N3	5.41	132.00	129.30
36	1	883	A	C8-N9-C4	-5.41	103.64	105.80
36	1	1414	G	C4-C5-N7	5.41	112.96	110.80
36	5	2283	G	N9-C4-C5	-5.41	103.24	105.40
36	1	928	C	C6-N1-C2	-5.41	118.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2901	G	O5'-P-OP2	-5.41	100.83	105.70
1	2	351	C	N1-C2-O2	5.41	122.14	118.90
1	2	453	U	C6-N1-C1'	-5.41	113.63	121.20
1	2	1489	U	C6-N1-C2	-5.41	117.76	121.00
36	1	1939	G	C4-C5-C6	5.41	122.04	118.80
1	6	275	C	N1-C2-O2	5.41	122.14	118.90
1	6	1700	C	N1-C2-O2	5.41	122.14	118.90
36	5	1406	A	C8-N9-C4	-5.41	103.64	105.80
36	5	2649	A	C5-C6-N1	5.41	120.40	117.70
36	5	3182	G	OP1-P-OP2	-5.41	111.49	119.60
36	1	2760	C	C6-N1-C2	5.40	122.46	120.30
36	5	2893	C	N3-C4-N4	5.40	121.78	118.00
36	1	941	G	C8-N9-C4	-5.40	104.24	106.40
36	1	2372	A	C5-C6-N6	-5.40	119.38	123.70
36	1	3104	U	C6-N1-C2	5.40	124.24	121.00
36	1	3128	G	N9-C4-C5	-5.40	103.24	105.40
36	5	1338	C	C5-C4-N4	-5.40	116.42	120.20
36	5	2620	G	N3-C4-N9	5.40	129.24	126.00
61	n5	34	LEU	CA-CB-CG	5.40	127.73	115.30
1	2	1488	G	C8-N9-C4	-5.40	104.24	106.40
36	1	400	G	C8-N9-C4	-5.40	104.24	106.40
36	1	901	G	C6-C5-N7	-5.40	127.16	130.40
36	1	1341	U	C4-C5-C6	5.40	122.94	119.70
1	6	64	U	C5-C6-N1	-5.40	120.00	122.70
1	6	268	C	N1-C2-O2	5.40	122.14	118.90
1	6	558	U	O4'-C1'-N1	5.40	112.52	108.20
36	5	651	G	N3-C4-N9	5.40	129.24	126.00
36	5	1149	G	N1-C2-N3	5.40	127.14	123.90
36	1	922	U	N3-C4-C5	-5.40	111.36	114.60
36	5	2996	U	N1-C2-O2	5.40	126.58	122.80
37	7	9	C	O5'-P-OP1	-5.40	100.84	105.70
1	2	1793	G	N3-C4-C5	-5.40	125.90	128.60
36	1	2194	G	C5-C6-O6	-5.40	125.36	128.60
36	1	2404	A	C2-N3-C4	5.40	113.30	110.60
36	1	2653	C	N3-C4-C5	5.40	124.06	121.90
36	1	2817	A	C2-N3-C4	5.40	113.30	110.60
36	5	170	G	C8-N9-C1'	-5.40	119.98	127.00
36	5	647	A	C5-C6-N1	-5.40	115.00	117.70
36	5	1832	C	C6-N1-C2	5.40	122.46	120.30
36	5	3148	U	C5-C6-N1	-5.40	120.00	122.70
38	8	80	A	N7-C8-N9	5.40	116.50	113.80
1	2	638	U	O4'-C1'-N1	5.40	112.52	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1012	U	N3-C4-C5	5.40	117.84	114.60
36	1	304	G	C6-C5-N7	5.39	133.64	130.40
36	1	331	G	N3-C2-N2	-5.39	116.12	119.90
36	1	1190	A	O4'-C1'-N9	-5.39	103.89	108.20
36	1	2176	U	O5'-P-OP1	-5.39	100.84	105.70
36	1	2647	A	C4-C5-C6	5.39	119.70	117.00
36	1	2719	U	C2-N1-C1'	-5.39	111.22	117.70
36	5	498	A	O5'-P-OP2	-5.39	100.84	105.70
36	5	1182	A	C5-C6-N6	-5.39	119.38	123.70
38	4	99	C	C6-N1-C2	5.39	122.46	120.30
1	6	334	G	N1-C2-N2	5.39	121.05	116.20
36	5	2704	A	N1-C6-N6	5.39	121.83	118.60
36	1	880	G	C8-N9-C4	5.39	108.56	106.40
36	1	1077	U	C6-N1-C2	5.39	124.23	121.00
36	1	1473	G	N9-C4-C5	-5.39	103.24	105.40
36	1	1836	C	C2-N1-C1'	5.39	124.73	118.80
36	5	776	U	C2-N3-C4	-5.39	123.77	127.00
36	5	2872	A	N3-C4-C5	5.39	130.57	126.80
37	7	5	G	C2-N3-C4	-5.39	109.20	111.90
1	2	1653	C	N3-C4-C5	-5.39	119.74	121.90
36	1	111	C	N1-C2-O2	-5.39	115.67	118.90
36	1	217	U	OP1-P-O3'	5.39	117.06	105.20
36	1	3266	G	N1-C6-O6	-5.39	116.67	119.90
1	6	60	U	C5-C6-N1	5.39	125.39	122.70
36	5	1611	G	C6-C5-N7	-5.39	127.17	130.40
36	5	2632	G	C2-N3-C4	-5.39	109.20	111.90
36	5	2699	G	N9-C4-C5	-5.39	103.24	105.40
36	5	3154	C	C6-N1-C1'	-5.39	114.33	120.80
48	m1	37	LEU	CA-CB-CG	-5.39	102.91	115.30
36	1	1868	G	N3-C2-N2	5.39	123.67	119.90
36	1	2970	C	C6-N1-C2	5.39	122.45	120.30
36	5	3076	C	C6-N1-C2	-5.39	118.14	120.30
1	2	1639	C	C2-N1-C1'	5.39	124.72	118.80
36	1	2321	A	N1-C6-N6	-5.39	115.37	118.60
36	5	2892	A	O5'-P-OP2	-5.39	100.85	105.70
36	1	1191	U	C5-C6-N1	-5.38	120.01	122.70
36	1	1497	C	N3-C4-C5	-5.38	119.75	121.90
36	1	2383	C	C4-C5-C6	-5.38	114.71	117.40
1	6	108	A	C4-C5-C6	5.38	119.69	117.00
36	5	2360	C	N3-C4-N4	5.38	121.77	118.00
36	5	2864	A	C6-C5-N7	-5.38	128.53	132.30
36	5	3264	G	O5'-P-OP1	-5.38	100.85	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	335	G	C4-C5-N7	5.38	112.95	110.80
36	1	1610	G	N1-C6-O6	5.38	123.13	119.90
1	6	1172	G	N3-C4-N9	5.38	129.23	126.00
36	1	1146	C	C5-C4-N4	-5.38	116.43	120.20
36	1	1929	G	C4-C5-N7	5.38	112.95	110.80
36	5	1161	G	C2-N3-C4	5.38	114.59	111.90
36	5	1519	G	C5-C6-O6	-5.38	125.37	128.60
36	5	2379	U	N3-C2-O2	-5.38	118.43	122.20
36	5	3183	A	N9-C4-C5	5.38	107.95	105.80
36	1	3002	C	C5-C6-N1	-5.38	118.31	121.00
1	6	384	G	N3-C4-N9	-5.38	122.77	126.00
38	8	64	U	C2-N1-C1'	5.38	124.16	117.70
36	1	2443	A	N1-C6-N6	5.38	121.83	118.60
36	5	924	G	O4'-C1'-N9	-5.38	103.90	108.20
36	5	1302	A	C5-C6-N1	-5.38	115.01	117.70
36	5	1830	G	C5-C6-N1	-5.38	108.81	111.50
36	5	1848	G	C5-C6-N1	5.38	114.19	111.50
36	5	2524	A	N7-C8-N9	5.38	116.49	113.80
36	5	2937	G	N3-C2-N2	-5.38	116.14	119.90
36	1	1352	A	P-O3'-C3'	5.38	126.15	119.70
36	1	1746	U	C6-N1-C2	-5.38	117.77	121.00
36	1	1863	G	C5-C6-O6	-5.38	125.38	128.60
36	5	1851	G	C6-C5-N7	-5.38	127.17	130.40
36	5	1878	G	C4-N9-C1'	5.38	133.49	126.50
36	5	1888	U	N1-C2-N3	5.38	118.13	114.90
36	5	2820	A	C5-N7-C8	-5.38	101.21	103.90
36	5	3033	A	C8-N9-C4	5.38	107.95	105.80
1	6	100	A	C4-C5-C6	5.38	119.69	117.00
36	5	1155	C	C5-C4-N4	-5.38	116.44	120.20
36	5	1407	A	O5'-P-OP2	-5.38	100.86	105.70
1	2	1284	C	N3-C2-O2	-5.37	118.14	121.90
36	1	1407	A	O5'-P-OP1	5.37	117.15	110.70
36	1	1792	C	N3-C4-C5	-5.37	119.75	121.90
36	1	2869	U	OP2-P-O3'	5.37	117.02	105.20
36	5	82	C	C6-N1-C2	-5.37	118.15	120.30
36	1	154	U	C5-C6-N1	-5.37	120.01	122.70
36	1	715	A	O4'-C1'-N9	5.37	112.50	108.20
36	1	936	A	N3-C4-C5	5.37	130.56	126.80
36	1	2616	C	N1-C2-O2	5.37	122.12	118.90
36	5	888	A	N9-C4-C5	-5.37	103.65	105.80
36	5	1556	C	N3-C2-O2	-5.37	118.14	121.90
36	5	3177	G	N1-C2-N3	5.37	127.12	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	80	G	N3-C4-N9	5.37	129.22	126.00
36	5	664	U	N3-C4-C5	-5.37	111.38	114.60
36	1	984	G	OP2-P-O3'	5.37	117.01	105.20
36	1	1315	U	C5-C6-N1	-5.37	120.02	122.70
1	6	1202	A	C2-N3-C4	5.37	113.28	110.60
36	5	1127	G	C5-C6-O6	5.37	131.82	128.60
36	5	1462	A	C2-N3-C4	-5.37	107.92	110.60
36	5	51	A	C4-C5-C6	5.37	119.68	117.00
36	5	646	A	N1-C2-N3	5.37	131.98	129.30
36	5	1296	C	N3-C4-N4	5.37	121.76	118.00
1	2	1568	C	C6-N1-C2	-5.37	118.15	120.30
1	6	1634	C	N3-C2-O2	-5.37	118.14	121.90
36	5	361	A	C8-N9-C4	5.37	107.95	105.80
36	5	3371	G	C5-C6-N1	-5.37	108.82	111.50
36	1	197	G	C5-N7-C8	-5.36	101.62	104.30
37	7	75	G	C4-N9-C1'	5.36	133.47	126.50
36	1	938	C	C6-N1-C2	-5.36	118.16	120.30
36	5	3218	A	C5-N7-C8	-5.36	101.22	103.90
36	1	1437	C	N3-C4-N4	5.36	121.75	118.00
47	MO	24	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	6	1039	A	O4'-C1'-N9	5.36	112.49	108.20
36	5	329	U	N1-C2-O2	5.36	126.55	122.80
36	5	3108	G	C6-C5-N7	-5.36	127.18	130.40
36	1	1144	U	O5'-P-OP1	-5.36	100.88	105.70
36	1	2639	G	C4-C5-C6	5.36	122.02	118.80
1	6	1730	A	N1-C2-N3	5.36	131.98	129.30
36	5	2297	U	C2-N1-C1'	-5.36	111.27	117.70
36	1	1340	G	C5-C6-N1	5.36	114.18	111.50
36	5	1372	C	N3-C4-C5	-5.36	119.76	121.90
36	5	2624	G	C8-N9-C4	-5.36	104.26	106.40
36	5	2628	A	O5'-P-OP1	5.36	117.13	110.70
1	2	1100	G	N3-C4-N9	5.36	129.21	126.00
1	2	1274	C	N3-C2-O2	-5.36	118.15	121.90
36	1	1431	G	N1-C6-O6	-5.36	116.69	119.90
38	4	51	G	C5-C6-O6	-5.36	125.39	128.60
1	6	1285	U	C6-N1-C2	-5.36	117.79	121.00
1	6	1600	A	N7-C8-N9	5.36	116.48	113.80
36	5	1846	C	C5-C6-N1	-5.36	118.32	121.00
36	1	977	C	C6-N1-C2	5.35	122.44	120.30
36	1	1445	U	C2-N1-C1'	-5.35	111.28	117.70
36	5	360	G	C4-C5-N7	-5.35	108.66	110.80
36	5	1481	A	N7-C8-N9	5.35	116.48	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	326	U	N3-C4-O4	5.35	123.15	119.40
36	1	586	C	C6-N1-C2	5.35	122.44	120.30
36	5	405	U	C5-C6-N1	5.35	125.38	122.70
36	5	2976	A	OP2-P-O3'	5.35	116.98	105.20
36	5	3388	C	C5-C6-N1	-5.35	118.32	121.00
36	1	2807	U	C5-C4-O4	-5.35	122.69	125.90
36	5	656	A	N9-C4-C5	-5.35	103.66	105.80
36	1	608	A	C5-C6-N1	-5.35	115.03	117.70
36	1	1505	C	OP2-P-O3'	5.35	116.97	105.20
36	1	1834	U	C4-C5-C6	5.35	122.91	119.70
36	1	2407	C	N1-C2-O2	-5.35	115.69	118.90
1	6	391	A	N7-C8-N9	-5.35	111.13	113.80
1	6	1614	A	N3-C4-C5	5.35	130.54	126.80
1	6	1648	A	N9-C4-C5	-5.35	103.66	105.80
36	5	2301	U	N1-C2-N3	-5.35	111.69	114.90
36	5	2550	U	C5-C4-O4	5.35	129.11	125.90
37	7	80	G	N3-C4-N9	5.35	129.21	126.00
1	2	1216	C	O5'-P-OP2	-5.35	100.89	105.70
1	2	1785	U	N1-C2-N3	5.35	118.11	114.90
36	5	3000	A	N1-C6-N6	5.35	121.81	118.60
1	6	1486	G	O5'-P-OP2	-5.35	100.89	105.70
36	5	1116	G	C4-N9-C1'	5.35	133.45	126.50
36	1	324	A	N1-C2-N3	5.34	131.97	129.30
36	1	1835	A	O5'-P-OP1	-5.34	100.89	105.70
36	1	2385	G	C8-N9-C1'	5.34	133.95	127.00
37	3	25	G	N3-C4-N9	5.34	129.21	126.00
36	5	96	G	C8-N9-C4	5.34	108.54	106.40
36	5	1326	A	N7-C8-N9	-5.34	111.13	113.80
36	5	3154	C	C5-C6-N1	5.34	123.67	121.00
36	1	1434	G	C8-N9-C4	-5.34	104.26	106.40
36	5	364	G	N9-C4-C5	-5.34	103.26	105.40
1	2	321	C	N1-C2-O2	5.34	122.11	118.90
36	1	211	A	O5'-P-OP1	-5.34	100.89	105.70
36	1	922	U	C5-C4-O4	5.34	129.10	125.90
36	1	1064	A	O4'-C1'-N9	-5.34	103.93	108.20
36	1	2367	A	C5-C6-N1	5.34	120.37	117.70
1	6	1258	U	N3-C2-O2	-5.34	118.46	122.20
36	5	513	G	C5-N7-C8	5.34	106.97	104.30
36	5	1064	A	P-O3'-C3'	5.34	126.11	119.70
36	5	2375	G	N1-C6-O6	-5.34	116.69	119.90
36	1	277	G	C8-N9-C4	-5.34	104.26	106.40
36	1	1365	G	N1-C2-N2	-5.34	111.39	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2812	C	C4-C5-C6	5.34	120.07	117.40
36	1	2959	C	N3-C2-O2	5.34	125.64	121.90
36	5	280	U	O5'-P-OP2	-5.34	100.89	105.70
36	5	388	G	C6-C5-N7	-5.34	127.20	130.40
36	5	920	A	OP1-P-OP2	-5.34	111.59	119.60
36	5	1301	A	N3-C4-C5	-5.34	123.06	126.80
36	5	2818	U	C5'-C4'-O4'	-5.34	102.69	109.10
1	2	1057	U	C2-N1-C1'	5.34	124.11	117.70
36	1	1001	G	C6-C5-N7	-5.34	127.20	130.40
36	1	3128	G	C8-N9-C1'	-5.34	120.06	127.00
1	6	407	A	O5'-P-OP1	5.34	117.11	110.70
1	6	886	U	O4'-C1'-N1	5.34	112.47	108.20
36	5	2850	G	OP1-P-OP2	5.34	127.61	119.60
1	2	1171	A	N1-C6-N6	-5.34	115.40	118.60
1	2	1782	A	C5-C6-N6	5.34	127.97	123.70
36	1	286	U	N3-C2-O2	-5.34	118.46	122.20
36	1	2764	C	N3-C4-N4	5.34	121.73	118.00
36	1	2899	C	N3-C4-C5	-5.34	119.77	121.90
36	5	61	A	N1-C2-N3	5.34	131.97	129.30
36	5	1340	G	C8-N9-C4	5.34	108.53	106.40
36	5	1519	G	C4-C5-N7	5.34	112.94	110.80
36	1	1741	A	N1-C2-N3	5.33	131.97	129.30
36	1	2144	A	O4'-C1'-N9	5.33	112.47	108.20
38	8	15	G	N1-C6-O6	-5.33	116.70	119.90
36	1	658	G	OP2-P-O3'	5.33	116.93	105.20
36	1	1507	G	N1-C6-O6	5.33	123.10	119.90
1	6	407	A	C8-N9-C4	-5.33	103.67	105.80
36	5	2341	A	N7-C8-N9	-5.33	111.13	113.80
36	1	636	C	C5-C4-N4	-5.33	116.47	120.20
36	1	648	C	O5'-P-OP1	-5.33	100.90	105.70
36	1	804	C	C5-C4-N4	-5.33	116.47	120.20
36	1	1520	G	C5-N7-C8	5.33	106.97	104.30
36	1	2288	G	C8-N9-C1'	-5.33	120.07	127.00
36	1	2617	U	C4-C5-C6	5.33	122.90	119.70
36	5	973	A	C6-C5-N7	-5.33	128.57	132.30
36	5	1129	A	C5-N7-C8	-5.33	101.23	103.90
36	5	2406	C	N1-C2-O2	-5.33	115.70	118.90
36	5	2993	G	C5-C6-O6	-5.33	125.40	128.60
1	2	704	C	C6-N1-C2	-5.33	118.17	120.30
1	2	1031	U	OP2-P-O3'	5.33	116.93	105.20
36	5	218	G	O5'-P-OP2	-5.33	100.90	105.70
36	5	3029	A	N9-C4-C5	5.33	107.93	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	24	G	C8-N9-C1'	-5.33	120.07	127.00
36	1	2832	C	C5-C6-N1	-5.33	118.34	121.00
36	5	999	G	C8-N9-C4	5.33	108.53	106.40
36	5	1744	G	N3-C4-C5	-5.33	125.94	128.60
37	7	82	G	C4-C5-N7	5.33	112.93	110.80
1	6	542	A	O4'-C1'-N9	5.33	112.46	108.20
1	6	935	U	C6-N1-C2	-5.33	117.80	121.00
36	5	1184	A	C6-C5-N7	5.33	136.03	132.30
36	1	682	U	C6-N1-C1'	5.33	128.66	121.20
36	1	1400	G	N3-C4-N9	5.33	129.19	126.00
36	1	2646	C	N3-C4-C5	5.33	124.03	121.90
36	1	2811	A	N9-C4-C5	5.33	107.93	105.80
1	6	1199	G	N3-C4-C5	5.33	131.26	128.60
36	5	668	G	C5-N7-C8	5.33	106.96	104.30
36	5	869	G	N9-C4-C5	-5.33	103.27	105.40
36	5	2352	A	N1-C6-N6	5.33	121.80	118.60
36	5	2758	A	C4-C5-N7	-5.33	108.04	110.70
36	5	2994	A	N3-C4-C5	-5.33	123.07	126.80
1	6	29	U	N3-C4-C5	-5.32	111.41	114.60
1	6	55	A	N7-C8-N9	5.32	116.46	113.80
1	6	934	C	N3-C2-O2	-5.32	118.17	121.90
36	5	1127	G	N3-C2-N2	5.32	123.63	119.90
36	5	1405	U	O5'-P-OP2	-5.32	100.91	105.70
36	5	3109	G	N1-C6-O6	5.32	123.09	119.90
36	5	3295	A	C6-N1-C2	-5.32	115.41	118.60
1	6	1382	A	O4'-C1'-N9	5.32	112.46	108.20
1	2	305	C	C5-C6-N1	5.32	123.66	121.00
36	1	1331	U	O5'-P-OP2	-5.32	100.91	105.70
36	1	1341	U	N3-C4-C5	-5.32	111.41	114.60
36	1	1792	C	O4'-C1'-N1	5.32	112.46	108.20
36	1	2996	U	C5-C4-O4	-5.32	122.71	125.90
1	6	576	G	C6-C5-N7	-5.32	127.21	130.40
36	5	2407	C	N3-C4-C5	5.32	124.03	121.90
36	5	2813	A	N1-C6-N6	5.32	121.79	118.60
36	5	2827	U	C2-N1-C1'	5.32	124.08	117.70
1	2	1490	C	C6-N1-C2	-5.32	118.17	120.30
36	1	954	U	N1-C2-N3	5.32	118.09	114.90
36	5	2711	C	N3-C4-N4	5.32	121.72	118.00
1	2	274	G	C4-N9-C1'	5.32	133.41	126.50
1	2	394	C	C6-N1-C2	-5.32	118.17	120.30
36	1	720	A	C6-C5-N7	-5.32	128.58	132.30
36	1	2412	G	C8-N9-C4	-5.32	104.27	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2916	U	C2-N3-C4	5.32	130.19	127.00
37	3	82	G	N1-C2-N2	-5.32	111.42	116.20
1	6	536	C	C5-C6-N1	5.32	123.66	121.00
36	5	1116	G	O5'-P-OP1	-5.32	100.91	105.70
36	5	3173	G	OP1-P-OP2	5.32	127.58	119.60
1	2	75	U	C2-N1-C1'	5.32	124.08	117.70
36	1	878	G	N1-C2-N3	5.32	127.09	123.90
36	1	1074	U	N3-C4-C5	5.32	117.79	114.60
36	1	1520	G	N7-C8-N9	-5.32	110.44	113.10
1	6	1127	G	C6-C5-N7	-5.32	127.21	130.40
36	1	3224	G	C2-N3-C4	-5.31	109.24	111.90
37	7	93	C	N3-C2-O2	-5.31	118.18	121.90
36	1	509	U	O5'-P-OP1	5.31	117.08	110.70
36	1	635	G	C6-N1-C2	-5.31	121.91	125.10
36	1	2196	C	N3-C4-C5	5.31	124.03	121.90
1	6	934	C	N1-C2-O2	5.31	122.09	118.90
1	6	1119	G	N9-C4-C5	5.31	107.53	105.40
36	5	416	A	OP2-P-O3'	5.31	116.89	105.20
36	5	523	A	C5-C6-N6	5.31	127.95	123.70
36	5	834	U	N3-C4-C5	5.31	117.79	114.60
36	1	884	A	C5-C6-N6	-5.31	119.45	123.70
36	1	714	G	N3-C4-N9	5.31	129.19	126.00
36	1	1417	G	O4'-C1'-N9	-5.31	103.95	108.20
36	1	2245	C	N1-C2-O2	5.31	122.09	118.90
36	1	2924	U	C5-C6-N1	-5.31	120.05	122.70
36	1	2989	U	C6-N1-C2	-5.31	117.81	121.00
36	5	2864	A	C5-C6-N6	-5.31	119.45	123.70
36	5	3055	U	N3-C2-O2	5.31	125.92	122.20
36	1	2727	A	C2-N3-C4	5.31	113.25	110.60
54	M8	138	LEU	CA-CB-CG	5.31	127.51	115.30
1	6	65	A	N9-C4-C5	-5.31	103.68	105.80
1	6	314	C	N3-C4-C5	-5.31	119.78	121.90
1	6	1600	A	OP1-P-O3'	5.31	116.88	105.20
36	5	1354	G	N1-C6-O6	5.31	123.08	119.90
36	5	1413	G	C8-N9-C4	5.31	108.52	106.40
36	5	1770	G	C4-N9-C1'	5.31	133.40	126.50
36	5	2299	A	O5'-P-OP2	-5.31	100.92	105.70
36	5	2670	G	O5'-P-OP2	-5.31	100.92	105.70
36	5	2856	G	C5-C6-O6	-5.31	125.42	128.60
36	5	3204	C	C5-C6-N1	-5.31	118.35	121.00
36	1	2324	A	N9-C4-C5	5.31	107.92	105.80
36	1	2899	C	OP2-P-O3'	5.31	116.87	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	541	A	C8-N9-C4	-5.31	103.68	105.80
36	1	224	C	N1-C2-O2	-5.30	115.72	118.90
36	1	1581	C	N1-C2-O2	5.30	122.08	118.90
36	1	3270	U	C2-N1-C1'	-5.30	111.33	117.70
1	6	20	G	N3-C4-C5	5.30	131.25	128.60
36	5	877	C	N3-C4-N4	-5.30	114.29	118.00
36	5	953	G	C8-N9-C4	5.30	108.52	106.40
36	5	3153	U	C2-N1-C1'	5.30	124.06	117.70
1	6	1112	G	N3-C2-N2	5.30	123.61	119.90
36	5	2283	G	C5-N7-C8	-5.30	101.65	104.30
1	2	1488	G	N7-C8-N9	5.30	115.75	113.10
36	1	2953	U	N3-C4-O4	5.30	123.11	119.40
1	6	447	U	C6-N1-C2	-5.30	117.82	121.00
36	5	421	G	C8-N9-C4	-5.30	104.28	106.40
36	5	629	U	N1-C2-N3	5.30	118.08	114.90
36	5	873	C	N1-C2-O2	5.30	122.08	118.90
36	5	2607	G	C6-C5-N7	-5.30	127.22	130.40
36	1	3011	A	C8-N9-C4	5.30	107.92	105.80
36	5	1298	C	C6-N1-C2	-5.30	118.18	120.30
36	5	2123	G	C5-N7-C8	5.30	106.95	104.30
36	5	2966	G	C4-N9-C1'	5.30	133.39	126.50
36	1	679	U	N1-C2-O2	5.30	126.51	122.80
36	1	2358	A	C2-N3-C4	-5.30	107.95	110.60
36	5	2617	U	N3-C4-O4	5.30	123.11	119.40
38	8	104	A	C8-N9-C4	5.30	107.92	105.80
36	1	642	U	N1-C2-N3	5.30	118.08	114.90
36	1	2356	A	C5-N7-C8	-5.30	101.25	103.90
36	1	2968	G	C4-C5-N7	5.30	112.92	110.80
1	6	1573	A	P-O3'-C3'	5.30	126.06	119.70
36	5	27	C	N1-C2-O2	-5.30	115.72	118.90
36	5	1528	G	C4-N9-C1'	5.30	133.38	126.50
36	5	2959	C	OP2-P-O3'	5.30	116.85	105.20
38	8	96	A	N1-C6-N6	5.30	121.78	118.60
36	1	2850	G	C6-C5-N7	-5.29	127.22	130.40
38	4	16	G	N7-C8-N9	-5.29	110.45	113.10
38	4	20	U	N1-C2-N3	5.29	118.08	114.90
36	5	2817	A	N3-C4-C5	-5.29	123.09	126.80
36	1	1383	G	C8-N9-C4	-5.29	104.28	106.40
36	5	645	A	C5-C6-N1	5.29	120.35	117.70
36	5	1116	G	C8-N9-C1'	-5.29	120.12	127.00
36	5	1476	G	N1-C2-N2	-5.29	111.44	116.20
36	5	2744	U	N3-C2-O2	-5.29	118.50	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2878	G	C2-N3-C4	5.29	114.55	111.90
36	5	3107	U	C2-N1-C1'	5.29	124.05	117.70
36	5	3301	U	C6-N1-C2	5.29	124.18	121.00
36	1	1005	G	N7-C8-N9	-5.29	110.45	113.10
36	1	2874	G	C4-C5-C6	5.29	121.97	118.80
37	3	9	C	N3-C4-C5	-5.29	119.78	121.90
1	6	272	U	C5-C6-N1	5.29	125.35	122.70
36	5	1369	A	C4-C5-C6	5.29	119.65	117.00
1	2	331	A	N9-C4-C5	5.29	107.92	105.80
36	1	1389	G	N1-C6-O6	5.29	123.07	119.90
36	5	2900	A	N1-C6-N6	-5.29	115.43	118.60
36	5	2930	A	C8-N9-C4	5.29	107.92	105.80
38	8	17	A	C6-C5-N7	-5.29	128.60	132.30
1	2	950	C	C6-N1-C2	-5.29	118.18	120.30
1	2	1168	U	OP1-P-O3'	5.29	116.83	105.20
36	1	59	G	C5-C6-O6	-5.29	125.43	128.60
36	1	2927	C	N1-C2-O2	-5.29	115.73	118.90
36	5	84	U	N3-C2-O2	-5.29	118.50	122.20
36	5	3261	C	C6-N1-C2	-5.29	118.19	120.30
67	o1	97	LEU	CA-CB-CG	5.29	127.47	115.30
36	1	2611	U	N3-C4-C5	-5.29	111.43	114.60
36	1	2787	G	N1-C6-O6	5.29	123.07	119.90
36	1	2875	U	C6-N1-C2	-5.29	117.83	121.00
36	5	2754	G	C8-N9-C4	5.29	108.52	106.40
1	2	1401	A	N1-C6-N6	-5.29	115.43	118.60
36	1	687	U	OP2-P-O3'	5.29	116.83	105.20
36	1	906	A	C6-N1-C2	-5.29	115.43	118.60
36	1	970	A	C4-C5-N7	5.29	113.34	110.70
36	1	1607	U	N3-C2-O2	-5.29	118.50	122.20
36	1	2247	G	C5-C6-N1	-5.29	108.86	111.50
36	1	2400	G	N3-C4-C5	5.29	131.24	128.60
36	1	2779	A	C8-N9-C4	5.29	107.91	105.80
36	5	1605	A	O4'-C1'-N9	5.29	112.43	108.20
36	1	336	A	N9-C4-C5	-5.28	103.69	105.80
36	1	410	U	N1-C2-N3	5.28	118.07	114.90
36	1	1402	C	N3-C4-C5	5.28	124.01	121.90
52	M6	133	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	6	405	C	C6-N1-C2	5.28	122.41	120.30
36	5	804	C	C6-N1-C2	5.28	122.41	120.30
36	5	1896	A	C5-N7-C8	-5.28	101.26	103.90
36	1	2122	G	O5'-P-OP2	-5.28	100.95	105.70
36	1	2169	G	N1-C6-O6	-5.28	116.73	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2403	G	C6-C5-N7	-5.28	127.23	130.40
36	1	2731	U	OP2-P-O3'	5.28	116.82	105.20
36	1	2812	C	C5-C6-N1	-5.28	118.36	121.00
36	5	437	G	N3-C2-N2	-5.28	116.20	119.90
36	5	2679	A	N7-C8-N9	-5.28	111.16	113.80
37	7	105	C	C4-C5-C6	5.28	120.04	117.40
36	1	53	G	C8-N9-C1'	-5.28	120.14	127.00
36	1	343	U	N1-C2-N3	5.28	118.07	114.90
36	1	2323	G	C5-C6-N1	5.28	114.14	111.50
36	5	1081	U	C5-C6-N1	5.28	125.34	122.70
37	7	1	G	C6-C5-N7	-5.28	127.23	130.40
37	7	73	C	C2-N1-C1'	5.28	124.61	118.80
36	1	1393	A	N1-C2-N3	5.28	131.94	129.30
37	3	38	U	C5-C6-N1	5.28	125.34	122.70
38	4	14	C	C5-C6-N1	-5.28	118.36	121.00
36	5	63	A	N1-C6-N6	5.28	121.77	118.60
37	7	49	G	N3-C4-C5	5.28	131.24	128.60
36	1	1904	C	C5-C6-N1	5.28	123.64	121.00
36	1	2132	C	O5'-P-OP2	-5.28	100.95	105.70
36	5	2398	A	C4-C5-N7	-5.28	108.06	110.70
37	7	14	U	C6-N1-C2	5.28	124.17	121.00
36	1	2586	G	N1-C6-O6	-5.27	116.74	119.90
36	5	1181	U	N1-C2-N3	5.27	118.06	114.90
36	5	1501	U	C5-C4-O4	5.27	129.06	125.90
36	5	2889	C	OP1-P-OP2	-5.27	111.69	119.60
36	5	2953	U	C5-C4-O4	-5.27	122.74	125.90
1	2	1137	A	N3-C4-C5	5.27	130.49	126.80
36	1	885	U	OP1-P-O3'	5.27	116.80	105.20
36	1	979	U	O4'-C1'-N1	5.27	112.42	108.20
36	1	1192	C	C5-C6-N1	5.27	123.64	121.00
36	1	2537	U	P-O3'-C3'	5.27	126.03	119.70
36	5	31	C	OP2-P-O3'	5.27	116.80	105.20
36	5	3164	C	O4'-C1'-N1	5.27	112.42	108.20
52	m6	133	ARG	NE-CZ-NH2	-5.27	117.66	120.30
36	1	721	G	C8-N9-C4	-5.27	104.29	106.40
36	1	1119	C	C5-C4-N4	5.27	123.89	120.20
1	6	85	A	N9-C4-C5	5.27	107.91	105.80
36	1	3000	A	N3-C4-C5	5.27	130.49	126.80
1	6	390	G	C4-C5-N7	5.27	112.91	110.80
36	5	2142	A	C6-N1-C2	-5.27	115.44	118.60
36	5	3035	A	N9-C4-C5	-5.27	103.69	105.80
36	5	3067	C	N3-C2-O2	-5.27	118.21	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	863	A	N3-C4-C5	5.27	130.49	126.80
36	1	1306	G	N3-C2-N2	-5.27	116.21	119.90
36	1	1604	G	C8-N9-C1'	-5.27	120.15	127.00
36	5	776	U	N3-C4-O4	-5.27	115.71	119.40
36	1	921	A	C5-C6-N6	5.27	127.91	123.70
36	1	1217	A	OP2-P-O3'	5.27	116.79	105.20
36	1	1422	G	N1-C6-O6	5.27	123.06	119.90
37	3	120	C	N3-C2-O2	-5.27	118.21	121.90
17	c5	36	LEU	CA-CB-CG	5.27	127.41	115.30
36	5	2775	U	C5-C4-O4	5.27	129.06	125.90
36	5	3092	C	C2-N3-C4	-5.27	117.27	119.90
36	1	2602	G	C4-C5-N7	-5.26	108.69	110.80
36	1	2630	C	O5'-P-OP1	-5.26	100.96	105.70
1	6	1130	G	C6-C5-N7	5.26	133.56	130.40
36	5	317	A	N1-C6-N6	-5.26	115.44	118.60
36	5	934	G	C2-N3-C4	5.26	114.53	111.90
36	5	1599	G	N9-C4-C5	-5.26	103.29	105.40
36	5	2524	A	C5-N7-C8	-5.26	101.27	103.90
36	1	594	U	C5-C4-O4	5.26	129.06	125.90
36	1	2643	A	O5'-P-OP1	-5.26	100.97	105.70
38	4	25	G	N9-C4-C5	5.26	107.50	105.40
36	5	644	G	N9-C4-C5	5.26	107.50	105.40
36	5	1332	A	C6-C5-N7	-5.26	128.62	132.30
36	5	2855	U	N1-C2-O2	-5.26	119.12	122.80
36	5	3389	U	C5-C4-O4	5.26	129.06	125.90
1	2	25	C	C2-N1-C1'	5.26	124.59	118.80
1	2	1274	C	C2-N1-C1'	5.26	124.58	118.80
22	D0	34	LEU	CA-CB-CG	5.26	127.40	115.30
36	1	2400	G	C6-C5-N7	-5.26	127.24	130.40
36	5	1839	A	O5'-P-OP1	-5.26	100.97	105.70
1	2	829	A	P-O3'-C3'	5.26	126.01	119.70
36	1	1748	G	C6-C5-N7	-5.26	127.25	130.40
36	1	2136	C	C5-C4-N4	5.26	123.88	120.20
36	1	2365	C	C5-C6-N1	-5.26	118.37	121.00
1	6	1521	G	N1-C6-O6	-5.26	116.75	119.90
36	5	508	U	C5-C6-N1	5.26	125.33	122.70
36	5	1075	A	N7-C8-N9	-5.26	111.17	113.80
36	5	1513	G	N3-C4-N9	5.26	129.15	126.00
36	5	1514	G	OP1-P-O3'	5.26	116.77	105.20
36	1	871	U	OP2-P-O3'	5.25	116.76	105.20
1	6	192	U	P-O3'-C3'	5.25	126.01	119.70
1	6	1550	A	N7-C8-N9	5.25	116.43	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1169	A	O5'-P-OP2	-5.25	100.97	105.70
36	5	2826	U	C5-C6-N1	-5.25	120.07	122.70
36	5	2892	A	C6-C5-N7	-5.25	128.62	132.30
1	2	1297	G	C5-C6-O6	-5.25	125.45	128.60
36	1	1807	G	C8-N9-C4	-5.25	104.30	106.40
36	1	2633	U	O5'-P-OP2	5.25	117.00	110.70
36	1	2889	C	N3-C4-C5	5.25	124.00	121.90
1	6	767	U	N3-C2-O2	-5.25	118.52	122.20
36	5	639	G	O5'-P-OP1	-5.25	100.97	105.70
36	1	396	A	C8-N9-C4	-5.25	103.70	105.80
36	1	1429	G	C5-N7-C8	5.25	106.93	104.30
36	1	2942	C	C6-N1-C1'	5.25	127.10	120.80
1	6	455	C	C6-N1-C2	-5.25	118.20	120.30
1	6	1773	C	C5-C6-N1	5.25	123.63	121.00
36	1	2626	A	N1-C6-N6	-5.25	115.45	118.60
38	4	26	U	C2-N1-C1'	5.25	124.00	117.70
36	5	699	A	C2-N3-C4	-5.25	107.97	110.60
36	5	1054	A	OP2-P-O3'	5.25	116.75	105.20
38	8	97	A	C8-N9-C4	5.25	107.90	105.80
1	2	163	G	O4'-C1'-N9	5.25	112.40	108.20
1	2	1636	C	N3-C4-N4	5.25	121.67	118.00
36	1	1413	G	N3-C2-N2	-5.25	116.22	119.90
36	1	1495	U	C2-N1-C1'	-5.25	111.40	117.70
1	6	1600	A	C2-N3-C4	-5.25	107.98	110.60
36	5	1856	C	C6-N1-C2	-5.25	118.20	120.30
1	2	278	U	N1-C2-O2	5.25	126.47	122.80
37	3	92	A	C5-C6-N1	-5.25	115.08	117.70
37	3	93	C	N1-C2-O2	5.25	122.05	118.90
36	5	869	G	C4-C5-N7	5.25	112.90	110.80
36	5	999	G	C5-C6-O6	-5.25	125.45	128.60
36	5	1116	G	N1-C2-N2	-5.25	111.48	116.20
36	5	1190	A	N7-C8-N9	5.25	116.42	113.80
1	6	687	G	N3-C4-N9	-5.25	122.85	126.00
36	5	520	U	C2-N1-C1'	-5.25	111.41	117.70
36	5	842	G	C5-C6-O6	-5.25	125.45	128.60
1	2	734	A	P-O3'-C3'	5.24	125.99	119.70
36	1	2370	G	C2-N3-C4	-5.24	109.28	111.90
1	6	620	A	C4-C5-C6	5.24	119.62	117.00
36	5	1443	G	C6-C5-N7	-5.24	127.25	130.40
36	1	2247	G	C4-C5-C6	5.24	121.94	118.80
36	5	2950	G	N1-C6-O6	5.24	123.05	119.90
36	1	670	C	N3-C2-O2	-5.24	118.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	908	G	C6-C5-N7	-5.24	127.26	130.40
36	5	886	C	C6-N1-C2	5.24	122.40	120.30
38	8	34	U	C5-C6-N1	-5.24	120.08	122.70
36	1	688	G	N3-C4-N9	5.24	129.14	126.00
36	1	1444	G	N1-C6-O6	5.24	123.04	119.90
1	6	391	A	C8-N9-C4	5.24	107.89	105.80
1	6	779	U	N1-C1'-C2'	5.24	120.81	114.00
36	5	1716	U	P-O3'-C3'	5.24	125.99	119.70
37	7	49	G	N3-C2-N2	-5.24	116.23	119.90
36	5	801	A	OP1-P-O3'	5.24	116.72	105.20
36	5	1348	U	C6-N1-C2	-5.24	117.86	121.00
36	5	2329	C	C6-N1-C2	5.24	122.39	120.30
36	5	2777	G	C5-C6-N1	-5.24	108.88	111.50
36	1	557	A	C8-N9-C4	5.24	107.89	105.80
36	1	870	G	N3-C4-N9	-5.24	122.86	126.00
36	1	2746	A	C2-N3-C4	-5.24	107.98	110.60
36	1	2983	C	O4'-C1'-N1	5.24	112.39	108.20
1	6	758	U	N3-C2-O2	-5.24	118.54	122.20
1	6	1608	U	C6-N1-C2	-5.24	117.86	121.00
36	5	1481	A	N1-C2-N3	5.24	131.92	129.30
36	5	1846	C	N3-C2-O2	-5.24	118.23	121.90
38	8	15	G	C5-C6-O6	5.24	131.74	128.60
36	1	3195	U	P-O3'-C3'	5.23	125.98	119.70
36	1	3375	A	OP1-P-O3'	5.23	116.72	105.20
36	5	2736	A	C4-C5-C6	5.23	119.62	117.00
36	1	1152	G	N3-C4-C5	-5.23	125.98	128.60
36	5	1865	A	C2-N3-C4	-5.23	107.98	110.60
1	2	501	U	P-O3'-C3'	5.23	125.98	119.70
1	2	1258	U	C2-N1-C1'	5.23	123.98	117.70
1	2	1462	G	C4-C5-N7	5.23	112.89	110.80
36	1	27	C	OP1-P-OP2	5.23	127.45	119.60
36	1	692	A	C5-C6-N1	-5.23	115.08	117.70
36	1	1327	C	N1-C2-O2	-5.23	115.76	118.90
36	1	2308	C	N3-C4-C5	5.23	123.99	121.90
36	1	2726	C	N1-C2-O2	5.23	122.04	118.90
1	6	1481	C	C6-N1-C2	-5.23	118.21	120.30
1	6	1697	G	N3-C4-C5	-5.23	125.98	128.60
36	5	197	G	N3-C2-N2	5.23	123.56	119.90
36	5	295	A	O5'-P-OP1	-5.23	100.99	105.70
36	5	1213	G	C2-N3-C4	5.23	114.52	111.90
36	5	1899	G	C5-C6-O6	5.23	131.74	128.60
36	1	2624	G	N1-C6-O6	5.23	123.04	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3182	G	N3-C4-N9	5.23	129.14	126.00
38	4	95	G	C4-N9-C1'	-5.23	119.70	126.50
1	6	543	C	C5-C4-N4	5.23	123.86	120.20
36	5	1177	G	N1-C2-N3	5.23	127.04	123.90
36	5	1186	G	C8-N9-C4	-5.23	104.31	106.40
36	5	1374	G	C8-N9-C4	5.23	108.49	106.40
36	1	2752	U	N1-C2-N3	5.23	118.04	114.90
36	1	2762	A	N1-C6-N6	-5.23	115.46	118.60
1	6	360	A	C5-C6-N6	-5.23	119.52	123.70
1	6	405	C	C5-C6-N1	-5.23	118.39	121.00
36	5	1200	A	N3-C4-N9	5.23	131.58	127.40
36	5	1440	G	N1-C2-N3	5.23	127.04	123.90
36	5	2278	C	N3-C4-C5	5.23	123.99	121.90
36	5	2945	G	N3-C2-N2	5.23	123.56	119.90
36	5	3104	U	O5'-P-OP2	-5.23	101.00	105.70
36	1	594	U	N3-C4-C5	-5.23	111.46	114.60
36	1	1504	A	N1-C6-N6	-5.23	115.46	118.60
36	5	807	A	C8-N9-C4	-5.23	103.71	105.80
36	5	1159	A	C5-N7-C8	-5.23	101.29	103.90
36	1	2946	A	C4-C5-C6	5.22	119.61	117.00
36	1	3100	U	C6-N1-C2	5.22	124.14	121.00
36	1	3302	U	C2-N3-C4	-5.22	123.86	127.00
36	1	3319	U	C2-N1-C1'	5.22	123.97	117.70
36	5	1462	A	N3-C4-C5	5.22	130.46	126.80
1	2	795	U	C4-C5-C6	5.22	122.83	119.70
36	1	1381	A	C4-C5-C6	5.22	119.61	117.00
36	1	1939	G	C8-N9-C1'	-5.22	120.21	127.00
1	6	1715	G	C4-N9-C1'	5.22	133.29	126.50
36	5	1445	U	C2-N3-C4	-5.22	123.87	127.00
1	2	426	G	N3-C4-N9	5.22	129.13	126.00
36	1	1371	G	C2-N3-C4	-5.22	109.29	111.90
36	1	2422	C	C2-N3-C4	-5.22	117.29	119.90
36	5	190	U	N1-C2-O2	5.22	126.45	122.80
36	5	1183	C	C5-C6-N1	-5.22	118.39	121.00
36	5	1891	A	N1-C6-N6	5.22	121.73	118.60
36	5	3017	A	C2-N3-C4	-5.22	107.99	110.60
37	7	101	G	C5-N7-C8	-5.22	101.69	104.30
36	1	1152	G	N3-C4-N9	5.22	129.13	126.00
36	1	1603	A	C8-N9-C4	-5.22	103.71	105.80
36	1	2143	A	C4-C5-N7	5.22	113.31	110.70
36	1	2808	A	N1-C6-N6	5.22	121.73	118.60
38	4	93	U	C2-N1-C1'	-5.22	111.44	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1798	U	C5-C6-N1	5.22	125.31	122.70
36	5	34	A	OP2-P-O3'	5.22	116.69	105.20
36	5	3301	U	C5-C6-N1	-5.22	120.09	122.70
36	1	2423	U	C5-C6-N1	5.22	125.31	122.70
36	5	1477	A	C6-N1-C2	-5.22	115.47	118.60
36	5	1917	C	C2-N1-C1'	-5.22	113.06	118.80
36	5	2870	C	C2-N1-C1'	-5.22	113.06	118.80
1	2	970	A	C4-C5-N7	5.22	113.31	110.70
1	2	1614	A	N1-C6-N6	5.22	121.73	118.60
36	1	1882	G	C5-C6-O6	-5.22	125.47	128.60
36	1	2752	U	C5-C4-O4	5.22	129.03	125.90
38	4	101	U	C6-N1-C2	-5.22	117.87	121.00
1	6	438	A	O5'-P-OP1	-5.22	101.00	105.70
1	6	1458	G	C4-N9-C1'	5.22	133.28	126.50
36	5	1352	A	OP1-P-O3'	5.22	116.67	105.20
36	5	1359	C	C6-N1-C2	5.22	122.39	120.30
36	5	2852	C	C6-N1-C2	5.22	122.39	120.30
36	1	1097	G	P-O3'-C3'	5.21	125.96	119.70
36	1	2138	A	C8-N9-C4	-5.21	103.71	105.80
36	1	2386	A	C8-N9-C4	-5.21	103.72	105.80
1	6	576	G	C5-C6-O6	-5.21	125.47	128.60
36	5	1368	U	N3-C4-O4	5.21	123.05	119.40
36	5	1404	G	N9-C4-C5	-5.21	103.31	105.40
1	2	278	U	N3-C2-O2	-5.21	118.55	122.20
36	1	1498	A	C6-N1-C2	-5.21	115.47	118.60
36	5	2832	C	C5-C6-N1	-5.21	118.39	121.00
1	2	559	C	C5-C6-N1	5.21	123.61	121.00
36	1	1296	C	N1-C2-O2	-5.21	115.77	118.90
1	6	1537	C	N1-C2-O2	-5.21	115.77	118.90
36	5	400	G	C6-C5-N7	5.21	133.53	130.40
36	5	1900	A	N9-C4-C5	-5.21	103.72	105.80
36	5	2801	A	O4'-C1'-N9	5.21	112.37	108.20
1	2	553	G	C5-N7-C8	-5.21	101.70	104.30
1	2	1555	A	C8-N9-C4	-5.21	103.72	105.80
36	1	222	A	N9-C4-C5	-5.21	103.72	105.80
36	1	2913	C	N3-C2-O2	-5.21	118.25	121.90
36	5	2836	C	N3-C4-C5	-5.21	119.82	121.90
1	2	89	G	O5'-P-OP1	-5.21	101.01	105.70
1	2	1082	C	C5-C6-N1	5.21	123.60	121.00
36	1	2612	U	C2-N1-C1'	-5.21	111.45	117.70
36	1	3118	C	C6-N1-C2	-5.21	118.22	120.30
36	1	3242	G	C6-C5-N7	5.21	133.52	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	311	U	N3-C2-O2	-5.21	118.56	122.20
36	5	718	G	C4-C5-C6	5.21	121.92	118.80
36	5	1367	G	C8-N9-C1'	-5.21	120.23	127.00
36	5	2167	A	N3-C4-C5	-5.21	123.16	126.80
36	5	2649	A	C2-N3-C4	5.21	113.20	110.60
36	5	2805	G	C6-C5-N7	-5.21	127.28	130.40
36	5	3028	G	N3-C4-N9	5.21	129.12	126.00
36	1	1149	G	C4-C5-N7	-5.21	108.72	110.80
1	6	44	U	N3-C2-O2	5.21	125.84	122.20
1	6	1120	U	N3-C2-O2	-5.21	118.56	122.20
36	5	1480	G	O4'-C1'-N9	5.21	112.36	108.20
1	2	1275	A	C4-C5-C6	5.20	119.60	117.00
36	1	1394	A	N3-C4-C5	5.20	130.44	126.80
36	1	2387	A	C8-N9-C4	5.20	107.88	105.80
36	1	2808	A	C5-N7-C8	-5.20	101.30	103.90
1	6	610	G	N3-C4-N9	5.20	129.12	126.00
1	6	1437	U	C5-C6-N1	-5.20	120.10	122.70
36	5	1321	G	C2-N3-C4	-5.20	109.30	111.90
36	1	1501	U	C6-N1-C2	5.20	124.12	121.00
36	5	757	C	C5-C6-N1	-5.20	118.40	121.00
36	5	1881	A	C6-N1-C2	-5.20	115.48	118.60
36	5	2761	G	C6-N1-C2	-5.20	121.98	125.10
38	8	114	G	N1-C6-O6	5.20	123.02	119.90
1	2	822	U	C5-C6-N1	5.20	125.30	122.70
36	1	1724	U	OP1-P-O3'	5.20	116.64	105.20
36	1	3093	C	C2-N1-C1'	-5.20	113.08	118.80
1	6	913	G	C5-C6-O6	-5.20	125.48	128.60
36	5	651	G	C4-N9-C1'	5.20	133.26	126.50
36	5	1377	G	C5-N7-C8	5.20	106.90	104.30
36	5	2601	A	C8-N9-C4	5.20	107.88	105.80
36	5	2757	U	N3-C4-O4	5.20	123.04	119.40
36	5	2759	U	C6-N1-C2	-5.20	117.88	121.00
1	2	1473	U	N1-C2-O2	5.20	126.44	122.80
1	2	1600	A	P-O3'-C3'	5.20	125.94	119.70
36	1	1411	C	OP1-P-O3'	5.20	116.64	105.20
36	1	2101	C	P-O3'-C3'	5.20	125.94	119.70
36	5	1913	A	N1-C6-N6	5.20	121.72	118.60
36	5	3099	C	N1-C2-O2	-5.20	115.78	118.90
36	1	2801	A	OP1-P-O3'	5.20	116.63	105.20
1	2	1616	G	C6-C5-N7	-5.20	127.28	130.40
36	1	940	G	C6-C5-N7	5.20	133.52	130.40
36	1	1178	G	N3-C4-N9	5.20	129.12	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1888	U	C2-N3-C4	-5.20	123.88	127.00
36	1	1912	U	C5-C4-O4	5.20	129.02	125.90
36	5	1185	C	N3-C4-N4	5.20	121.64	118.00
36	5	1878	G	C8-N9-C1'	-5.20	120.25	127.00
36	5	2705	A	N9-C4-C5	-5.20	103.72	105.80
36	5	2816	G	N9-C4-C5	-5.20	103.32	105.40
36	5	2924	U	C6-N1-C2	5.20	124.12	121.00
1	2	974	A	C8-N9-C4	5.19	107.88	105.80
1	2	1639	C	N3-C4-N4	5.19	121.64	118.00
36	1	993	G	N3-C4-N9	5.19	129.12	126.00
36	1	2812	C	OP2-P-O3'	5.19	116.63	105.20
37	3	92	A	C2-N3-C4	-5.19	108.00	110.60
36	5	50	U	N3-C2-O2	-5.19	118.56	122.20
36	5	2361	A	OP2-P-O3'	5.19	116.63	105.20
36	1	806	A	C8-N9-C4	5.19	107.88	105.80
36	1	1851	G	N1-C6-O6	5.19	123.02	119.90
1	6	1150	G	C4-N9-C1'	-5.19	119.75	126.50
36	5	1203	A	N1-C6-N6	5.19	121.72	118.60
36	1	70	A	O5'-P-OP2	5.19	116.93	110.70
36	1	1847	A	N1-C2-N3	5.19	131.90	129.30
36	1	1853	U	N3-C4-O4	-5.19	115.77	119.40
1	6	139	C	N3-C4-C5	5.19	123.98	121.90
1	6	1629	G	OP2-P-O3'	5.19	116.62	105.20
36	5	110	G	N7-C8-N9	-5.19	110.50	113.10
36	5	1450	G	C5-N7-C8	-5.19	101.70	104.30
36	5	2728	G	O4'-C1'-N9	5.19	112.35	108.20
36	1	2434	U	C5-C6-N1	-5.19	120.11	122.70
36	5	209	A	N1-C2-N3	5.19	131.90	129.30
36	5	523	A	C4-C5-N7	-5.19	108.11	110.70
36	5	2761	G	C8-N9-C1'	5.19	133.75	127.00
36	5	2821	C	N1-C2-O2	5.19	122.01	118.90
36	5	3192	U	C2-N1-C1'	-5.19	111.47	117.70
37	7	5	G	N3-C4-C5	5.19	131.19	128.60
1	2	56	U	N1-C2-O2	5.19	126.43	122.80
36	1	196	G	O5'-P-OP1	-5.19	101.03	105.70
36	1	645	A	N1-C2-N3	5.19	131.89	129.30
36	1	652	G	N1-C2-N2	-5.19	111.53	116.20
36	1	3005	A	OP1-P-OP2	5.19	127.38	119.60
36	5	2274	U	C5-C6-N1	5.19	125.29	122.70
36	5	2697	A	N1-C6-N6	5.19	121.71	118.60
36	5	2980	U	N1-C2-N3	5.19	118.01	114.90
36	5	3283	U	O4'-C1'-N1	5.19	112.35	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1184	A	N1-C6-N6	5.19	121.71	118.60
36	1	965	A	N7-C8-N9	5.19	116.39	113.80
36	1	1449	A	N1-C6-N6	-5.19	115.49	118.60
41	14	339	LEU	CA-CB-CG	5.19	127.23	115.30
36	1	890	C	N3-C2-O2	-5.18	118.27	121.90
36	1	1001	G	C4-C5-N7	5.18	112.87	110.80
36	1	2201	G	C6-C5-N7	-5.18	127.29	130.40
36	1	2679	A	O4'-C1'-N9	5.18	112.35	108.20
38	4	40	A	N3-C4-N9	5.18	131.55	127.40
38	4	58	G	C6-C5-N7	-5.18	127.29	130.40
1	6	297	U	N1-C2-O2	5.18	126.43	122.80
1	6	1569	A	C4-N9-C1'	5.18	135.63	126.30
36	5	1011	A	C8-N9-C4	-5.18	103.73	105.80
36	5	1114	U	O5'-P-OP2	-5.18	101.03	105.70
36	5	1137	C	N1-C2-O2	5.18	122.01	118.90
36	1	3011	A	N7-C8-N9	-5.18	111.21	113.80
36	1	3375	A	N1-C6-N6	-5.18	115.49	118.60
36	5	878	G	C8-N9-C4	-5.18	104.33	106.40
36	5	2353	G	C6-C5-N7	-5.18	127.29	130.40
36	5	2639	G	C8-N9-C4	-5.18	104.33	106.40
37	7	67	G	N1-C6-O6	5.18	123.01	119.90
1	2	768	C	N3-C4-C5	-5.18	119.83	121.90
1	6	17	C	N3-C2-O2	-5.18	118.27	121.90
36	5	436	A	N7-C8-N9	5.18	116.39	113.80
36	5	1190	A	O4'-C1'-N9	-5.18	104.06	108.20
38	8	25	G	OP2-P-O3'	-5.18	93.80	105.20
1	2	1600	A	OP1-P-O3'	5.18	116.59	105.20
36	1	928	C	N3-C2-O2	-5.18	118.27	121.90
36	1	1748	G	N1-C6-O6	5.18	123.01	119.90
36	1	3178	A	C8-N9-C4	5.18	107.87	105.80
36	1	3203	U	OP2-P-O3'	5.18	116.60	105.20
36	5	1417	G	C6-C5-N7	-5.18	127.29	130.40
36	5	3063	C	N1-C2-O2	-5.18	115.79	118.90
1	2	1745	G	C5-C6-O6	-5.18	125.49	128.60
36	5	842	G	C6-C5-N7	-5.18	127.29	130.40
36	5	2344	U	C5-C6-N1	-5.18	120.11	122.70
36	5	2709	C	C2-N3-C4	-5.18	117.31	119.90
36	5	3326	G	N1-C6-O6	5.18	123.01	119.90
1	2	543	C	N3-C2-O2	-5.18	118.28	121.90
36	1	1902	G	C4-C5-N7	5.18	112.87	110.80
36	1	2896	A	C2-N3-C4	-5.18	108.01	110.60
36	1	2984	C	C5-C4-N4	5.18	123.82	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	39	A	N9-C4-C5	5.18	107.87	105.80
1	6	384	G	N3-C4-C5	5.18	131.19	128.60
36	5	413	U	C5-C4-O4	-5.18	122.80	125.90
36	5	645	A	C8-N9-C4	-5.18	103.73	105.80
36	5	2281	A	C4-C5-N7	5.18	113.29	110.70
1	2	1596	C	N3-C2-O2	-5.17	118.28	121.90
36	1	1008	U	C6-N1-C2	5.17	124.11	121.00
36	1	1367	G	C8-N9-C1'	-5.17	120.27	127.00
1	6	467	G	N9-C4-C5	-5.17	103.33	105.40
36	5	1392	G	N7-C8-N9	-5.17	110.51	113.10
36	5	1903	U	N3-C4-C5	-5.17	111.50	114.60
36	5	2334	U	N3-C2-O2	-5.17	118.58	122.20
36	5	2878	G	OP1-P-OP2	-5.17	111.84	119.60
36	5	3009	G	C8-N9-C4	-5.17	104.33	106.40
36	5	3197	G	N3-C4-N9	-5.17	122.89	126.00
36	1	426	G	C8-N9-C4	-5.17	104.33	106.40
37	3	33	U	C2-N1-C1'	5.17	123.91	117.70
1	2	1615	C	P-O3'-C3'	5.17	125.91	119.70
36	1	222	A	O5'-P-OP2	-5.17	101.05	105.70
36	1	650	C	C6-N1-C2	5.17	122.37	120.30
36	1	1908	A	C6-C5-N7	-5.17	128.68	132.30
36	1	3144	G	N1-C6-O6	5.17	123.00	119.90
36	5	661	G	C4-N9-C1'	5.17	133.22	126.50
36	5	680	G	C4-N9-C1'	-5.17	119.78	126.50
36	5	934	G	N3-C4-C5	-5.17	126.01	128.60
36	5	1049	C	N3-C4-C5	-5.17	119.83	121.90
36	5	1107	C	C5-C6-N1	-5.17	118.41	121.00
36	5	1184	A	C8-N9-C4	5.17	107.87	105.80
36	5	1783	U	C5-C4-O4	5.17	129.00	125.90
36	5	3183	A	N1-C6-N6	-5.17	115.50	118.60
36	1	285	A	C2-N3-C4	-5.17	108.02	110.60
36	1	1113	G	C4-C5-N7	5.17	112.87	110.80
36	1	1379	G	C2-N3-C4	-5.17	109.31	111.90
1	2	576	G	N3-C4-C5	5.17	131.18	128.60
36	1	233	C	C5-C6-N1	-5.17	118.42	121.00
36	1	329	U	C2-N1-C1'	5.17	123.90	117.70
36	1	917	A	N9-C4-C5	5.17	107.87	105.80
36	1	1381	A	C6-C5-N7	-5.17	128.68	132.30
36	1	1394	A	C8-N9-C4	5.17	107.87	105.80
36	5	637	C	C4-C5-C6	-5.17	114.82	117.40
36	5	1159	A	N3-C4-N9	-5.17	123.27	127.40
36	1	170	G	O5'-P-OP1	-5.17	101.05	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	639	G	N9-C1'-C2'	-5.17	106.32	112.00
36	1	897	U	N3-C4-O4	-5.17	115.78	119.40
36	1	933	A	C4-C5-N7	5.17	113.28	110.70
36	1	1929	G	N3-C2-N2	5.17	123.52	119.90
1	6	1455	G	N1-C6-O6	5.17	123.00	119.90
36	5	406	G	O4'-C1'-N9	5.17	112.33	108.20
36	5	1794	G	N3-C4-C5	5.17	131.18	128.60
36	5	2379	U	C4-C5-C6	5.17	122.80	119.70
36	5	2978	U	C5-C6-N1	-5.17	120.12	122.70
36	5	3109	G	C5-N7-C8	-5.17	101.72	104.30
1	2	1428	G	O5'-P-OP1	-5.17	101.05	105.70
36	1	906	A	C6-C5-N7	-5.17	128.68	132.30
36	1	1301	A	C8-N9-C4	-5.17	103.73	105.80
1	6	76	A	OP1-P-O3'	5.17	116.56	105.20
36	5	1607	U	OP1-P-O3'	5.17	116.56	105.20
36	5	2211	U	C5-C4-O4	5.17	129.00	125.90
36	5	2641	U	C4-C5-C6	5.17	122.80	119.70
36	5	3330	A	C8-N9-C4	-5.17	103.73	105.80
38	8	16	G	O5'-P-OP1	-5.17	101.05	105.70
1	2	4	C	C6-N1-C2	-5.16	118.23	120.30
35	SM	134	ASP	CB-CG-OD2	5.16	122.95	118.30
36	1	699	A	N1-C2-N3	5.16	131.88	129.30
36	1	1643	A	N1-C6-N6	5.16	121.70	118.60
36	1	2148	U	O5'-P-OP2	5.16	116.90	110.70
36	1	2806	U	N1-C2-O2	-5.16	119.19	122.80
1	6	901	G	N9-C4-C5	-5.16	103.33	105.40
1	6	1187	U	C5-C6-N1	5.16	125.28	122.70
36	5	513	G	C4-C5-N7	-5.16	108.73	110.80
36	5	937	G	N3-C4-N9	5.16	129.10	126.00
36	1	498	A	C4-C5-C6	5.16	119.58	117.00
36	1	2622	C	N3-C4-C5	-5.16	119.83	121.90
36	1	3242	G	C8-N9-C1'	5.16	133.71	127.00
36	5	709	A	C5-C6-N6	-5.16	119.57	123.70
36	1	2306	C	C6-N1-C1'	-5.16	114.61	120.80
36	1	2612	U	C5-C6-N1	-5.16	120.12	122.70
1	6	1697	G	C2-N3-C4	5.16	114.48	111.90
36	5	917	A	C5-N7-C8	-5.16	101.32	103.90
36	5	1661	G	C5-C6-O6	-5.16	125.50	128.60
36	5	2310	U	N3-C2-O2	-5.16	118.59	122.20
36	5	3289	G	C8-N9-C4	-5.16	104.34	106.40
36	1	2245	C	C5-C6-N1	5.16	123.58	121.00
36	1	2283	G	C5-C6-O6	-5.16	125.50	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	75	G	C8-N9-C1'	-5.16	120.29	127.00
36	5	716	A	N9-C4-C5	-5.16	103.74	105.80
36	5	1852	G	C8-N9-C4	-5.16	104.34	106.40
36	1	123	A	C6-C5-N7	-5.16	128.69	132.30
1	6	217	A	P-O3'-C3'	5.16	125.89	119.70
1	6	1793	G	N1-C6-O6	-5.16	116.81	119.90
36	5	297	G	O4'-C1'-N9	5.16	112.33	108.20
36	5	1151	U	N3-C4-O4	5.16	123.01	119.40
36	5	1839	A	N7-C8-N9	-5.16	111.22	113.80
36	1	961	C	O4'-C1'-N1	-5.15	104.08	108.20
1	6	155	U	N3-C2-O2	-5.15	118.59	122.20
36	5	359	U	C5-C6-N1	5.15	125.28	122.70
36	5	979	U	O4'-C1'-N1	5.15	112.32	108.20
46	19	176	LEU	CA-CB-CG	-5.15	103.45	115.30
1	2	937	C	N1-C2-O2	5.15	121.99	118.90
36	1	2631	U	C2-N3-C4	-5.15	123.91	127.00
36	5	1832	C	C2-N1-C1'	-5.15	113.13	118.80
36	5	2316	G	N3-C4-N9	5.15	129.09	126.00
36	5	2351	U	N3-C4-O4	-5.15	115.79	119.40
37	7	87	G	C5-C6-N1	-5.15	108.92	111.50
78	q2	104	LEU	CA-CB-CG	5.15	127.15	115.30
36	1	199	A	O4'-C1'-N9	5.15	112.32	108.20
36	1	676	G	N1-C2-N2	-5.15	111.57	116.20
36	1	1103	A	N9-C4-C5	-5.15	103.74	105.80
1	2	599	A	OP2-P-O3'	5.15	116.53	105.20
36	1	335	G	C8-N9-C1'	5.15	133.69	127.00
36	1	908	G	N9-C4-C5	-5.15	103.34	105.40
36	1	914	A	C5-N7-C8	5.15	106.47	103.90
36	1	2427	U	N3-C2-O2	-5.15	118.60	122.20
36	1	2627	C	C5-C6-N1	-5.15	118.43	121.00
36	1	2848	G	OP2-P-O3'	5.15	116.53	105.20
37	3	98	C	N1-C2-O2	-5.15	115.81	118.90
38	4	27	U	N1-C2-O2	5.15	126.40	122.80
1	6	470	A	C8-N9-C4	-5.15	103.74	105.80
36	5	1101	G	C8-N9-C4	5.15	108.46	106.40
36	5	1368	U	O5'-P-OP1	-5.15	101.07	105.70
36	5	2973	G	C8-N9-C4	-5.15	104.34	106.40
36	5	3028	G	C6-C5-N7	-5.15	127.31	130.40
36	5	2807	U	N3-C4-O4	5.15	123.00	119.40
36	1	2261	G	C4-N9-C1'	5.14	133.19	126.50
1	6	6	G	O5'-P-OP1	-5.14	101.07	105.70
1	6	209	U	N1-C2-O2	-5.14	119.20	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	411	U	O5'-P-OP2	-5.14	101.07	105.70
36	5	991	G	C5-C6-O6	5.14	131.69	128.60
36	5	2195	C	C5-C4-N4	-5.14	116.60	120.20
36	5	2777	G	C8-N9-C1'	5.14	133.69	127.00
36	5	2982	A	C2-N3-C4	5.14	113.17	110.60
36	1	309	U	N3-C2-O2	-5.14	118.60	122.20
36	1	722	G	C2-N3-C4	-5.14	109.33	111.90
36	1	775	A	C2-N3-C4	-5.14	108.03	110.60
36	1	1889	G	C6-C5-N7	-5.14	127.31	130.40
36	1	2747	A	N9-C4-C5	5.14	107.86	105.80
36	1	2918	G	C4-N9-C1'	5.14	133.19	126.50
1	6	337	G	N3-C2-N2	5.14	123.50	119.90
36	5	1744	G	C6-C5-N7	-5.14	127.31	130.40
36	1	2632	G	C6-C5-N7	-5.14	127.31	130.40
36	1	49	A	C2-N3-C4	-5.14	108.03	110.60
36	1	934	G	C5-C6-O6	-5.14	125.52	128.60
36	1	2531	C	C2-N1-C1'	5.14	124.45	118.80
36	1	2595	A	O4'-C1'-N9	5.14	112.31	108.20
1	6	1662	G	O5'-P-OP2	-5.14	101.07	105.70
36	5	712	G	O5'-P-OP2	-5.14	101.08	105.70
36	5	1359	C	C5-C6-N1	-5.14	118.43	121.00
36	5	1406	A	N9-C4-C5	5.14	107.86	105.80
36	5	2855	U	N1-C2-N3	5.14	117.98	114.90
37	7	8	G	N1-C2-N2	-5.14	111.57	116.20
36	5	967	A	N9-C4-C5	5.14	107.86	105.80
36	5	2938	G	C8-N9-C4	-5.14	104.34	106.40
36	1	780	A	C4-C5-C6	5.14	119.57	117.00
36	1	923	C	C6-N1-C2	5.14	122.35	120.30
36	1	1492	G	N9-C4-C5	-5.14	103.34	105.40
1	6	1297	G	N1-C6-O6	-5.14	116.82	119.90
36	5	22	G	N1-C6-O6	5.14	122.98	119.90
36	5	2322	C	N3-C4-N4	5.14	121.60	118.00
36	1	62	A	O5'-P-OP1	5.13	116.86	110.70
36	1	3173	G	C4-N9-C1'	5.13	133.18	126.50
1	6	1016	C	C6-N1-C2	-5.13	118.25	120.30
1	6	1481	C	N1-C2-O2	5.13	121.98	118.90
36	5	1049	C	C6-N1-C2	-5.13	118.25	120.30
36	5	2885	C	N3-C4-N4	5.13	121.59	118.00
36	5	3122	A	O5'-P-OP1	-5.13	101.08	105.70
1	2	1611	A	N1-C2-N3	5.13	131.87	129.30
36	1	860	G	N3-C2-N2	-5.13	116.31	119.90
36	1	1581	C	C2-N1-C1'	5.13	124.45	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	N5	115	ARG	NE-CZ-NH1	5.13	122.87	120.30
36	5	2282	U	N3-C2-O2	5.13	125.79	122.20
36	1	2905	U	N3-C2-O2	5.13	125.79	122.20
36	1	3178	A	N1-C6-N6	5.13	121.68	118.60
1	6	976	G	C6-C5-N7	-5.13	127.32	130.40
1	6	1081	A	O4'-C1'-N9	5.13	112.31	108.20
5	s3	161	GLY	N-CA-C	5.13	125.93	113.10
36	1	2261	G	C8-N9-C1'	-5.13	120.33	127.00
36	1	2363	A	C5-C6-N1	-5.13	115.14	117.70
36	1	2370	G	C4-C5-N7	-5.13	108.75	110.80
36	5	2183	A	C8-N9-C4	5.13	107.85	105.80
36	5	2303	A	C5-C6-N6	-5.13	119.60	123.70
1	2	1284	C	N1-C2-O2	5.13	121.98	118.90
36	1	110	G	C6-C5-N7	-5.13	127.32	130.40
36	1	340	C	N3-C2-O2	-5.13	118.31	121.90
36	1	698	U	C6-N1-C1'	5.13	128.38	121.20
1	6	477	A	N1-C6-N6	5.13	121.68	118.60
36	5	995	U	C5-C6-N1	-5.13	120.14	122.70
36	5	1500	G	C5-C6-O6	-5.13	125.52	128.60
36	1	725	G	C5-C6-O6	-5.13	125.52	128.60
36	1	757	C	N1-C2-O2	-5.13	115.82	118.90
36	1	2911	A	N1-C6-N6	-5.13	115.52	118.60
1	6	647	G	N3-C4-N9	-5.13	122.92	126.00
1	6	1036	A	O5'-P-OP2	-5.13	101.09	105.70
1	6	1146	G	N1-C6-O6	5.13	122.97	119.90
1	6	1663	G	C8-N9-C4	-5.13	104.35	106.40
36	5	2526	C	N1-C2-O2	5.13	121.98	118.90
36	5	3294	A	N1-C2-N3	5.13	131.86	129.30
36	5	3362	A	C4-C5-N7	5.13	113.26	110.70
13	C1	90	TYR	CA-CB-CG	5.12	123.14	113.40
36	1	1912	U	N3-C4-C5	-5.12	111.53	114.60
38	4	95	G	N3-C4-C5	5.12	131.16	128.60
1	6	539	G	O4'-C1'-N9	-5.12	104.10	108.20
1	6	1028	C	N3-C4-C5	5.12	123.95	121.90
36	5	1213	G	C5-C6-N1	5.12	114.06	111.50
1	2	1778	G	C4-C5-N7	5.12	112.85	110.80
36	1	780	A	C6-C5-N7	-5.12	128.71	132.30
36	1	1154	A	O5'-P-OP1	-5.12	101.09	105.70
41	L4	57	GLY	N-CA-C	-5.12	100.29	113.10
1	2	1127	G	C5-C6-N1	-5.12	108.94	111.50
36	1	947	G	C4-N9-C1'	5.12	133.16	126.50
36	1	2610	G	C6-C5-N7	-5.12	127.33	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3155	U	N1-C2-O2	5.12	126.39	122.80
36	5	1115	G	C6-C5-N7	-5.12	127.33	130.40
36	5	1317	A	C8-N9-C4	-5.12	103.75	105.80
36	5	1927	G	N3-C4-N9	5.12	129.07	126.00
36	1	404	G	C8-N9-C4	-5.12	104.35	106.40
36	5	2141	U	N1-C2-N3	5.12	117.97	114.90
36	5	2413	A	N7-C8-N9	-5.12	111.24	113.80
36	1	99	A	C5'-C4'-O4'	5.12	115.24	109.10
36	1	880	G	N1-C6-O6	-5.12	116.83	119.90
36	1	1404	G	C5-C6-O6	5.12	131.67	128.60
36	1	1556	C	N3-C2-O2	-5.12	118.32	121.90
36	1	2858	U	C5-C4-O4	5.12	128.97	125.90
49	M3	67	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	6	275	C	C2-N1-C1'	5.12	124.43	118.80
36	5	728	G	C8-N9-C1'	-5.12	120.35	127.00
36	5	895	A	C2-N3-C4	-5.12	108.04	110.60
36	5	1147	G	N7-C8-N9	5.12	115.66	113.10
36	5	1178	G	C5-C6-N1	-5.12	108.94	111.50
36	5	1620	U	N3-C2-O2	-5.12	118.62	122.20
36	5	2385	G	C8-N9-C4	5.12	108.45	106.40
36	5	2675	C	C6-N1-C2	-5.12	118.25	120.30
36	1	2209	U	C5-C6-N1	5.12	125.26	122.70
36	5	661	G	O5'-P-OP1	-5.12	101.09	105.70
36	5	1853	U	N1-C2-O2	-5.12	119.22	122.80
36	5	2794	G	N9-C4-C5	-5.12	103.35	105.40
36	5	2885	C	N3-C2-O2	5.12	125.48	121.90
36	1	18	G	N3-C4-C5	5.12	131.16	128.60
36	1	517	G	N1-C6-O6	-5.12	116.83	119.90
36	1	637	C	C2-N1-C1'	5.12	124.43	118.80
36	1	1321	G	O4'-C1'-N9	5.12	112.29	108.20
36	1	1375	G	C6-C5-N7	-5.12	127.33	130.40
36	1	1694	U	N3-C2-O2	-5.12	118.62	122.20
36	1	2727	A	C5-N7-C8	5.12	106.46	103.90
36	1	2828	G	C8-N9-C1'	-5.12	120.35	127.00
38	4	7	U	N1-C2-O2	-5.12	119.22	122.80
38	4	66	A	N7-C8-N9	5.12	116.36	113.80
36	5	938	C	C5-C4-N4	-5.12	116.62	120.20
36	5	1342	C	C2-N3-C4	-5.12	117.34	119.90
36	5	2994	A	C5-C6-N1	5.12	120.26	117.70
36	1	1010	G	N1-C6-O6	5.11	122.97	119.90
36	1	2807	U	C5-C6-N1	5.11	125.26	122.70
1	6	116	U	N1-C2-N3	5.11	117.97	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	609	G	O5'-P-OP2	-5.11	101.10	105.70
36	5	1119	C	OP2-P-O3'	5.11	116.45	105.20
36	5	1432	C	C6-N1-C2	-5.11	118.25	120.30
36	5	2672	G	C5-C6-O6	-5.11	125.53	128.60
53	m7	41	LEU	CA-CB-CG	5.11	127.06	115.30
1	2	75	U	N3-C2-O2	-5.11	118.62	122.20
36	1	2524	A	O4'-C1'-N9	5.11	112.29	108.20
1	6	25	C	OP2-P-O3'	5.11	116.45	105.20
1	6	39	A	O4'-C1'-N9	5.11	112.29	108.20
36	5	437	G	N7-C8-N9	5.11	115.66	113.10
36	5	2237	C	C6-N1-C2	5.11	122.34	120.30
36	5	3030	G	O5'-P-OP1	-5.11	101.10	105.70
1	2	1748	G	C2-N3-C4	-5.11	109.34	111.90
36	1	1048	A	N1-C6-N6	-5.11	115.53	118.60
36	1	1417	G	N3-C4-C5	5.11	131.16	128.60
36	1	1496	C	C2-N1-C1'	5.11	124.42	118.80
36	1	2647	A	C6-C5-N7	-5.11	128.72	132.30
36	5	1214	U	C2-N1-C1'	5.11	123.83	117.70
36	5	1548	C	N3-C2-O2	5.11	125.48	121.90
38	4	60	U	N3-C2-O2	-5.11	118.62	122.20
36	5	1902	G	N1-C2-N3	5.11	126.97	123.90
36	1	282	G	C2'-C3'-O3'	5.11	121.87	113.70
36	1	394	G	C8-N9-C1'	5.11	133.64	127.00
36	1	638	C	C6-N1-C1'	-5.11	114.67	120.80
36	1	863	C	C5-C4-N4	-5.11	116.62	120.20
36	1	1661	G	N1-C2-N2	-5.11	111.60	116.20
1	6	603	U	N3-C4-O4	5.11	122.98	119.40
1	6	1517	U	C2-N1-C1'	5.11	123.83	117.70
36	5	2145	A	N7-C8-N9	5.11	116.35	113.80
51	m5	96	ARG	NE-CZ-NH1	5.11	122.85	120.30
36	1	75	G	O5'-P-OP1	5.11	116.83	110.70
36	1	1385	C	N3-C4-C5	-5.11	119.86	121.90
36	5	87	U	C2-N1-C1'	5.11	123.83	117.70
36	5	726	G	N3-C4-C5	5.11	131.15	128.60
36	5	726	G	N3-C4-N9	-5.11	122.94	126.00
36	5	1450	G	N1-C2-N2	5.11	120.80	116.20
36	5	3098	G	N9-C4-C5	5.11	107.44	105.40
36	5	3214	U	O4'-C1'-N1	5.11	112.28	108.20
1	2	1412	G	C8-N9-C4	5.10	108.44	106.40
36	1	1472	U	N1-C2-O2	-5.10	119.23	122.80
1	6	457	G	N1-C6-O6	5.10	122.96	119.90
36	5	1667	A	C8-N9-C4	5.10	107.84	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2190	U	N1-C2-N3	5.10	117.96	114.90
1	6	1196	A	N1-C6-N6	-5.10	115.54	118.60
36	5	879	U	C5-C4-O4	-5.10	122.84	125.90
36	5	1331	U	C2-N3-C4	-5.10	123.94	127.00
36	5	1335	C	N3-C4-N4	5.10	121.57	118.00
36	5	3055	U	C5-C4-O4	-5.10	122.84	125.90
36	5	3344	A	C8-N9-C4	-5.10	103.76	105.80
37	7	37	G	C4-C5-N7	5.10	112.84	110.80
36	1	2732	G	N1-C6-O6	-5.10	116.84	119.90
36	5	1142	G	C8-N9-C4	-5.10	104.36	106.40
36	5	1375	G	OP2-P-O3'	5.10	116.42	105.20
36	5	3354	U	N3-C2-O2	-5.10	118.63	122.20
1	2	1116	A	C2-N3-C4	-5.10	108.05	110.60
36	1	968	G	C4-C5-C6	5.10	121.86	118.80
51	M5	93	LYS	N-CA-C	5.10	124.77	111.00
36	5	364	G	C5-C6-O6	-5.10	125.54	128.60
36	5	567	G	C8-N9-C1'	-5.10	120.37	127.00
36	5	2827	U	C6-N1-C1'	-5.10	114.06	121.20
36	5	3361	G	N3-C4-C5	-5.10	126.05	128.60
36	1	2354	C	N3-C4-C5	-5.10	119.86	121.90
37	3	119	U	C5-C6-N1	-5.10	120.15	122.70
38	4	105	A	C8-N9-C4	-5.10	103.76	105.80
36	5	1379	G	N3-C4-N9	5.10	129.06	126.00
36	5	3040	A	N1-C2-N3	5.10	131.85	129.30
38	4	95	G	N3-C4-N9	-5.10	122.94	126.00
36	5	2859	U	C5-C6-N1	-5.10	120.15	122.70
1	2	318	U	N3-C2-O2	5.09	125.77	122.20
36	1	189	G	N9-C4-C5	5.09	107.44	105.40
36	1	282	G	N7-C8-N9	5.09	115.65	113.10
36	1	663	C	C4-C5-C6	5.09	119.95	117.40
36	1	1400	G	C8-N9-C1'	-5.09	120.38	127.00
36	1	1404	G	C5-N7-C8	5.09	106.85	104.30
36	1	2519	A	N1-C6-N6	5.09	121.66	118.60
36	5	400	G	N3-C4-N9	-5.09	122.94	126.00
36	5	1858	A	C2-N3-C4	5.09	113.15	110.60
36	5	2123	G	N3-C4-N9	5.09	129.06	126.00
36	5	2565	U	O4'-C1'-N1	5.09	112.28	108.20
36	5	2755	C	O5'-P-OP1	-5.09	101.11	105.70
1	2	1633	A	N1-C6-N6	-5.09	115.54	118.60
36	1	1106	G	N3-C2-N2	-5.09	116.33	119.90
36	1	1307	G	N3-C2-N2	-5.09	116.33	119.90
36	1	2370	G	O5'-P-OP1	-5.09	101.12	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	349	A	C5-C6-N1	5.09	120.25	117.70
36	1	895	A	N7-C8-N9	5.09	116.35	113.80
36	1	2175	U	N3-C2-O2	-5.09	118.64	122.20
36	1	3140	G	C5-C6-O6	-5.09	125.55	128.60
51	M5	68	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	6	346	G	N3-C4-C5	-5.09	126.05	128.60
36	5	813	G	N9-C4-C5	-5.09	103.36	105.40
36	5	2928	C	N3-C4-N4	5.09	121.56	118.00
36	5	1473	G	C8-N9-C4	5.09	108.44	106.40
36	5	1546	A	C4-C5-C6	5.09	119.55	117.00
36	5	2624	G	C4-C5-N7	5.09	112.84	110.80
36	5	2695	A	O4'-C1'-N9	5.09	112.27	108.20
36	5	3096	C	N1-C2-O2	-5.09	115.85	118.90
1	2	1644	C	N3-C2-O2	-5.09	118.34	121.90
36	1	32	U	N3-C4-O4	5.09	122.96	119.40
36	1	320	G	OP2-P-O3'	5.09	116.39	105.20
36	1	1386	A	C6-C5-N7	-5.09	128.74	132.30
1	6	1595	U	N3-C4-C5	-5.09	111.55	114.60
36	5	220	G	C4-C5-N7	5.09	112.83	110.80
1	2	139	C	C6-N1-C2	-5.09	118.27	120.30
36	1	2572	C	N3-C2-O2	-5.09	118.34	121.90
36	5	1143	A	N1-C6-N6	5.09	121.65	118.60
36	5	2938	G	N1-C6-O6	5.09	122.95	119.90
36	1	1192	C	O5'-P-OP2	-5.08	101.12	105.70
36	1	3243	A	C6-C5-N7	-5.08	128.74	132.30
36	5	1838	G	N1-C6-O6	5.08	122.95	119.90
36	1	38	U	N1-C2-N3	-5.08	111.85	114.90
36	1	1364	C	OP2-P-O3'	5.08	116.38	105.20
36	5	757	C	C2-N3-C4	-5.08	117.36	119.90
36	1	2153	U	C6-N1-C2	-5.08	117.95	121.00
36	1	2309	A	C4-C5-N7	5.08	113.24	110.70
36	1	2601	A	N1-C6-N6	5.08	121.65	118.60
36	1	3121	U	OP1-P-O3'	5.08	116.38	105.20
36	5	1043	C	OP2-P-O3'	5.08	116.38	105.20
36	5	1169	A	N7-C8-N9	-5.08	111.26	113.80
36	5	3294	A	C8-N9-C4	-5.08	103.77	105.80
37	3	80	G	C4-C5-C6	5.08	121.85	118.80
1	6	614	C	N1-C2-O2	5.08	121.95	118.90
1	2	1539	G	C8-N9-C4	-5.08	104.37	106.40
1	2	1773	C	N1-C2-O2	-5.08	115.85	118.90
36	1	281	G	C8-N9-C4	-5.08	104.37	106.40
36	1	669	U	N3-C4-C5	5.08	117.65	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2549	G	N3-C4-C5	-5.08	126.06	128.60
36	5	110	G	C5-N7-C8	5.08	106.84	104.30
36	5	968	G	C4-N9-C1'	5.08	133.10	126.50
36	5	1373	A	C6-C5-N7	-5.08	128.75	132.30
36	5	2673	A	N1-C6-N6	-5.08	115.55	118.60
36	1	1012	G	C8-N9-C4	5.08	108.43	106.40
36	1	1145	G	C2-N3-C4	5.08	114.44	111.90
36	1	1844	C	N1-C2-O2	-5.08	115.85	118.90
36	1	3206	C	N1-C2-O2	5.08	121.95	118.90
36	5	574	U	C5-C6-N1	-5.08	120.16	122.70
1	2	1169	G	N1-C6-O6	-5.08	116.86	119.90
1	2	1297	G	C4-C5-N7	5.08	112.83	110.80
36	1	1190	A	C8-N9-C1'	-5.08	118.56	127.70
54	M8	140	LEU	CA-CB-CG	-5.08	103.62	115.30
36	5	999	G	N9-C4-C5	-5.08	103.37	105.40
1	2	16	G	C8-N9-C1'	-5.07	120.41	127.00
36	1	1137	C	C6-N1-C2	5.07	122.33	120.30
36	1	1307	G	C4-C5-N7	-5.07	108.77	110.80
36	1	1309	U	N3-C2-O2	-5.07	118.65	122.20
36	1	1892	G	C4-C5-N7	-5.07	108.77	110.80
36	1	3182	G	C4-C5-N7	5.07	112.83	110.80
1	6	965	U	C4-C5-C6	-5.07	116.66	119.70
36	5	692	A	O5'-P-OP1	-5.07	101.13	105.70
36	5	2198	A	C5-N7-C8	-5.07	101.36	103.90
37	7	52	G	C8-N9-C4	5.07	108.43	106.40
36	1	1581	C	N3-C2-O2	-5.07	118.35	121.90
36	5	86	G	N3-C4-N9	5.07	129.04	126.00
36	1	1515	A	N1-C6-N6	5.07	121.64	118.60
1	6	557	G	N1-C6-O6	-5.07	116.86	119.90
36	5	39	A	C5-N7-C8	-5.07	101.36	103.90
36	5	2726	C	C4-C5-C6	5.07	119.94	117.40
36	5	2748	A	C5-C6-N6	-5.07	119.64	123.70
37	3	89	G	N3-C4-N9	5.07	129.04	126.00
1	6	1130	G	N3-C4-N9	-5.07	122.96	126.00
36	5	1211	U	C4-C5-C6	-5.07	116.66	119.70
36	5	2908	G	N3-C4-N9	-5.07	122.96	126.00
1	2	913	G	P-O3'-C3'	5.07	125.78	119.70
1	2	1600	A	C5-N7-C8	-5.07	101.37	103.90
36	1	614	C	C6-N1-C2	5.07	122.33	120.30
36	1	941	G	C6-C5-N7	-5.07	127.36	130.40
36	1	1939	G	N3-C4-C5	-5.07	126.07	128.60
36	1	2257	C	O4'-C1'-N1	5.07	112.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2311	G	N9-C4-C5	5.07	107.43	105.40
36	1	2937	G	N7-C8-N9	-5.07	110.57	113.10
36	1	3173	G	C8-N9-C1'	-5.07	120.41	127.00
36	1	3375	A	C5'-C4'-C3'	-5.07	107.89	116.00
1	6	7	G	N3-C4-C5	-5.07	126.07	128.60
1	6	359	A	N3-C4-N9	-5.07	123.35	127.40
36	5	991	G	C4-C5-N7	-5.07	108.77	110.80
36	5	1193	A	C4-C5-C6	5.07	119.53	117.00
36	5	1306	G	N7-C8-N9	5.07	115.63	113.10
36	1	2400	G	OP2-P-O3'	5.07	116.35	105.20
36	1	2683	U	C5-C6-N1	-5.07	120.17	122.70
37	3	58	C	N3-C2-O2	-5.07	118.35	121.90
1	6	985	G	C2-N3-C4	-5.07	109.37	111.90
36	5	396	A	C5-C6-N1	-5.07	115.17	117.70
36	5	1177	G	N9-C4-C5	5.07	107.43	105.40
36	5	3315	G	N1-C2-N3	5.07	126.94	123.90
36	1	1119	C	C2-N1-C1'	-5.06	113.23	118.80
36	1	1389	G	C8-N9-C4	5.06	108.43	106.40
36	1	3277	U	N1-C2-O2	5.06	126.34	122.80
36	5	83	U	N3-C2-O2	-5.06	118.66	122.20
36	1	1207	G	N1-C6-O6	5.06	122.94	119.90
1	6	431	C	N1-C2-O2	-5.06	115.86	118.90
36	5	1101	G	N1-C2-N2	-5.06	111.64	116.20
36	5	1507	G	N1-C2-N2	-5.06	111.64	116.20
37	7	35	C	N3-C2-O2	-5.06	118.36	121.90
36	1	634	C	C5-C6-N1	-5.06	118.47	121.00
38	4	112	U	C2-N1-C1'	-5.06	111.63	117.70
1	6	1653	C	C6-N1-C2	-5.06	118.28	120.30
36	5	2932	U	O5'-P-OP2	-5.06	101.14	105.70
36	1	1587	A	N1-C6-N6	-5.06	115.56	118.60
36	1	2860	U	N3-C4-C5	5.06	117.64	114.60
36	1	3054	U	N3-C2-O2	-5.06	118.66	122.20
36	1	3243	A	N9-C4-C5	-5.06	103.78	105.80
1	6	620	A	C8-N9-C4	-5.06	103.78	105.80
1	6	1354	G	C4-N9-C1'	5.06	133.08	126.50
36	5	922	U	C2-N3-C4	-5.06	123.96	127.00
36	5	1665	C	N3-C2-O2	-5.06	118.36	121.90
36	5	3296	A	OP2-P-O3'	5.06	116.33	105.20
36	1	940	G	C5-C6-O6	5.06	131.63	128.60
36	1	2688	U	O4'-C1'-N1	-5.06	104.15	108.20
36	1	2989	U	C2-N1-C1'	5.06	123.77	117.70
38	4	52	A	C4-C5-N7	-5.06	108.17	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	96	G	OP1-P-OP2	5.06	127.19	119.60
36	5	927	C	O5'-P-OP1	-5.06	101.15	105.70
36	5	2377	G	N3-C2-N2	5.06	123.44	119.90
36	5	3247	G	C8-N9-C4	5.06	108.42	106.40
1	2	933	A	C8-N9-C4	-5.06	103.78	105.80
1	2	1778	G	N7-C8-N9	5.06	115.63	113.10
36	5	524	U	O5'-P-OP2	-5.06	101.15	105.70
36	1	1084	A	C6-C5-N7	-5.05	128.76	132.30
36	1	1401	A	C2-N3-C4	-5.05	108.07	110.60
36	1	1451	C	N1-C2-O2	5.05	121.93	118.90
36	1	1820	U	OP2-P-O3'	5.05	116.32	105.20
36	1	1851	G	N7-C8-N9	5.05	115.63	113.10
36	1	2194	G	C4-C5-N7	5.05	112.82	110.80
36	1	2415	C	C2-N1-C1'	-5.05	113.24	118.80
36	1	2897	A	C8-N9-C4	5.05	107.82	105.80
1	6	1274	C	C6-N1-C1'	-5.05	114.73	120.80
36	5	331	G	O5'-P-OP1	-5.05	101.15	105.70
36	5	666	A	C5-C6-N6	5.05	127.74	123.70
36	5	852	U	OP2-P-O3'	5.05	116.32	105.20
36	5	1370	G	N1-C6-O6	-5.05	116.87	119.90
36	5	1420	C	C2-N1-C1'	-5.05	113.24	118.80
36	5	1502	C	N1-C2-O2	5.05	121.93	118.90
1	2	9	U	O5'-P-OP1	-5.05	101.15	105.70
36	1	1157	G	C6-N1-C2	-5.05	122.07	125.10
36	1	2804	A	N1-C2-N3	5.05	131.83	129.30
36	5	1178	G	O5'-P-OP1	-5.05	101.15	105.70
36	5	1452	A	C5-N7-C8	-5.05	101.37	103.90
36	5	2195	C	N3-C4-N4	5.05	121.54	118.00
36	5	2857	C	N3-C4-C5	5.05	123.92	121.90
1	6	351	C	O4'-C1'-N1	-5.05	104.16	108.20
1	6	565	C	C2-N3-C4	-5.05	117.38	119.90
36	5	411	U	C2-N1-C1'	-5.05	111.64	117.70
36	5	691	A	OP1-P-O3'	5.05	116.31	105.20
1	2	1370	U	P-O3'-C3'	5.05	125.76	119.70
1	2	1615	C	C6-N1-C2	-5.05	118.28	120.30
36	1	2865	U	N1-C2-O2	5.05	126.33	122.80
36	1	3178	A	N9-C4-C5	-5.05	103.78	105.80
1	6	1744	A	C8-N9-C4	5.05	107.82	105.80
36	5	2374	C	O5'-P-OP2	-5.05	101.16	105.70
36	5	2888	U	C2-N1-C1'	5.05	123.76	117.70
36	1	996	A	OP2-P-O3'	5.05	116.31	105.20
36	1	1351	U	C2-N1-C1'	5.05	123.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2395	G	OP2-P-O3'	5.05	116.31	105.20
38	4	85	G	N7-C8-N9	5.05	115.62	113.10
1	6	1150	G	N3-C4-N9	-5.05	122.97	126.00
36	5	283	G	O4'-C1'-N9	-5.05	104.16	108.20
36	5	2796	G	N3-C4-C5	-5.05	126.08	128.60
36	5	2849	C	N3-C4-C5	-5.05	119.88	121.90
36	5	3164	C	C6-N1-C2	5.05	122.32	120.30
1	2	318	U	C6-N1-C2	5.05	124.03	121.00
36	1	349	A	OP2-P-O3'	5.05	116.30	105.20
36	1	1227	C	C5-C6-N1	5.05	123.52	121.00
36	1	1592	G	C5-C6-N1	-5.05	108.98	111.50
36	1	2714	G	C4-C5-C6	-5.05	115.77	118.80
1	6	344	A	C8-N9-C4	5.05	107.82	105.80
1	2	1535	U	O5'-P-OP1	5.04	116.75	110.70
36	1	304	G	N3-C2-N2	-5.04	116.37	119.90
36	1	1440	G	C8-N9-C4	5.04	108.42	106.40
36	5	523	A	N9-C4-C5	5.04	107.82	105.80
36	1	511	G	C6-C5-N7	-5.04	127.37	130.40
36	1	1198	C	N3-C4-C5	-5.04	119.88	121.90
36	1	1311	G	C4-C5-N7	5.04	112.82	110.80
36	1	1323	G	C8-N9-C4	5.04	108.42	106.40
36	1	1446	A	N9-C4-C5	5.04	107.82	105.80
36	1	2978	U	O4'-C1'-N1	5.04	112.23	108.20
1	6	20	G	N1-C6-O6	5.04	122.93	119.90
36	5	2952	G	C8-N9-C4	-5.04	104.38	106.40
36	5	3091	A	C4-C5-C6	5.04	119.52	117.00
1	2	1486	G	C4-N9-C1'	5.04	133.05	126.50
36	1	342	A	N3-C4-N9	-5.04	123.37	127.40
36	1	1850	A	O5'-P-OP2	-5.04	101.16	105.70
36	1	2989	U	C5-C6-N1	5.04	125.22	122.70
1	6	41	A	N1-C6-N6	5.04	121.62	118.60
1	6	1285	U	N1-C2-O2	5.04	126.33	122.80
1	6	1539	G	O4'-C1'-N9	-5.04	104.17	108.20
36	5	2897	A	O4'-C1'-N9	5.04	112.23	108.20
36	1	2525	G	C4-N9-C1'	5.04	133.05	126.50
1	6	2	A	N1-C6-N6	5.04	121.62	118.60
1	6	711	U	C2-N1-C1'	5.04	123.75	117.70
36	5	639	G	C6-C5-N7	-5.04	127.38	130.40
36	5	3149	G	O5'-P-OP1	5.04	116.75	110.70
1	6	154	G	C8-N9-C4	-5.04	104.39	106.40
36	5	970	A	C4-C5-N7	5.04	113.22	110.70
36	5	3085	G	C5-C6-N1	-5.04	108.98	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1052	U	N1-C2-O2	5.04	126.33	122.80
36	1	808	A	C8-N9-C4	5.04	107.81	105.80
36	1	691	A	C4-C5-C6	5.04	119.52	117.00
36	1	1143	A	N9-C4-C5	5.04	107.81	105.80
36	1	2684	C	C4-C5-C6	5.04	119.92	117.40
36	1	2989	U	C5-C4-O4	-5.04	122.88	125.90
36	5	41	G	O5'-P-OP2	-5.04	101.17	105.70
36	5	2403	G	N3-C4-N9	5.04	129.02	126.00
36	1	358	G	C2-N3-C4	-5.03	109.38	111.90
36	1	695	C	O5'-P-OP1	-5.03	101.17	105.70
36	1	936	A	C2-N3-C4	-5.03	108.08	110.60
36	1	1142	G	O5'-P-OP2	-5.03	101.17	105.70
36	1	1172	G	N1-C2-N2	5.03	120.73	116.20
36	1	1874	A	N1-C2-N3	5.03	131.82	129.30
36	1	2197	C	C6-N1-C2	5.03	122.31	120.30
36	1	2371	G	O5'-P-OP2	-5.03	101.17	105.70
36	1	2661	G	C6-C5-N7	-5.03	127.38	130.40
36	1	2687	G	C5-C6-O6	5.03	131.62	128.60
36	1	2824	G	C5-C6-N1	-5.03	108.98	111.50
36	1	2936	A	C8-N9-C4	-5.03	103.79	105.80
38	4	97	A	N1-C2-N3	5.03	131.82	129.30
1	6	530	C	C2-N1-C1'	-5.03	113.26	118.80
36	5	994	G	OP1-P-O3'	5.03	116.27	105.20
36	5	1494	U	O5'-P-OP2	5.03	116.74	110.70
36	5	2725	U	C4-C5-C6	-5.03	116.68	119.70
36	5	3164	C	N3-C4-C5	5.03	123.91	121.90
1	2	875	G	C6-C5-N7	-5.03	127.38	130.40
1	2	1412	G	N7-C8-N9	-5.03	110.58	113.10
1	2	1793	G	O4'-C1'-N9	5.03	112.23	108.20
36	1	551	A	O4'-C1'-N9	5.03	112.23	108.20
36	1	1112	A	N1-C2-N3	5.03	131.82	129.30
36	1	1518	U	C5-C6-N1	-5.03	120.18	122.70
36	1	2881	C	C2-N1-C1'	-5.03	113.27	118.80
36	1	3091	A	C5-N7-C8	-5.03	101.38	103.90
36	1	3228	C	C2-N1-C1'	5.03	124.33	118.80
37	3	105	C	C6-N1-C2	5.03	122.31	120.30
38	4	10	A	N7-C8-N9	-5.03	111.28	113.80
38	4	103	G	N3-C4-N9	5.03	129.02	126.00
36	5	339	C	C2-N1-C1'	-5.03	113.26	118.80
36	5	2322	C	C5-C6-N1	5.03	123.52	121.00
1	2	334	G	C2-N3-C4	-5.03	109.38	111.90
36	1	1544	G	N1-C6-O6	5.03	122.92	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2321	A	N9-C4-C5	5.03	107.81	105.80
36	1	2627	C	OP2-P-O3'	5.03	116.27	105.20
44	L7	110	ARG	NE-CZ-NH2	-5.03	117.78	120.30
36	5	821	U	N3-C2-O2	-5.03	118.68	122.20
36	5	1374	G	N3-C4-C5	5.03	131.12	128.60
36	5	2160	G	C8-N9-C1'	-5.03	120.46	127.00
1	6	577	G	N3-C4-C5	5.03	131.12	128.60
36	5	842	G	N9-C4-C5	-5.03	103.39	105.40
36	5	3045	G	N3-C2-N2	-5.03	116.38	119.90
36	1	2343	C	OP2-P-O3'	5.03	116.26	105.20
36	1	2857	C	N1-C2-O2	5.03	121.92	118.90
36	5	2834	G	O5'-P-OP2	-5.03	101.18	105.70
36	5	2871	G	C5-C6-N1	5.03	114.01	111.50
36	5	2891	U	N1-C2-O2	5.03	126.32	122.80
36	5	2900	A	C5-C6-N6	5.03	127.72	123.70
1	2	49	C	C6-N1-C2	-5.03	118.29	120.30
36	1	1807	G	C8-N9-C1'	-5.03	120.47	127.00
36	1	2614	G	C8-N9-C4	5.03	108.41	106.40
36	1	2918	G	C4-C5-C6	5.03	121.82	118.80
36	1	3138	U	OP2-P-O3'	5.03	116.25	105.20
52	M6	84	LEU	CB-CG-CD2	-5.03	102.46	111.00
36	5	1148	G	C5-C6-N1	5.03	114.01	111.50
36	5	1889	G	C6-C5-N7	-5.03	127.39	130.40
1	6	969	C	N1-C2-O2	-5.02	115.89	118.90
36	5	2849	C	C5-C6-N1	5.02	123.51	121.00
36	1	1896	A	N7-C8-N9	5.02	116.31	113.80
37	3	87	G	OP2-P-O3'	5.02	116.25	105.20
36	5	413	U	N3-C4-O4	5.02	122.92	119.40
36	5	607	A	C5-C6-N6	5.02	127.72	123.70
36	5	2947	G	C5-N7-C8	-5.02	101.79	104.30
36	1	647	A	C2-N3-C4	-5.02	108.09	110.60
36	5	727	G	O5'-P-OP1	-5.02	101.18	105.70
36	1	2145	A	C4-C5-C6	5.02	119.51	117.00
36	1	2585	G	C8-N9-C4	-5.02	104.39	106.40
36	5	1292	C	N3-C2-O2	5.02	125.41	121.90
36	5	2347	U	C6-N1-C2	-5.02	117.99	121.00
1	2	1554	U	N1-C2-O2	-5.02	119.29	122.80
36	1	51	A	C2-N3-C4	-5.02	108.09	110.60
36	1	86	G	C4-C5-C6	-5.02	115.79	118.80
36	1	145	G	C5-N7-C8	-5.02	101.79	104.30
36	1	709	A	C4-C5-N7	5.02	113.21	110.70
36	1	1404	G	N7-C8-N9	-5.02	110.59	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1694	U	C2-N1-C1'	5.02	123.72	117.70
36	5	2415	C	OP1-P-O3'	5.02	116.24	105.20
1	2	587	C	C2-N1-C1'	5.02	124.32	118.80
1	2	736	C	C2-N1-C1'	5.02	124.32	118.80
1	2	1479	A	N1-C6-N6	5.02	121.61	118.60
36	1	1725	C	C6-N1-C2	5.02	122.31	120.30
37	3	106	U	C5-C6-N1	5.02	125.21	122.70
36	5	658	G	C5-N7-C8	-5.02	101.79	104.30
36	5	2777	G	OP1-P-O3'	5.02	116.23	105.20
36	5	2813	A	C6-C5-N7	-5.02	128.79	132.30
36	5	2843	U	C2-N1-C1'	5.02	123.72	117.70
1	2	852	C	N1-C2-O2	5.01	121.91	118.90
36	1	766	U	C6-N1-C2	-5.01	117.99	121.00
37	3	45	A	N1-C6-N6	-5.01	115.59	118.60
1	6	1317	C	C6-N1-C2	-5.01	118.29	120.30
1	6	1696	G	P-O3'-C3'	5.01	125.72	119.70
36	5	8	C	C6-N1-C2	-5.01	118.29	120.30
36	5	912	G	OP2-P-O3'	5.01	116.23	105.20
36	5	1662	G	C6-C5-N7	-5.01	127.39	130.40
36	5	2815	G	C8-N9-C4	5.01	108.41	106.40
36	5	3337	G	C8-N9-C1'	-5.01	120.48	127.00
1	2	425	A	C5-C6-N6	-5.01	119.69	123.70
36	1	1184	A	O5'-P-OP2	-5.01	101.19	105.70
36	1	1435	A	N7-C8-N9	5.01	116.31	113.80
36	1	2610	G	C5-C6-O6	-5.01	125.59	128.60
36	5	1362	G	OP2-P-O3'	5.01	116.23	105.20
36	5	1920	U	C5-C4-O4	5.01	128.91	125.90
1	2	93	A	N7-C8-N9	5.01	116.31	113.80
1	2	163	G	C8-N9-C4	-5.01	104.39	106.40
36	1	80	G	N1-C2-N2	-5.01	111.69	116.20
36	1	1940	G	N1-C2-N3	5.01	126.91	123.90
36	1	2379	U	N3-C4-O4	5.01	122.91	119.40
36	1	2920	U	C2-N3-C4	-5.01	123.99	127.00
36	1	3134	A	N9-C4-C5	-5.01	103.80	105.80
57	N1	89	LEU	CA-CB-CG	5.01	126.83	115.30
1	6	364	G	C8-N9-C4	5.01	108.41	106.40
36	5	2321	A	OP2-P-O3'	5.01	116.23	105.20
36	5	2892	A	C2-N3-C4	-5.01	108.09	110.60
36	5	2946	A	C2-N3-C4	-5.01	108.09	110.60
36	5	3214	U	N1-C2-O2	5.01	126.31	122.80
36	5	3313	U	OP1-P-OP2	5.01	127.12	119.60
1	2	109	G	N1-C6-O6	5.01	122.91	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	636	C	C5-C6-N1	-5.01	118.50	121.00
36	1	703	G	C8-N9-C4	5.01	108.40	106.40
1	6	1127	G	C2-N3-C4	-5.01	109.40	111.90
1	6	1198	G	N3-C4-N9	-5.01	122.99	126.00
36	5	98	G	N3-C2-N2	5.01	123.41	119.90
36	5	1906	G	C4-C5-N7	5.01	112.80	110.80
36	5	2340	U	O5'-P-OP1	-5.01	101.19	105.70
36	1	2549	G	N9-C4-C5	-5.01	103.40	105.40
37	3	56	A	C8-N9-C4	5.01	107.80	105.80
38	4	27	U	N3-C2-O2	-5.01	118.69	122.20
36	5	660	A	C4-C5-N7	-5.01	108.20	110.70
1	6	96	G	OP2-P-O3'	5.01	116.21	105.20
36	5	567	G	C4-C5-C6	5.01	121.80	118.80
36	5	655	C	N1-C2-N3	5.01	122.70	119.20
36	5	1190	A	N9-C4-C5	5.01	107.80	105.80
36	5	1292	C	N3-C4-C5	5.01	123.90	121.90
36	5	3001	C	C6-N1-C2	5.01	122.30	120.30
36	1	1137	C	C5-C4-N4	-5.00	116.70	120.20
37	3	86	U	C2-N3-C4	-5.00	124.00	127.00
36	5	2627	C	N3-C4-C5	-5.00	119.90	121.90
36	5	3181	C	N1-C2-N3	5.00	122.70	119.20
36	1	1848	G	N1-C2-N2	-5.00	111.70	116.20
1	6	1725	U	C2-N1-C1'	5.00	123.70	117.70
36	5	1395	G	C6-C5-N7	-5.00	127.40	130.40
36	5	1695	U	N3-C2-O2	-5.00	118.70	122.20
36	5	2152	A	O4'-C1'-N9	5.00	112.20	108.20
36	5	2572	C	N1-C2-O2	5.00	121.90	118.90
36	5	2978	U	O4'-C1'-N1	5.00	112.20	108.20
36	5	3039	C	C6-N1-C2	-5.00	118.30	120.30
1	2	1595	U	O4'-C1'-N1	5.00	112.20	108.20
36	1	546	C	C6-N1-C2	-5.00	118.30	120.30
36	1	609	G	N3-C4-N9	5.00	129.00	126.00
36	1	1126	G	N9-C4-C5	-5.00	103.40	105.40
36	1	2647	A	O5'-P-OP2	5.00	116.70	110.70
1	6	620	A	OP2-P-O3'	5.00	116.20	105.20
1	6	913	G	N1-C6-O6	5.00	122.90	119.90
36	5	1009	A	O5'-P-OP1	5.00	116.70	110.70
36	5	3234	A	O4'-C1'-N9	5.00	112.20	108.20
36	5	3309	G	N3-C4-N9	5.00	129.00	126.00

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
18	C6	113	ASP	Peptide
19	C7	84	TYR	Peptide
27	D5	54	VAL	Peptide
27	D5	94	LYS	Peptide
33	E1	146	SER	Peptide
39	L2	19	HIS	Peptide
40	L3	248	LYS	Peptide
42	L5	257	GLU	Peptide
43	L6	17	ALA	Peptide
45	L8	30	THR	Peptide
47	M0	188	GLY	Peptide
48	M1	8	PRO	Peptide
50	M4	112	LEU	Peptide
52	M6	110	PRO	Peptide
65	N9	19	ASN	Peptide
67	O1	5	LYS	Peptide
3	S1	177	GLN	Peptide
9	S7	131	PHE	Peptide
10	S8	8	ARG	Peptide
11	S9	137	GLY	Peptide
18	c6	40	GLU	Peptide
20	c8	144	ARG	Peptide
22	d0	70	THR	Peptide
26	d4	29	HIS	Peptide
80	e0	61	SER	Peptide
39	l2	215	ASN	Peptide
40	l3	234	GLY	Peptide
44	l7	226	GLY	Peptide
48	m1	8	PRO	Peptide
56	n0	133	ALA	Peptide
56	n0	152	LEU	Peptide
64	n8	66	ALA	Peptide
69	o3	105	SER	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide
9	s7	30	SER	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	142 (70%)	37 (18%)	25 (12%)	0	4
2	s0	204/251 (81%)	150 (74%)	36 (18%)	18 (9%)	1	7
3	S1	212/254 (84%)	142 (67%)	42 (20%)	28 (13%)	0	3
3	s1	214/254 (84%)	165 (77%)	37 (17%)	12 (6%)	2	15
4	S2	215/253 (85%)	175 (81%)	23 (11%)	17 (8%)	1	9
4	s2	215/253 (85%)	169 (79%)	28 (13%)	18 (8%)	1	8
5	S3	221/239 (92%)	170 (77%)	37 (17%)	14 (6%)	1	13
5	s3	221/239 (92%)	174 (79%)	25 (11%)	22 (10%)	0	6
6	S4	258/260 (99%)	201 (78%)	43 (17%)	14 (5%)	2	16
6	s4	258/260 (99%)	206 (80%)	35 (14%)	17 (7%)	1	12
7	S5	204/224 (91%)	150 (74%)	33 (16%)	21 (10%)	0	6
7	s5	204/224 (91%)	140 (69%)	41 (20%)	23 (11%)	0	5
8	S6	224/236 (95%)	181 (81%)	33 (15%)	10 (4%)	2	20
8	s6	216/236 (92%)	172 (80%)	34 (16%)	10 (5%)	2	20
9	S7	182/189 (96%)	137 (75%)	27 (15%)	18 (10%)	0	6
9	s7	184/189 (97%)	133 (72%)	34 (18%)	17 (9%)	1	7
10	S8	184/200 (92%)	145 (79%)	29 (16%)	10 (5%)	2	16
10	s8	184/200 (92%)	149 (81%)	27 (15%)	8 (4%)	2	21
11	S9	183/196 (93%)	144 (79%)	27 (15%)	12 (7%)	1	12
11	s9	183/196 (93%)	133 (73%)	40 (22%)	10 (6%)	2	16
12	C0	94/105 (90%)	68 (72%)	19 (20%)	7 (7%)	1	10
12	c0	92/105 (88%)	68 (74%)	11 (12%)	13 (14%)	0	3
13	C1	153/155 (99%)	107 (70%)	27 (18%)	19 (12%)	0	4
13	c1	144/155 (93%)	114 (79%)	23 (16%)	7 (5%)	2	18
14	C2	122/142 (86%)	66 (54%)	39 (32%)	17 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/142 (86%)	72 (59%)	30 (25%)	20 (16%)	0	2
15	C3	148/150 (99%)	117 (79%)	24 (16%)	7 (5%)	2	19
15	c3	148/150 (99%)	107 (72%)	28 (19%)	13 (9%)	1	7
16	C4	125/136 (92%)	93 (74%)	23 (18%)	9 (7%)	1	10
16	c4	126/136 (93%)	99 (79%)	18 (14%)	9 (7%)	1	11
17	C5	122/141 (86%)	84 (69%)	24 (20%)	14 (12%)	0	5
17	c5	133/141 (94%)	92 (69%)	24 (18%)	17 (13%)	0	3
18	C6	139/142 (98%)	117 (84%)	16 (12%)	6 (4%)	2	21
18	c6	140/142 (99%)	106 (76%)	23 (16%)	11 (8%)	1	9
19	C7	116/136 (85%)	85 (73%)	18 (16%)	13 (11%)	0	5
19	c7	113/136 (83%)	84 (74%)	22 (20%)	7 (6%)	1	13
20	C8	143/145 (99%)	107 (75%)	23 (16%)	13 (9%)	1	7
20	c8	143/145 (99%)	105 (73%)	25 (18%)	13 (9%)	1	7
21	C9	141/143 (99%)	108 (77%)	27 (19%)	6 (4%)	2	21
21	c9	141/143 (99%)	114 (81%)	21 (15%)	6 (4%)	2	21
22	D0	105/120 (88%)	79 (75%)	20 (19%)	6 (6%)	1	15
22	d0	108/120 (90%)	83 (77%)	14 (13%)	11 (10%)	0	6
23	D1	85/87 (98%)	58 (68%)	19 (22%)	8 (9%)	0	7
23	d1	85/87 (98%)	68 (80%)	12 (14%)	5 (6%)	1	14
24	D2	127/129 (98%)	103 (81%)	17 (13%)	7 (6%)	2	16
24	d2	127/129 (98%)	101 (80%)	23 (18%)	3 (2%)	6	34
25	D3	142/144 (99%)	107 (75%)	22 (16%)	13 (9%)	1	7
25	d3	142/144 (99%)	115 (81%)	19 (13%)	8 (6%)	2	15
26	D4	132/134 (98%)	105 (80%)	17 (13%)	10 (8%)	1	9
26	d4	132/134 (98%)	100 (76%)	15 (11%)	17 (13%)	0	3
27	D5	68/107 (64%)	44 (65%)	14 (21%)	10 (15%)	0	2
27	d5	67/107 (63%)	47 (70%)	15 (22%)	5 (8%)	1	10
28	D6	95/97 (98%)	59 (62%)	23 (24%)	13 (14%)	0	3
28	d6	95/97 (98%)	70 (74%)	18 (19%)	7 (7%)	1	10
29	D7	79/81 (98%)	55 (70%)	18 (23%)	6 (8%)	1	9
29	d7	79/81 (98%)	53 (67%)	21 (27%)	5 (6%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	D8	61/66 (92%)	42 (69%)	14 (23%)	5 (8%)	1	8
30	d8	61/66 (92%)	43 (70%)	14 (23%)	4 (7%)	1	12
31	D9	51/55 (93%)	37 (72%)	10 (20%)	4 (8%)	1	9
31	d9	51/55 (93%)	39 (76%)	8 (16%)	4 (8%)	1	9
32	E0	58/60 (97%)	43 (74%)	10 (17%)	5 (9%)	1	8
33	E1	69/76 (91%)	32 (46%)	20 (29%)	17 (25%)	0	0
33	e1	74/76 (97%)	33 (45%)	21 (28%)	20 (27%)	0	0
34	SR	316/318 (99%)	231 (73%)	58 (18%)	27 (8%)	1	8
34	sR	316/318 (99%)	255 (81%)	49 (16%)	12 (4%)	3	24
35	SM	155/273 (57%)	99 (64%)	34 (22%)	22 (14%)	0	3
35	sM	98/273 (36%)	63 (64%)	23 (24%)	12 (12%)	0	4
39	L2	250/253 (99%)	214 (86%)	28 (11%)	8 (3%)	4	28
39	l2	250/253 (99%)	200 (80%)	32 (13%)	18 (7%)	1	10
40	L3	384/386 (100%)	324 (84%)	45 (12%)	15 (4%)	3	24
40	l3	384/386 (100%)	323 (84%)	42 (11%)	19 (5%)	2	18
41	L4	359/361 (99%)	279 (78%)	54 (15%)	26 (7%)	1	10
41	l4	359/361 (99%)	277 (77%)	56 (16%)	26 (7%)	1	10
42	L5	294/296 (99%)	237 (81%)	34 (12%)	23 (8%)	1	9
42	l5	292/296 (99%)	240 (82%)	39 (13%)	13 (4%)	2	20
43	L6	152/175 (87%)	121 (80%)	26 (17%)	5 (3%)	4	27
43	l6	153/175 (87%)	121 (79%)	25 (16%)	7 (5%)	2	20
44	L7	220/243 (90%)	183 (83%)	24 (11%)	13 (6%)	1	14
44	l7	221/243 (91%)	177 (80%)	30 (14%)	14 (6%)	1	13
45	L8	231/255 (91%)	179 (78%)	35 (15%)	17 (7%)	1	10
45	l8	229/255 (90%)	176 (77%)	36 (16%)	17 (7%)	1	10
46	L9	189/191 (99%)	150 (79%)	28 (15%)	11 (6%)	1	15
46	l9	189/191 (99%)	153 (81%)	27 (14%)	9 (5%)	2	19
47	M0	207/220 (94%)	167 (81%)	30 (14%)	10 (5%)	2	19
47	m0	209/220 (95%)	163 (78%)	27 (13%)	19 (9%)	1	7
48	M1	167/173 (96%)	126 (75%)	31 (19%)	10 (6%)	1	14
48	m1	167/173 (96%)	127 (76%)	25 (15%)	15 (9%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	140 (73%)	37 (19%)	14 (7%)	1	10
49	m3	192/198 (97%)	150 (78%)	24 (12%)	18 (9%)	0	7
50	M4	134/137 (98%)	106 (79%)	19 (14%)	9 (7%)	1	12
50	m4	135/137 (98%)	116 (86%)	16 (12%)	3 (2%)	6	35
51	M5	201/203 (99%)	170 (85%)	24 (12%)	7 (4%)	3	26
51	m5	201/203 (99%)	171 (85%)	25 (12%)	5 (2%)	5	32
52	M6	195/198 (98%)	167 (86%)	22 (11%)	6 (3%)	4	29
52	m6	195/198 (98%)	164 (84%)	23 (12%)	8 (4%)	3	23
53	M7	181/183 (99%)	142 (78%)	27 (15%)	12 (7%)	1	12
53	m7	153/183 (84%)	130 (85%)	20 (13%)	3 (2%)	7	37
54	M8	183/185 (99%)	148 (81%)	28 (15%)	7 (4%)	3	24
54	m8	183/185 (99%)	140 (76%)	30 (16%)	13 (7%)	1	11
55	M9	186/188 (99%)	160 (86%)	17 (9%)	9 (5%)	2	19
55	m9	186/188 (99%)	156 (84%)	26 (14%)	4 (2%)	6	35
56	N0	170/172 (99%)	149 (88%)	14 (8%)	7 (4%)	3	23
56	n0	170/172 (99%)	146 (86%)	19 (11%)	5 (3%)	4	30
57	N1	157/159 (99%)	136 (87%)	16 (10%)	5 (3%)	4	28
57	n1	157/159 (99%)	125 (80%)	26 (17%)	6 (4%)	3	24
58	N2	98/120 (82%)	74 (76%)	16 (16%)	8 (8%)	1	8
58	n2	96/120 (80%)	76 (79%)	17 (18%)	3 (3%)	4	29
59	N3	134/136 (98%)	114 (85%)	14 (10%)	6 (4%)	2	20
59	n3	134/136 (98%)	116 (87%)	9 (7%)	9 (7%)	1	12
60	N4	96/155 (62%)	68 (71%)	20 (21%)	8 (8%)	1	8
60	n4	133/155 (86%)	99 (74%)	21 (16%)	13 (10%)	0	6
61	N5	119/141 (84%)	98 (82%)	17 (14%)	4 (3%)	3	27
61	n5	118/141 (84%)	97 (82%)	16 (14%)	5 (4%)	3	22
62	N6	124/126 (98%)	99 (80%)	16 (13%)	9 (7%)	1	10
62	n6	124/126 (98%)	100 (81%)	16 (13%)	8 (6%)	1	12
63	N7	133/135 (98%)	104 (78%)	20 (15%)	9 (7%)	1	12
63	n7	133/135 (98%)	91 (68%)	30 (23%)	12 (9%)	1	7
64	N8	146/148 (99%)	114 (78%)	23 (16%)	9 (6%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	n8	146/148 (99%)	119 (82%)	19 (13%)	8 (6%)	2	16
65	N9	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	0	5
65	n9	56/58 (97%)	36 (64%)	11 (20%)	9 (16%)	0	2
66	O0	95/104 (91%)	76 (80%)	17 (18%)	2 (2%)	7	36
66	o0	98/104 (94%)	83 (85%)	11 (11%)	4 (4%)	3	23
67	O1	107/112 (96%)	87 (81%)	13 (12%)	7 (6%)	1	12
67	o1	107/112 (96%)	87 (81%)	12 (11%)	8 (8%)	1	10
68	O2	125/129 (97%)	99 (79%)	18 (14%)	8 (6%)	1	13
68	o2	125/129 (97%)	102 (82%)	14 (11%)	9 (7%)	1	10
69	O3	104/106 (98%)	86 (83%)	13 (12%)	5 (5%)	2	19
69	o3	104/106 (98%)	95 (91%)	7 (7%)	2 (2%)	8	38
70	O4	110/120 (92%)	92 (84%)	16 (14%)	2 (2%)	8	39
70	o4	110/120 (92%)	90 (82%)	15 (14%)	5 (4%)	2	20
71	O5	117/119 (98%)	99 (85%)	13 (11%)	5 (4%)	2	21
71	o5	117/119 (98%)	89 (76%)	22 (19%)	6 (5%)	2	17
72	O6	97/99 (98%)	70 (72%)	15 (16%)	12 (12%)	0	4
72	o6	97/99 (98%)	83 (86%)	10 (10%)	4 (4%)	3	23
73	O7	85/87 (98%)	66 (78%)	18 (21%)	1 (1%)	13	48
73	o7	85/87 (98%)	69 (81%)	12 (14%)	4 (5%)	2	19
74	O8	75/77 (97%)	61 (81%)	11 (15%)	3 (4%)	3	23
74	o8	75/77 (97%)	63 (84%)	10 (13%)	2 (3%)	5	31
75	O9	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	36
75	o9	48/50 (96%)	38 (79%)	6 (12%)	4 (8%)	1	8
76	Q0	50/52 (96%)	42 (84%)	3 (6%)	5 (10%)	0	6
76	q0	50/52 (96%)	40 (80%)	8 (16%)	2 (4%)	3	23
77	Q1	23/25 (92%)	16 (70%)	5 (22%)	2 (9%)	1	8
77	q1	23/25 (92%)	19 (83%)	2 (9%)	2 (9%)	1	8
78	Q2	103/105 (98%)	77 (75%)	18 (18%)	8 (8%)	1	9
78	q2	103/105 (98%)	87 (84%)	11 (11%)	5 (5%)	2	18
79	Q3	89/91 (98%)	74 (83%)	8 (9%)	7 (8%)	1	9
79	q3	89/91 (98%)	70 (79%)	13 (15%)	6 (7%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	e0	60/62 (97%)	39 (65%)	15 (25%)	6 (10%)	0	6
81	p0	139/311 (45%)	108 (78%)	24 (17%)	7 (5%)	2	18
All	All	22333/24143 (92%)	17400 (78%)	3410 (15%)	1523 (7%)	1	12

All (1523) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	68	PRO
2	S0	139	VAL
2	S0	158	VAL
3	S1	49	ASN
3	S1	58	SER
3	S1	63	GLY
3	S1	79	HIS
3	S1	132	ASP
3	S1	148	ASN
3	S1	158	SER
3	S1	179	SER
3	S1	182	ALA
3	S1	206	PRO
3	S1	223	PHE
4	S2	80	VAL
4	S2	81	MET
4	S2	163	GLY
5	S3	65	ARG
5	S3	93	ASP
5	S3	220	PRO
6	S4	12	LEU
6	S4	69	HIS
6	S4	96	ASN
7	S5	35	GLN
7	S5	39	GLU
7	S5	43	PHE
7	S5	51	VAL
7	S5	58	LEU
8	S6	122	GLU
8	S6	173	PRO
8	S6	174	LYS
9	S7	31	SER

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Mol	Chain	Res	Type
9	S7	32	PRO
9	S7	63	PRO
9	S7	112	ARG
9	S7	116	ARG
9	S7	131	PHE
9	S7	186	PRO
10	S8	81	VAL
10	S8	152	ILE
11	S9	134	ILE
12	C0	87	VAL
12	C0	88	PRO
13	C1	4	GLU
13	C1	7	VAL
13	C1	55	ASP
13	C1	95	PRO
13	C1	96	LYS
13	C1	140	VAL
13	C1	146	ALA
13	C1	154	ALA
14	C2	91	VAL
15	C3	138	ASN
16	C4	42	VAL
16	C4	124	ASP
16	C4	126	THR
17	C5	125	PRO
17	C5	126	VAL
18	C6	41	PRO
18	C6	114	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	104	ASN
19	C7	124	VAL
20	C8	91	ASP
20	C8	92	ILE
21	C9	53	TRP
21	C9	69	LYS
23	D1	6	GLY
24	D2	57	ARG
24	D2	78	ARG

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Mol	Chain	Res	Type
24	D2	83	ILE
25	D3	70	LYS
25	D3	112	LYS
25	D3	114	LYS
25	D3	128	SER
25	D3	137	LYS
25	D3	144	ARG
26	D4	5	VAL
26	D4	53	ASP
26	D4	58	PHE
27	D5	37	GLN
27	D5	43	ASP
27	D5	56	THR
27	D5	71	ILE
28	D6	36	ILE
28	D6	45	VAL
28	D6	84	VAL
28	D6	86	VAL
29	D7	38	PRO
29	D7	62	ILE
29	D7	75	GLU
31	D9	8	PHE
31	D9	47	ALA
32	E0	13	LYS
32	E0	47	VAL
33	E1	98	VAL
33	E1	102	VAL
33	E1	103	LEU
33	E1	105	TYR
33	E1	106	TYR
33	E1	110	ALA
33	E1	111	GLU
33	E1	138	ARG
34	SR	155	ARG
34	SR	161	LYS
34	SR	188	ILE
34	SR	231	MET
34	SR	318	ALA
35	SM	52	PRO
35	SM	86	ASN
35	SM	87	THR
35	SM	140	ASP

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Mol	Chain	Res	Type
35	SM	166	VAL
35	SM	167	PRO
40	L3	140	ASP
40	L3	348	ARG
40	L3	385	LYS
41	L4	24	ALA
41	L4	83	GLY
41	L4	132	ALA
41	L4	146	PRO
41	L4	183	LYS
41	L4	265	GLU
41	L4	270	SER
41	L4	292	SER
41	L4	311	HIS
42	L5	6	ASP
42	L5	59	ASP
42	L5	178	ASN
42	L5	215	ASP
42	L5	234	ASP
42	L5	253	PHE
42	L5	258	LYS
42	L5	292	ALA
42	L5	293	LEU
43	L6	94	GLU
43	L6	98	VAL
44	L7	24	GLU
44	L7	191	VAL
45	L8	25	PRO
45	L8	31	PRO
45	L8	36	ILE
45	L8	37	GLY
45	L8	40	VAL
45	L8	156	ASP
45	L8	255	SER
46	L9	50	ASN
47	M0	145	LYS
47	M0	207	GLU
48	M1	8	PRO
48	M1	145	LYS
48	M1	165	GLN
49	M3	129	ASN
50	M4	6	ILE

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Mol	Chain	Res	Type
50	M4	8	LYS
50	M4	9	ALA
50	M4	135	LEU
50	M4	136	ALA
51	M5	40	ALA
52	M6	111	PRO
53	M7	88	VAL
53	M7	109	ALA
53	M7	157	VAL
55	M9	61	SER
55	M9	85	ARG
56	N0	2	ALA
57	N1	159	PHE
58	N2	51	GLY
59	N3	3	GLY
60	N4	26	SER
60	N4	81	PRO
61	N5	26	VAL
61	N5	50	ALA
62	N6	53	ASP
63	N7	30	ASP
63	N7	125	GLY
63	N7	129	TRP
64	N8	24	LYS
67	O1	5	LYS
67	O1	6	ASP
67	O1	83	GLU
68	O2	30	GLU
69	O3	94	PHE
71	O5	96	GLU
72	O6	27	SER
73	O7	12	HIS
75	O9	4	GLN
76	Q0	78	ILE
76	Q0	120	GLN
77	Q1	4	LYS
78	Q2	30	ALA
78	Q2	100	LYS
79	Q3	58	SER
2	s0	4	PRO
2	s0	68	PRO
2	s0	158	VAL

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Mol	Chain	Res	Type
2	s0	191	ARG
2	s0	203	PHE
2	s0	206	ASP
3	s1	132	ASP
3	s1	147	ALA
3	s1	206	PRO
3	s1	232	HIS
4	s2	76	LEU
4	s2	92	ALA
4	s2	134	LEU
4	s2	148	LEU
4	s2	150	GLN
4	s2	207	LEU
5	s3	92	GLN
5	s3	144	ALA
5	s3	161	GLY
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
5	s3	221	SER
6	s4	95	THR
6	s4	104	ASP
6	s4	118	GLU
6	s4	163	ASP
6	s4	195	ILE
6	s4	196	VAL
6	s4	240	LYS
7	s5	28	PRO
7	s5	35	GLN
7	s5	36	ALA
7	s5	39	GLU
7	s5	81	ARG
7	s5	154	ALA
7	s5	184	PHE
7	s5	204	GLY
7	s5	209	TYR
8	s6	70	PRO
8	s6	153	VAL
8	s6	173	PRO
9	s7	64	VAL
9	s7	66	SER

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Mol	Chain	Res	Type
9	s7	67	LEU
9	s7	106	SER
9	s7	112	ARG
9	s7	131	PHE
9	s7	163	ASP
10	s8	13	ALA
10	s8	36	THR
11	s9	5	PRO
12	c0	2	LEU
12	c0	28	ASN
12	c0	32	HIS
12	c0	83	PRO
12	c0	88	PRO
12	c0	92	ILE
12	c0	97	PRO
13	c1	114	ALA
13	c1	129	ARG
14	c2	89	ILE
14	c2	93	ASP
15	c3	60	VAL
15	c3	66	ILE
15	c3	139	TRP
16	c4	51	ASP
16	c4	132	ARG
17	c5	11	VAL
17	c5	49	MET
17	c5	51	SER
17	c5	52	LYS
17	c5	125	PRO
17	c5	128	HIS
18	c6	39	VAL
18	c6	116	LEU
19	c7	67	ARG
19	c7	88	VAL
19	c7	99	VAL
20	c8	18	LEU
20	c8	61	LEU
20	c8	91	ASP
20	c8	92	ILE
22	d0	17	GLN
22	d0	51	VAL
22	d0	52	LYS

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Mol	Chain	Res	Type
22	d0	118	VAL
23	d1	4	ASP
25	d3	70	LYS
26	d4	30	PRO
26	d4	35	VAL
26	d4	52	LYS
26	d4	63	GLN
27	d5	85	LYS
27	d5	87	GLY
27	d5	104	ALA
28	d6	63	ALA
29	d7	18	LYS
29	d7	38	PRO
29	d7	60	SER
31	d9	6	VAL
31	d9	7	TRP
31	d9	19	ARG
33	e1	83	LYS
33	e1	84	VAL
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	100	LEU
33	e1	102	VAL
33	e1	103	LEU
33	e1	106	TYR
34	sR	4	ASN
34	sR	165	ASP
34	sR	282	SER
35	sM	47	ALA
35	sM	50	ASN
35	sM	163	PHE
39	l2	24	GLN
39	l2	96	LEU
39	l2	144	ASN
39	l2	160	SER
39	l2	215	ASN
39	l2	238	ILE
39	l2	249	SER
40	l3	129	ALA
40	l3	140	ASP
40	l3	142	ALA

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Mol	Chain	Res	Type
40	l3	188	ILE
40	l3	200	GLU
40	l3	235	THR
40	l3	347	SER
41	l4	14	GLU
41	l4	24	ALA
41	l4	90	PHE
41	l4	193	LYS
41	l4	268	ALA
41	l4	277	PRO
41	l4	311	HIS
41	l4	329	PRO
41	l4	338	LYS
41	l4	339	LEU
41	l4	345	GLU
42	l5	178	ASN
42	l5	279	LYS
43	l6	3	ALA
43	l6	98	VAL
44	l7	178	ILE
44	l7	193	PRO
45	l8	25	PRO
45	l8	122	LYS
45	l8	208	GLU
45	l8	240	ASN
46	l9	141	LYS
46	l9	177	ASP
47	m0	82	ARG
47	m0	156	ARG
47	m0	157	TYR
48	m1	8	PRO
48	m1	9	MET
48	m1	10	ARG
48	m1	94	ARG
48	m1	173	ASP
49	m3	25	HIS
49	m3	47	ALA
49	m3	50	PRO
49	m3	133	PRO
49	m3	134	GLU
49	m3	150	PRO
49	m3	152	THR

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Mol	Chain	Res	Type
49	m3	193	ALA
50	m4	78	THR
51	m5	76	PRO
51	m5	81	TYR
51	m5	187	ARG
52	m6	16	VAL
52	m6	90	HIS
52	m6	186	ALA
54	m8	84	VAL
54	m8	95	GLU
54	m8	112	ALA
55	m9	182	ASP
56	n0	87	THR
56	n0	139	TYR
57	n1	122	GLN
57	n1	144	GLU
57	n1	146	ASN
58	n2	50	LEU
60	n4	25	ASP
60	n4	63	ILE
60	n4	64	THR
60	n4	76	VAL
61	n5	40	LEU
61	n5	55	ASN
62	n6	6	LEU
62	n6	62	SER
62	n6	83	ASP
62	n6	84	LYS
62	n6	90	VAL
62	n6	97	ILE
63	n7	5	LEU
63	n7	7	ALA
63	n7	90	GLU
63	n7	125	GLY
63	n7	129	TRP
64	n8	76	ASP
65	n9	21	ILE
65	n9	23	LYS
65	n9	24	PRO
65	n9	39	PHE
68	o2	4	LEU
68	o2	5	PRO

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Mol	Chain	Res	Type
70	o4	33	GLN
71	o5	43	LYS
71	o5	119	LYS
72	o6	12	ASN
72	o6	98	ARG
73	o7	68	LYS
73	o7	84	SER
73	o7	85	LYS
74	o8	16	ARG
75	o9	35	ILE
79	q3	52	ALA
81	p0	93	LEU
2	S0	5	ALA
2	S0	33	GLN
2	S0	43	ASP
2	S0	64	ILE
2	S0	111	ILE
2	S0	185	ARG
2	S0	190	ASP
2	S0	202	TYR
3	S1	54	LEU
3	S1	181	LEU
3	S1	218	LEU
3	S1	221	PRO
4	S2	78	ASP
4	S2	106	ASP
4	S2	107	SER
4	S2	148	LEU
5	S3	62	ASN
5	S3	137	VAL
5	S3	218	LEU
6	S4	17	HIS
6	S4	77	ARG
6	S4	153	ASN
6	S4	205	PHE
6	S4	228	ILE
7	S5	33	VAL
7	S5	50	GLU
7	S5	54	LYS
7	S5	63	GLN
7	S5	127	GLN
7	S5	153	GLY

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Mol	Chain	Res	Type
7	S5	204	GLY
8	S6	70	PRO
8	S6	138	ALA
8	S6	152	ASP
8	S6	165	GLY
9	S7	8	ILE
9	S7	30	SER
9	S7	35	LYS
9	S7	52	ALA
9	S7	64	VAL
9	S7	73	VAL
9	S7	110	GLN
9	S7	132	PRO
10	S8	22	ARG
10	S8	40	ALA
10	S8	149	SER
11	S9	98	ALA
11	S9	164	PHE
12	C0	60	SER
13	C1	51	GLY
13	C1	72	THR
13	C1	89	ALA
13	C1	139	VAL
13	C1	145	ALA
14	C2	87	PRO
14	C2	89	ILE
14	C2	101	ALA
14	C2	106	ILE
14	C2	119	SER
14	C2	126	TRP
14	C2	131	ASP
15	C3	22	ALA
15	C3	27	LYS
16	C4	50	ALA
16	C4	92	LYS
17	C5	48	GLY
17	C5	53	PRO
17	C5	80	MET
18	C6	39	VAL
19	C7	23	LYS
20	C8	7	GLU
20	C8	14	ILE

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Mol	Chain	Res	Type
20	C8	60	GLU
20	C8	82	PRO
20	C8	142	GLY
20	C8	144	ARG
22	D0	21	LYS
22	D0	72	ASN
23	D1	12	TYR
26	D4	36	SER
26	D4	59	GLY
27	D5	44	GLN
27	D5	55	PRO
27	D5	88	ILE
28	D6	39	MET
28	D6	82	ARG
28	D6	85	ARG
29	D7	4	VAL
29	D7	63	LEU
30	D8	22	ARG
30	D8	36	THR
32	E0	3	LYS
32	E0	9	ALA
33	E1	84	VAL
33	E1	85	TYR
33	E1	87	THR
33	E1	127	GLY
33	E1	128	ALA
34	SR	24	ALA
34	SR	141	LEU
34	SR	166	SER
35	SM	101	ASP
35	SM	139	GLU
35	SM	154	TYR
39	L2	13	GLY
39	L2	234	LYS
40	L3	4	ARG
40	L3	155	ALA
40	L3	186	GLY
40	L3	333	LYS
41	L4	82	THR
41	L4	90	PHE
41	L4	130	ALA
41	L4	143	GLU

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Mol	Chain	Res	Type
41	L4	175	HIS
41	L4	293	SER
42	L5	7	ALA
42	L5	9	SER
42	L5	57	ASN
42	L5	91	GLY
42	L5	93	THR
43	L6	130	ILE
44	L7	26	VAL
44	L7	159	GLN
44	L7	241	LYS
45	L8	39	ALA
45	L8	157	VAL
46	L9	49	ASN
46	L9	151	VAL
46	L9	189	GLU
47	M0	146	ASP
47	M0	194	GLY
48	M1	39	GLN
48	M1	115	LYS
49	M3	19	GLN
49	M3	47	ALA
50	M4	109	ARG
51	M5	141	ALA
51	M5	184	LYS
52	M6	178	VAL
53	M7	160	ALA
53	M7	164	LYS
54	M8	98	LYS
55	M9	128	LYS
56	N0	118	PHE
56	N0	130	GLU
56	N0	166	LYS
57	N1	124	VAL
58	N2	11	ILE
58	N2	50	LEU
58	N2	60	GLY
58	N2	70	LYS
58	N2	107	PHE
59	N3	131	SER
60	N4	72	SER
61	N5	117	ASN

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Mol	Chain	Res	Type
62	N6	84	LYS
63	N7	102	GLU
64	N8	47	LYS
64	N8	66	ALA
65	N9	5	LYS
65	N9	24	PRO
65	N9	25	LYS
66	O0	20	SER
67	O1	84	ASP
68	O2	13	HIS
68	O2	27	ARG
69	O3	40	ASP
70	O4	77	GLY
71	O5	94	LYS
71	O5	97	ALA
71	O5	119	LYS
72	O6	3	VAL
72	O6	21	THR
72	O6	33	ALA
72	O6	64	SER
74	O8	75	VAL
78	Q2	15	LYS
78	Q2	17	CYS
78	Q2	94	GLY
79	Q3	60	CYS
79	Q3	71	VAL
79	Q3	90	VAL
2	s0	29	VAL
2	s0	189	VAL
3	s1	63	GLY
3	s1	81	PHE
3	s1	93	GLY
3	s1	223	PHE
4	s2	163	GLY
5	s3	44	THR
5	s3	142	LEU
5	s3	195	SER
5	s3	203	PRO
6	s4	164	LEU
6	s4	245	LYS
7	s5	43	PHE
7	s5	75	GLY

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Mol	Chain	Res	Type
7	s5	101	GLY
7	s5	196	GLU
7	s5	217	LEU
8	s6	9	VAL
8	s6	123	GLY
8	s6	154	ARG
8	s6	174	LYS
9	s7	15	GLU
9	s7	74	GLN
9	s7	155	ASP
9	s7	156	SER
10	s8	94	ASN
10	s8	162	ALA
10	s8	199	LYS
11	s9	99	LEU
11	s9	122	VAL
11	s9	167	ALA
13	c1	7	VAL
13	c1	24	LYS
13	c1	55	ASP
13	c1	144	ALA
14	c2	101	ALA
15	c3	21	ASN
15	c3	35	GLU
15	c3	87	ASP
15	c3	140	LYS
16	c4	32	ASP
17	c5	17	TYR
17	c5	50	THR
17	c5	69	GLU
17	c5	126	VAL
18	c6	42	GLU
18	c6	113	ASP
18	c6	115	THR
18	c6	120	ASP
19	c7	63	LYS
20	c8	4	VAL
20	c8	29	VAL
20	c8	55	HIS
20	c8	90	ASN
20	c8	139	LYS
21	c9	29	GLU

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Mol	Chain	Res	Type
21	c9	142	GLU
22	d0	15	GLN
22	d0	16	GLN
23	d1	42	GLU
25	d3	3	LYS
25	d3	47	SER
25	d3	65	ASN
25	d3	138	GLU
26	d4	32	ARG
26	d4	33	ALA
26	d4	36	SER
26	d4	51	GLU
26	d4	58	PHE
26	d4	64	PHE
26	d4	65	GLY
26	d4	84	LYS
26	d4	121	THR
26	d4	123	LYS
27	d5	38	HIS
80	e0	44	PHE
80	e0	51	ASN
33	e1	128	ALA
34	sR	149	ASP
34	sR	194	GLY
35	sM	33	LYS
35	sM	65	THR
35	sM	168	GLU
39	l2	54	ARG
39	l2	172	GLY
39	l2	194	ASN
40	l3	23	ALA
40	l3	66	LYS
40	l3	230	THR
40	l3	385	LYS
40	l3	386	ASP
41	l4	15	ALA
41	l4	145	ILE
41	l4	341	SER
41	l4	342	LYS
42	l5	9	SER
42	l5	115	LEU
42	l5	256	THR

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Mol	Chain	Res	Type
42	l5	260	PHE
43	l6	24	ALA
43	l6	32	ALA
44	l7	91	GLY
44	l7	130	ILE
45	l8	26	LEU
45	l8	112	GLU
45	l8	120	LYS
45	l8	133	LYS
45	l8	182	GLY
45	l8	203	VAL
46	l9	144	ILE
47	m0	3	ARG
47	m0	25	ALA
47	m0	83	ASP
47	m0	101	LYS
47	m0	174	THR
47	m0	187	ALA
47	m0	196	PHE
48	m1	95	ASN
48	m1	108	GLU
48	m1	114	ILE
49	m3	76	THR
49	m3	101	ARG
49	m3	122	LYS
51	m5	183	THR
52	m6	139	GLY
53	m7	34	GLN
54	m8	70	ALA
54	m8	99	THR
54	m8	181	SER
56	n0	129	ILE
58	n2	91	ASP
59	n3	54	LEU
59	n3	134	GLY
60	n4	34	SER
60	n4	71	ARG
60	n4	77	LYS
60	n4	98	PRO
60	n4	126	GLU
61	n5	41	ALA
62	n6	61	GLY

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Mol	Chain	Res	Type
63	n7	6	LYS
63	n7	102	GLU
63	n7	128	GLN
64	n8	15	VAL
64	n8	24	LYS
65	n9	6	ASN
65	n9	52	LYS
66	o0	49	PRO
67	o1	26	LYS
67	o1	45	GLY
67	o1	84	ASP
68	o2	124	GLY
70	o4	79	SER
74	o8	18	ALA
75	o9	4	GLN
78	q2	15	LYS
78	q2	17	CYS
79	q3	9	GLY
81	p0	102	SER
2	S0	30	GLN
2	S0	49	ASN
2	S0	66	ALA
2	S0	103	THR
2	S0	163	ASN
2	S0	192	THR
2	S0	195	TRP
3	S1	35	PRO
3	S1	81	PHE
3	S1	130	SER
3	S1	154	SER
3	S1	213	ARG
4	S2	91	ARG
4	S2	146	THR
4	S2	150	GLN
5	S3	31	GLU
5	S3	44	THR
5	S3	195	SER
5	S3	217	ILE
6	S4	104	ASP
6	S4	195	ILE
7	S5	49	GLU
7	S5	64	VAL

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Mol	Chain	Res	Type
7	S5	81	ARG
8	S6	151	ASP
9	S7	36	ALA
9	S7	118	LEU
10	S8	52	ASN
10	S8	68	ALA
10	S8	120	THR
11	S9	9	SER
11	S9	163	PRO
12	C0	54	TYR
12	C0	81	ASN
12	C0	90	THR
13	C1	29	LYS
13	C1	30	ARG
14	C2	22	VAL
14	C2	105	LYS
14	C2	107	ASP
15	C3	68	GLY
15	C3	149	LEU
16	C4	18	ARG
16	C4	40	ALA
17	C5	25	LEU
17	C5	29	SER
17	C5	39	ALA
17	C5	51	SER
17	C5	54	ALA
17	C5	69	GLU
17	C5	101	ALA
18	C6	113	ASP
18	C6	142	TYR
19	C7	87	GLU
19	C7	113	LEU
19	C7	115	LEU
20	C8	8	GLN
20	C8	61	LEU
20	C8	110	ARG
21	C9	31	PRO
21	C9	39	THR
23	D1	2	GLU
24	D2	77	PRO
24	D2	91	ALA
24	D2	92	ASN

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Mol	Chain	Res	Type
26	D4	6	THR
26	D4	68	LYS
27	D5	39	ALA
27	D5	94	LYS
28	D6	63	ALA
29	D7	48	SER
31	D9	20	GLN
33	E1	86	THR
33	E1	90	LYS
34	SR	22	SER
34	SR	70	ASP
34	SR	76	ASP
34	SR	140	CYS
34	SR	150	TRP
34	SR	162	ALA
34	SR	163	ASP
34	SR	194	GLY
34	SR	242	SER
35	SM	81	THR
35	SM	102	THR
39	L2	47	GLN
39	L2	152	SER
40	L3	3	HIS
40	L3	171	LEU
40	L3	299	ASP
40	L3	300	ARG
40	L3	347	SER
41	L4	15	ALA
41	L4	64	SER
41	L4	103	THR
41	L4	181	VAL
41	L4	190	GLY
42	L5	58	LYS
42	L5	157	ALA
42	L5	213	ASP
42	L5	259	LYS
42	L5	260	PHE
42	L5	276	LYS
44	L7	158	LYS
45	L8	135	GLY
45	L8	227	ASP
46	L9	117	PHE

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Mol	Chain	Res	Type
46	L9	120	ASP
47	M0	16	PRO
47	M0	82	ARG
47	M0	161	GLY
47	M0	218	ALA
48	M1	38	GLU
48	M1	151	SER
49	M3	58	VAL
49	M3	62	THR
49	M3	176	GLU
50	M4	29	ALA
50	M4	105	GLN
51	M5	94	TYR
51	M5	192	LYS
52	M6	63	ALA
52	M6	188	SER
53	M7	3	ARG
53	M7	30	ARG
53	M7	51	VAL
53	M7	161	ALA
54	M8	74	GLU
55	M9	97	ARG
57	N1	132	PRO
58	N2	84	LEU
59	N3	16	GLY
59	N3	67	PRO
60	N4	34	SER
60	N4	97	LYS
62	N6	3	LYS
62	N6	52	ARG
62	N6	92	GLY
63	N7	3	LYS
64	N8	96	LYS
67	O1	7	VAL
72	O6	34	SER
72	O6	96	ALA
72	O6	97	SER
74	O8	33	LYS
76	Q0	79	GLU
76	Q0	114	LYS
78	Q2	34	SER
2	s0	7	PHE

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Mol	Chain	Res	Type
2	s0	10	THR
2	s0	152	PRO
2	s0	186	GLY
3	s1	94	LYS
3	s1	154	SER
4	s2	83	ILE
4	s2	91	ARG
4	s2	151	PRO
4	s2	196	VAL
4	s2	204	THR
4	s2	205	ARG
4	s2	238	SER
5	s3	61	GLU
5	s3	90	ARG
5	s3	93	ASP
5	s3	179	GLN
5	s3	204	ASP
6	s4	12	LEU
7	s5	34	GLN
7	s5	84	LYS
7	s5	98	MET
11	s9	43	TYR
11	s9	64	GLU
11	s9	78	ARG
11	s9	169	PRO
12	c0	30	ALA
13	c1	28	SER
14	c2	39	ASP
14	c2	45	LEU
14	c2	106	ILE
14	c2	108	ARG
14	c2	119	SER
14	c2	131	ASP
15	c3	29	SER
15	c3	137	PRO
16	c4	12	GLN
16	c4	96	PRO
17	c5	8	LYS
17	c5	130	ARG
20	c8	65	GLU
21	c9	66	TYR
22	d0	49	ASN

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Mol	Chain	Res	Type
25	d3	66	SER
25	d3	99	ASN
26	d4	49	LYS
28	d6	5	ARG
28	d6	8	ASN
28	d6	27	SER
29	d7	59	CYS
30	d8	33	LEU
30	d8	57	MET
80	e0	56	MET
33	e1	107	LYS
33	e1	111	GLU
33	e1	112	GLY
33	e1	125	THR
33	e1	131	PHE
33	e1	136	LYS
33	e1	145	HIS
34	sR	96	THR
34	sR	163	ASP
34	sR	186	PHE
34	sR	277	GLU
35	sM	171	LYS
39	l2	17	THR
39	l2	56	ALA
39	l2	70	ARG
39	l2	127	ALA
40	l3	12	GLY
40	l3	291	GLU
40	l3	302	LYS
41	l4	330	TYR
41	l4	361	HIS
42	l5	269	SER
43	l6	10	TYR
44	l7	53	LYS
44	l7	191	VAL
45	l8	69	LEU
45	l8	237	ILE
45	l8	239	GLY
46	l9	2	LYS
47	m0	78	THR
47	m0	176	LEU
47	m0	207	GLU

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Mol	Chain	Res	Type
47	m0	219	ALA
48	m1	82	ARG
48	m1	111	ASP
48	m1	151	SER
48	m1	153	LYS
49	m3	93	ILE
49	m3	163	GLY
50	m4	8	LYS
51	m5	49	ARG
52	m6	110	PRO
52	m6	162	VAL
54	m8	41	ASP
54	m8	69	ARG
55	m9	142	ILE
59	n3	4	ASN
59	n3	27	ASP
59	n3	28	ASN
59	n3	68	GLU
59	n3	69	LEU
60	n4	130	SER
61	n5	47	ALA
62	n6	126	LEU
63	n7	14	VAL
63	n7	41	ALA
63	n7	103	GLN
64	n8	110	GLY
65	n9	25	LYS
65	n9	33	LYS
67	o1	47	ASP
67	o1	82	GLU
67	o1	83	GLU
69	o3	59	VAL
70	o4	12	PRO
71	o5	16	GLN
71	o5	81	ARG
71	o5	105	ARG
76	q0	78	ILE
77	q1	3	ALA
77	q1	4	LYS
78	q2	74	CYS
78	q2	78	LYS
79	q3	20	SER

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Mol	Chain	Res	Type
81	p0	206	ASP
2	S0	7	PHE
2	S0	78	SER
2	S0	126	PRO
3	S1	156	ALA
4	S2	39	THR
4	S2	235	LEU
5	S3	118	ALA
5	S3	129	SER
6	S4	237	SER
7	S5	31	GLU
7	S5	36	ALA
7	S5	202	ALA
7	S5	210	ALA
9	S7	98	ILE
10	S8	136	SER
11	S9	56	ALA
11	S9	100	LYS
11	S9	119	ALA
11	S9	162	SER
13	C1	3	THR
13	C1	82	ARG
13	C1	153	PHE
15	C3	3	ARG
16	C4	51	ASP
16	C4	114	ARG
17	C5	24	LYS
19	C7	73	LEU
20	C8	118	LYS
20	C8	134	ARG
21	C9	25	GLN
22	D0	17	GLN
22	D0	55	PRO
22	D0	73	GLY
23	D1	7	GLN
23	D1	82	VAL
25	D3	4	GLY
25	D3	41	SER
25	D3	139	LYS
27	D5	41	ILE
28	D6	18	VAL
28	D6	61	GLU

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Mol	Chain	Res	Type
28	D6	64	LEU
28	D6	65	PRO
30	D8	16	LEU
30	D8	61	ARG
32	E0	23	LYS
33	E1	100	LEU
33	E1	137	ASP
34	SR	15	GLY
34	SR	189	GLU
35	SM	53	ARG
35	SM	100	THR
35	SM	119	ALA
35	SM	136	ALA
35	SM	168	GLU
35	SM	172	VAL
35	SM	173	GLU
35	SM	174	LEU
39	L2	153	GLY
39	L2	231	SER
40	L3	244	ARG
41	L4	140	HIS
41	L4	182	LEU
41	L4	184	SER
42	L5	137	ASP
42	L5	212	ALA
43	L6	6	ALA
44	L7	128	LYS
45	L8	136	LEU
45	L8	163	VAL
46	L9	5	GLN
46	L9	96	HIS
46	L9	110	LYS
46	L9	190	ASP
48	M1	114	ILE
48	M1	117	ASP
49	M3	76	THR
49	M3	128	ARG
49	M3	164	GLU
49	M3	175	SER
51	M5	77	LYS
51	M5	81	TYR
53	M7	63	PHE

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Mol	Chain	Res	Type
53	M7	133	HIS
54	M8	162	ALA
55	M9	3	ASN
55	M9	53	LYS
56	N0	24	LEU
56	N0	34	GLU
59	N3	46	LEU
59	N3	54	LEU
62	N6	38	GLU
63	N7	35	SER
63	N7	103	GLN
65	N9	33	LYS
67	O1	97	LEU
68	O2	122	PRO
68	O2	127	ALA
69	O3	59	VAL
70	O4	81	CYS
71	O5	75	TYR
72	O6	32	ALA
74	O8	37	PRO
77	Q1	3	ALA
78	Q2	78	LYS
2	s0	9	LEU
2	s0	49	ASN
2	s0	103	THR
3	s1	22	ASP
3	s1	60	ALA
4	s2	234	PRO
5	s3	43	PRO
5	s3	64	ARG
6	s4	30	ARG
6	s4	90	ILE
6	s4	117	GLU
6	s4	168	LYS
6	s4	223	ASN
7	s5	29	ILE
7	s5	118	LEU
8	s6	216	LEU
9	s7	11	GLN
9	s7	41	LEU
9	s7	130	VAL
9	s7	133	THR

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Mol	Chain	Res	Type
12	c0	23	ALA
12	c0	35	ILE
12	c0	54	TYR
14	c2	21	GLU
14	c2	40	GLY
14	c2	107	ASP
14	c2	127	GLY
15	c3	26	PHE
17	c5	12	PHE
17	c5	14	THR
17	c5	68	PRO
19	c7	103	ASP
20	c8	14	ILE
22	d0	120	SER
23	d1	9	VAL
23	d1	10	GLU
24	d2	68	ARG
24	d2	99	PHE
25	d3	13	ARG
26	d4	50	ALA
27	d5	81	ARG
28	d6	34	LYS
28	d6	59	TYR
30	d8	62	GLU
31	d9	11	PRO
33	e1	81	LYS
33	e1	85	TYR
33	e1	148	TYR
34	sR	166	SER
35	sM	43	ASP
35	sM	84	LYS
39	l2	80	GLU
39	l2	213	GLY
40	l3	155	ALA
40	l3	206	ASP
41	l4	197	ARG
41	l4	301	PRO
41	l4	305	ALA
42	l5	189	GLU
42	l5	215	ASP
42	l5	245	GLU
43	l6	97	ASN

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Mol	Chain	Res	Type
44	l7	159	GLN
45	l8	39	ALA
45	l8	196	ALA
46	l9	107	ASP
47	m0	27	PRO
47	m0	175	ASN
47	m0	195	ALA
47	m0	220	GLN
48	m1	115	LYS
49	m3	60	ALA
49	m3	62	THR
49	m3	135	ALA
50	m4	86	ALA
52	m6	196	ALA
54	m8	49	LEU
54	m8	97	PRO
54	m8	105	ARG
54	m8	149	ALA
55	m9	28	GLU
55	m9	183	ALA
56	n0	110	MET
56	n0	154	HIS
57	n1	58	GLN
58	n2	60	GLY
60	n4	83	THR
64	n8	48	TYR
66	o0	46	ALA
66	o0	47	ASN
68	o2	6	HIS
68	o2	27	ARG
69	o3	60	ARG
70	o4	32	ALA
71	o5	82	ALA
73	o7	65	ARG
75	o9	3	ALA
75	o9	18	LYS
78	q2	77	CYS
81	p0	68	SER
3	S1	22	ASP
3	S1	59	ASP
3	S1	101	HIS
3	S1	131	ASP

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Mol	Chain	Res	Type
3	S1	210	ILE
4	S2	47	ALA
5	S3	72	LEU
5	S3	216	PRO
6	S4	5	PRO
6	S4	11	ARG
11	S9	110	GLN
11	S9	147	MET
14	C2	23	THR
14	C2	83	GLU
17	C5	38	PRO
18	C6	33	GLY
19	C7	72	LYS
21	C9	122	ARG
22	D0	119	ALA
23	D1	42	GLU
24	D2	100	GLY
25	D3	3	LYS
25	D3	20	ARG
25	D3	21	ASN
26	D4	54	ALA
31	D9	11	PRO
34	SR	98	GLU
34	SR	120	SER
34	SR	152	SER
34	SR	237	GLN
34	SR	247	PRO
35	SM	12	VAL
35	SM	85	SER
35	SM	155	LEU
39	L2	127	ALA
40	L3	141	GLY
40	L3	317	ILE
41	L4	14	GLU
42	L5	251	PRO
43	L6	36	PRO
44	L7	25	GLN
44	L7	54	GLU
44	L7	163	LEU
44	L7	217	PRO
45	L8	80	TYR
45	L8	122	LYS

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Mol	Chain	Res	Type
48	M1	108	GLU
49	M3	46	ILE
50	M4	28	SER
52	M6	16	VAL
53	M7	75	GLU
55	M9	131	ALA
57	N1	127	GLN
62	N6	126	LEU
63	N7	36	HIS
64	N8	76	ASP
67	O1	60	TRP
69	O3	90	PRO
72	O6	12	ASN
72	O6	36	ARG
72	O6	78	GLY
78	Q2	104	LEU
79	Q3	12	GLY
79	Q3	91	GLU
2	s0	162	CYS
5	s3	45	LYS
5	s3	56	GLN
7	s5	21	THR
7	s5	57	SER
7	s5	74	ALA
8	s6	165	GLY
10	s8	20	GLN
10	s8	52	ASN
10	s8	78	ILE
11	s9	162	SER
12	c0	26	ASP
12	c0	82	LEU
14	c2	66	VAL
14	c2	90	LYS
14	c2	91	VAL
15	c3	12	SER
15	c3	22	ALA
15	c3	148	ALA
16	c4	131	GLY
17	c5	31	GLU
18	c6	61	SER
18	c6	97	VAL
19	c7	86	PRO

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Mol	Chain	Res	Type
20	c8	60	GLU
21	c9	49	ASP
22	d0	53	LYS
22	d0	96	PRO
35	sM	46	LYS
39	l2	98	VAL
41	l4	146	PRO
41	l4	176	SER
41	l4	328	ASN
41	l4	353	ALA
42	l5	174	PRO
42	l5	258	LYS
43	l6	31	ARG
44	l7	27	ALA
44	l7	217	PRO
46	l9	30	PRO
46	l9	31	ARG
46	l9	167	VAL
48	m1	12	LEU
48	m1	117	ASP
49	m3	51	LEU
53	m7	6	ALA
57	n1	83	ARG
57	n1	148	PRO
60	n4	59	HIS
60	n4	132	GLY
61	n5	97	LYS
63	n7	124	ALA
64	n8	70	LYS
65	n9	37	PRO
67	o1	44	MET
68	o2	69	SER
68	o2	70	GLY
72	o6	4	LYS
72	o6	33	ALA
79	q3	3	LYS
79	q3	17	ARG
2	S0	189	VAL
3	S1	21	VAL
4	S2	153	SER
4	S2	248	SER
7	S5	26	ALA

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Mol	Chain	Res	Type
8	S6	146	GLY
10	S8	10	LYS
12	C0	92	ILE
13	C1	5	LEU
14	C2	108	ARG
15	C3	79	GLY
23	D1	10	GLU
23	D1	46	ILE
26	D4	34	ASN
26	D4	133	ASN
34	SR	113	VAL
41	L4	328	ASN
44	L7	91	GLY
44	L7	178	ILE
46	L9	4	ILE
47	M0	47	PRO
49	M3	136	GLU
52	M6	139	GLY
54	M8	84	VAL
54	M8	99	THR
56	N0	167	ARG
61	N5	44	PRO
64	N8	15	VAL
64	N8	70	LYS
64	N8	116	GLY
66	O0	96	GLY
68	O2	45	ARG
76	Q0	88	LYS
2	s0	139	VAL
2	s0	185	ARG
4	s2	93	GLY
4	s2	236	PRO
6	s4	241	GLY
9	s7	177	THR
11	s9	42	ILE
14	c2	103	LEU
16	c4	11	SER
16	c4	50	ALA
17	c5	6	ASN
18	c6	40	GLU
19	c7	98	GLY
21	c9	118	PRO

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Mol	Chain	Res	Type
23	d1	44	ARG
24	d2	8	ALA
26	d4	78	SER
28	d6	35	ALA
30	d8	58	GLU
80	e0	47	VAL
80	e0	54	ARG
41	l4	331	ALA
44	l7	54	GLU
45	l8	34	PHE
46	l9	172	ILE
49	m3	13	HIS
52	m6	5	PRO
53	m7	37	ASN
59	n3	3	GLY
64	n8	47	LYS
64	n8	120	ASN
67	o1	86	LYS
68	o2	17	PHE
70	o4	59	PRO
81	p0	33	VAL
2	S0	50	VAL
4	S2	74	PRO
7	S5	150	GLY
30	D8	23	GLY
34	SR	67	ILE
60	N4	63	ILE
62	N6	101	PRO
65	N9	21	ILE
68	O2	108	ILE
6	s4	135	GLY
9	s7	73	VAL
14	c2	63	VAL
14	c2	82	PRO
22	d0	97	VAL
80	e0	60	PRO
35	sM	167	PRO
42	l5	125	VAL
54	m8	43	PRO
59	n3	13	ILE
68	o2	122	PRO
4	S2	182	PRO

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Mol	Chain	Res	Type
6	S4	111	VAL
14	C2	115	VAL
34	SR	63	GLY
39	L2	15	ILE
57	N1	123	GLY
62	N6	49	PRO
68	O2	124	GLY
14	c2	22	VAL
16	c4	39	ILE
29	d7	4	VAL
66	o0	96	GLY
81	p0	101	VAL
3	S1	93	GLY
8	S6	181	PRO
14	C2	66	VAL
45	L8	30	THR
47	M0	117	GLY
49	M3	132	ALA
54	M8	160	GLY
54	M8	183	GLY
55	M9	57	VAL
58	N2	22	PRO
60	N4	90	ILE
63	N7	70	PRO
69	O3	76	GLY
79	Q3	50	GLY
4	s2	68	ILE
8	s6	69	LEU
18	c6	4	VAL
21	c9	100	ILE
34	sR	138	GLY
35	sM	52	PRO
40	l3	141	GLY
40	l3	186	GLY
28	D6	59	TYR
41	L4	4	PRO
49	M3	33	VAL
64	N8	29	PRO
65	N9	29	TYR
5	s3	81	PRO
7	s5	89	ILE
18	c6	33	GLY

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Mol	Chain	Res	Type
20	c8	69	ILE
34	sR	247	PRO
39	l2	49	VAL
44	l7	89	ILE
44	l7	204	PRO
44	l7	210	PRO
44	l7	240	VAL
45	l8	119	GLY
47	m0	16	PRO
79	q3	71	VAL
81	p0	30	VAL
11	S9	168	ARG
14	C2	117	GLY
25	D3	96	VAL
45	L8	167	PRO
55	M9	14	VAL
60	N4	76	VAL
41	l4	190	GLY
76	q0	123	PRO

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%)	125 (76%)	39 (24%)	0	3
2	s0	165/209 (79%)	135 (82%)	30 (18%)	1	8
3	S1	191/223 (86%)	146 (76%)	45 (24%)	1	3
3	s1	192/223 (86%)	147 (77%)	45 (23%)	1	3
4	S2	176/204 (86%)	136 (77%)	40 (23%)	1	3
4	s2	176/204 (86%)	128 (73%)	48 (27%)	0	2
5	S3	182/194 (94%)	140 (77%)	42 (23%)	1	3
5	s3	182/194 (94%)	140 (77%)	42 (23%)	1	3
6	S4	221/221 (100%)	175 (79%)	46 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	s4	221/221 (100%)	173 (78%)	48 (22%)	1	4
7	S5	173/190 (91%)	139 (80%)	34 (20%)	1	6
7	s5	173/190 (91%)	136 (79%)	37 (21%)	1	4
8	S6	188/201 (94%)	151 (80%)	37 (20%)	1	6
8	s6	187/201 (93%)	153 (82%)	34 (18%)	1	8
9	S7	165/169 (98%)	135 (82%)	30 (18%)	1	8
9	s7	165/169 (98%)	130 (79%)	35 (21%)	1	4
10	S8	150/161 (93%)	123 (82%)	27 (18%)	1	8
10	s8	150/161 (93%)	127 (85%)	23 (15%)	2	15
11	S9	158/165 (96%)	119 (75%)	39 (25%)	0	3
11	s9	158/165 (96%)	128 (81%)	30 (19%)	1	7
12	C0	77/98 (79%)	61 (79%)	16 (21%)	1	5
12	c0	73/98 (74%)	60 (82%)	13 (18%)	2	8
13	C1	129/136 (95%)	105 (81%)	24 (19%)	1	7
13	c1	129/136 (95%)	108 (84%)	21 (16%)	2	12
14	C2	88/118 (75%)	67 (76%)	21 (24%)	0	3
14	c2	88/118 (75%)	71 (81%)	17 (19%)	1	6
15	C3	127/127 (100%)	96 (76%)	31 (24%)	0	3
15	c3	127/127 (100%)	102 (80%)	25 (20%)	1	6
16	C4	81/104 (78%)	67 (83%)	14 (17%)	2	10
16	c4	97/104 (93%)	76 (78%)	21 (22%)	1	4
17	C5	101/117 (86%)	79 (78%)	22 (22%)	1	4
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	9
18	C6	117/118 (99%)	97 (83%)	20 (17%)	2	10
18	c6	118/118 (100%)	96 (81%)	22 (19%)	1	7
19	C7	94/124 (76%)	70 (74%)	24 (26%)	0	2
19	c7	92/124 (74%)	72 (78%)	20 (22%)	1	4
20	C8	128/128 (100%)	95 (74%)	33 (26%)	0	2
20	c8	128/128 (100%)	94 (73%)	34 (27%)	0	2
21	C9	115/115 (100%)	86 (75%)	29 (25%)	0	3
21	c9	115/115 (100%)	96 (84%)	19 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	D0	100/113 (88%)	76 (76%)	24 (24%)	0	3
22	d0	103/113 (91%)	72 (70%)	31 (30%)	0	2
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	9
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	4
24	D2	110/110 (100%)	90 (82%)	20 (18%)	1	8
24	d2	110/110 (100%)	89 (81%)	21 (19%)	1	6
25	D3	119/119 (100%)	95 (80%)	24 (20%)	1	5
25	d3	119/119 (100%)	91 (76%)	28 (24%)	1	3
26	D4	112/112 (100%)	93 (83%)	19 (17%)	2	10
26	d4	112/112 (100%)	93 (83%)	19 (17%)	2	10
27	D5	61/88 (69%)	46 (75%)	15 (25%)	0	3
27	d5	61/88 (69%)	48 (79%)	13 (21%)	1	4
28	D6	83/83 (100%)	61 (74%)	22 (26%)	0	2
28	d6	83/83 (100%)	65 (78%)	18 (22%)	1	4
29	D7	70/70 (100%)	59 (84%)	11 (16%)	2	14
29	d7	70/70 (100%)	55 (79%)	15 (21%)	1	4
30	D8	56/59 (95%)	45 (80%)	11 (20%)	1	6
30	d8	56/59 (95%)	43 (77%)	13 (23%)	1	3
31	D9	47/48 (98%)	40 (85%)	7 (15%)	3	16
31	d9	47/48 (98%)	36 (77%)	11 (23%)	1	3
32	E0	51/51 (100%)	42 (82%)	9 (18%)	2	9
33	E1	62/66 (94%)	48 (77%)	14 (23%)	1	3
33	e1	66/66 (100%)	49 (74%)	17 (26%)	0	2
34	SR	260/261 (100%)	223 (86%)	37 (14%)	3	17
34	sR	260/261 (100%)	222 (85%)	38 (15%)	3	16
35	SM	97/228 (42%)	72 (74%)	25 (26%)	0	2
35	sM	54/228 (24%)	45 (83%)	9 (17%)	2	11
39	L2	193/195 (99%)	143 (74%)	50 (26%)	0	2
39	l2	192/195 (98%)	144 (75%)	48 (25%)	0	3
40	L3	320/322 (99%)	256 (80%)	64 (20%)	1	5
40	l3	320/322 (99%)	248 (78%)	72 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	L4	288/288 (100%)	223 (77%)	65 (23%)	1	3
41	l4	288/288 (100%)	229 (80%)	59 (20%)	1	5
42	L5	244/244 (100%)	191 (78%)	53 (22%)	1	4
42	l5	243/244 (100%)	198 (82%)	45 (18%)	1	7
43	L6	134/152 (88%)	108 (81%)	26 (19%)	1	6
43	l6	135/152 (89%)	102 (76%)	33 (24%)	0	3
44	L7	186/204 (91%)	154 (83%)	32 (17%)	2	10
44	l7	187/204 (92%)	152 (81%)	35 (19%)	1	7
45	L8	187/207 (90%)	150 (80%)	37 (20%)	1	5
45	l8	177/207 (86%)	141 (80%)	36 (20%)	1	5
46	L9	171/171 (100%)	127 (74%)	44 (26%)	0	2
46	l9	171/171 (100%)	128 (75%)	43 (25%)	0	3
47	M0	177/186 (95%)	137 (77%)	40 (23%)	1	3
47	m0	179/186 (96%)	144 (80%)	35 (20%)	1	6
48	M1	147/150 (98%)	112 (76%)	35 (24%)	0	3
48	m1	147/150 (98%)	111 (76%)	36 (24%)	0	3
49	M3	154/158 (98%)	122 (79%)	32 (21%)	1	5
49	m3	154/158 (98%)	120 (78%)	34 (22%)	1	4
50	M4	107/108 (99%)	85 (79%)	22 (21%)	1	5
50	m4	108/108 (100%)	86 (80%)	22 (20%)	1	5
51	M5	175/175 (100%)	132 (75%)	43 (25%)	0	3
51	m5	175/175 (100%)	141 (81%)	34 (19%)	1	6
52	M6	160/161 (99%)	121 (76%)	39 (24%)	0	3
52	m6	160/161 (99%)	120 (75%)	40 (25%)	0	3
53	M7	140/145 (97%)	111 (79%)	29 (21%)	1	5
53	m7	125/145 (86%)	101 (81%)	24 (19%)	1	6
54	M8	150/150 (100%)	116 (77%)	34 (23%)	1	3
54	m8	150/150 (100%)	116 (77%)	34 (23%)	1	3
55	M9	153/153 (100%)	124 (81%)	29 (19%)	1	7
55	m9	153/153 (100%)	125 (82%)	28 (18%)	1	7
56	N0	156/156 (100%)	122 (78%)	34 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	n0	156/156 (100%)	122 (78%)	34 (22%)	1	4
57	N1	136/136 (100%)	102 (75%)	34 (25%)	0	3
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	4
58	N2	87/106 (82%)	73 (84%)	14 (16%)	2	13
58	n2	85/106 (80%)	58 (68%)	27 (32%)	0	2
59	N3	104/104 (100%)	84 (81%)	20 (19%)	1	6
59	n3	104/104 (100%)	85 (82%)	19 (18%)	1	7
60	N4	57/129 (44%)	47 (82%)	10 (18%)	2	9
60	n4	100/129 (78%)	79 (79%)	21 (21%)	1	4
61	N5	104/117 (89%)	78 (75%)	26 (25%)	0	3
61	n5	104/117 (89%)	85 (82%)	19 (18%)	1	7
62	N6	109/109 (100%)	88 (81%)	21 (19%)	1	6
62	n6	109/109 (100%)	85 (78%)	24 (22%)	1	4
63	N7	115/115 (100%)	94 (82%)	21 (18%)	1	7
63	n7	115/115 (100%)	87 (76%)	28 (24%)	0	3
64	N8	118/118 (100%)	98 (83%)	20 (17%)	2	11
64	n8	118/118 (100%)	91 (77%)	27 (23%)	1	3
65	N9	46/46 (100%)	35 (76%)	11 (24%)	0	3
65	n9	46/46 (100%)	30 (65%)	16 (35%)	0	1
66	O0	81/87 (93%)	66 (82%)	15 (18%)	1	7
66	o0	84/87 (97%)	69 (82%)	15 (18%)	2	8
67	O1	92/96 (96%)	69 (75%)	23 (25%)	0	3
67	o1	94/96 (98%)	63 (67%)	31 (33%)	0	1
68	O2	109/110 (99%)	87 (80%)	22 (20%)	1	5
68	o2	109/110 (99%)	81 (74%)	28 (26%)	0	2
69	O3	90/90 (100%)	71 (79%)	19 (21%)	1	4
69	o3	90/90 (100%)	75 (83%)	15 (17%)	2	11
70	O4	95/102 (93%)	75 (79%)	20 (21%)	1	4
70	o4	95/102 (93%)	82 (86%)	13 (14%)	3	18
71	O5	104/104 (100%)	83 (80%)	21 (20%)	1	5
71	o5	103/104 (99%)	76 (74%)	27 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	O6	81/81 (100%)	56 (69%)	25 (31%)	0	2
72	o6	80/81 (99%)	53 (66%)	27 (34%)	0	1
73	O7	70/70 (100%)	55 (79%)	15 (21%)	1	4
73	o7	70/70 (100%)	52 (74%)	18 (26%)	0	2
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0	2
74	o8	67/68 (98%)	49 (73%)	18 (27%)	0	2
75	O9	45/45 (100%)	40 (89%)	5 (11%)	6	26
75	o9	45/45 (100%)	33 (73%)	12 (27%)	0	2
76	Q0	47/47 (100%)	41 (87%)	6 (13%)	4	20
76	q0	47/47 (100%)	32 (68%)	15 (32%)	0	2
77	Q1	23/23 (100%)	16 (70%)	7 (30%)	0	2
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	1
78	Q2	90/90 (100%)	67 (74%)	23 (26%)	0	2
78	q2	90/90 (100%)	70 (78%)	20 (22%)	1	4
79	Q3	71/71 (100%)	55 (78%)	16 (22%)	1	3
79	q3	71/71 (100%)	54 (76%)	17 (24%)	0	3
80	e0	53/53 (100%)	38 (72%)	15 (28%)	0	2
81	p0	105/253 (42%)	84 (80%)	21 (20%)	1	5
All	All	18728/20241 (92%)	14710 (78%)	4018 (22%)	1	4

All (4018) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	6	THR
2	S0	10	THR
2	S0	12	GLU
2	S0	18	LEU
2	S0	32	HIS
2	S0	37	VAL
2	S0	49	ASN
2	S0	50	VAL
2	S0	59	LEU
2	S0	62	ARG
2	S0	71	GLU
2	S0	78	SER
2	S0	84	ARG

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Mol	Chain	Res	Type
2	S0	86	VAL
2	S0	88	LYS
2	S0	96	THR
2	S0	98	ILE
2	S0	103	THR
2	S0	110	TYR
2	S0	112	THR
2	S0	123	VAL
2	S0	124	THR
2	S0	140	ASN
2	S0	144	ILE
2	S0	146	LEU
2	S0	153	SER
2	S0	156	VAL
2	S0	157	ASP
2	S0	162	CYS
2	S0	168	HIS
2	S0	172	LEU
2	S0	177	LEU
2	S0	184	LEU
2	S0	185	ARG
2	S0	188	LEU
2	S0	196	SER
2	S0	197	ILE
2	S0	198	MET
2	S0	200	ASP
3	S1	21	VAL
3	S1	22	ASP
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	39	GLU
3	S1	46	THR
3	S1	51	SER
3	S1	61	LEU
3	S1	65	VAL
3	S1	70	LEU
3	S1	72	ASP
3	S1	74	GLN
3	S1	76	SER
3	S1	77	GLU
3	S1	78	ASP

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Mol	Chain	Res	Type
3	S1	79	HIS
3	S1	81	PHE
3	S1	89	ASP
3	S1	97	LEU
3	S1	105	PHE
3	S1	111	ARG
3	S1	115	ARG
3	S1	116	LYS
3	S1	125	VAL
3	S1	126	THR
3	S1	135	LEU
3	S1	140	ILE
3	S1	148	ASN
3	S1	149	GLN
3	S1	170	GLU
3	S1	173	THR
3	S1	180	THR
3	S1	181	LEU
3	S1	184	LEU
3	S1	191	GLU
3	S1	198	GLU
3	S1	202	LYS
3	S1	212	VAL
3	S1	215	VAL
3	S1	218	LEU
3	S1	219	LYS
3	S1	222	LYS
3	S1	223	PHE
3	S1	229	MET
4	S2	41	LEU
4	S2	54	GLU
4	S2	58	LEU
4	S2	69	ILE
4	S2	72	LEU
4	S2	73	LEU
4	S2	77	GLN
4	S2	81	MET
4	S2	87	GLN
4	S2	89	GLN
4	S2	90	THR
4	S2	95	ARG
4	S2	96	THR

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Mol	Chain	Res	Type
4	S2	97	ARG
4	S2	106	ASP
4	S2	108	ASN
4	S2	111	VAL
4	S2	113	LEU
4	S2	117	THR
4	S2	134	LEU
4	S2	140	ARG
4	S2	141	ARG
4	S2	146	THR
4	S2	147	ASN
4	S2	148	LEU
4	S2	166	THR
4	S2	198	THR
4	S2	201	ASN
4	S2	207	LEU
4	S2	210	THR
4	S2	221	THR
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	227	PRO
4	S2	235	LEU
4	S2	237	VAL
4	S2	238	SER
4	S2	240	LEU
4	S2	245	ASP
5	S3	4	LEU
5	S3	10	LYS
5	S3	14	ASP
5	S3	21	LEU
5	S3	23	GLU
5	S3	26	THR
5	S3	37	VAL
5	S3	44	THR
5	S3	59	LEU
5	S3	64	ARG
5	S3	65	ARG
5	S3	76	ARG
5	S3	84	ILE
5	S3	92	GLN
5	S3	94	ARG

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Mol	Chain	Res	Type
5	S3	105	MET
5	S3	111	ASN
5	S3	117	ARG
5	S3	120	TYR
5	S3	143	ARG
5	S3	146	ARG
5	S3	151	LYS
5	S3	154	ASP
5	S3	158	ILE
5	S3	172	THR
5	S3	175	VAL
5	S3	176	LEU
5	S3	177	MET
5	S3	178	ARG
5	S3	179	GLN
5	S3	181	VAL
5	S3	190	ARG
5	S3	195	SER
5	S3	196	ARG
5	S3	202	LEU
5	S3	209	ILE
5	S3	210	GLU
5	S3	218	LEU
5	S3	220	PRO
5	S3	222	VAL
5	S3	223	LYS
5	S3	225	TYR
6	S4	6	LYS
6	S4	7	LYS
6	S4	12	LEU
6	S4	23	LEU
6	S4	26	CYS
6	S4	38	LEU
6	S4	42	LEU
6	S4	45	ILE
6	S4	48	LEU
6	S4	52	LEU
6	S4	56	LEU
6	S4	65	LEU
6	S4	68	ARG
6	S4	69	HIS
6	S4	70	VAL

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Mol	Chain	Res	Type
6	S4	76	VAL
6	S4	77	ARG
6	S4	78	THR
6	S4	81	THR
6	S4	87	MET
6	S4	95	THR
6	S4	116	ASP
6	S4	123	LEU
6	S4	128	LYS
6	S4	129	VAL
6	S4	133	LYS
6	S4	158	ASP
6	S4	160	VAL
6	S4	170	THR
6	S4	180	LEU
6	S4	187	ARG
6	S4	192	ILE
6	S4	206	ASP
6	S4	211	LYS
6	S4	214	LEU
6	S4	215	ASP
6	S4	225	VAL
6	S4	226	PHE
6	S4	227	VAL
6	S4	228	ILE
6	S4	240	LYS
6	S4	242	LYS
6	S4	247	SER
6	S4	248	ILE
6	S4	259	GLN
6	S4	261	LEU
7	S5	23	VAL
7	S5	25	LEU
7	S5	38	THR
7	S5	39	GLU
7	S5	40	ILE
7	S5	41	LYS
7	S5	42	LEU
7	S5	43	PHE
7	S5	45	LYS
7	S5	50	GLU
7	S5	53	VAL

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Mol	Chain	Res	Type
7	S5	63	GLN
7	S5	76	ARG
7	S5	79	ASN
7	S5	86	GLN
7	S5	87	CYS
7	S5	89	ILE
7	S5	90	ILE
7	S5	93	LEU
7	S5	94	THR
7	S5	97	LEU
7	S5	99	MET
7	S5	112	ARG
7	S5	119	ASP
7	S5	122	ASN
7	S5	123	VAL
7	S5	148	ARG
7	S5	156	ARG
7	S5	157	ARG
7	S5	161	ASP
7	S5	169	ASN
7	S5	186	ASN
7	S5	219	ARG
7	S5	225	ARG
8	S6	12	SER
8	S6	13	GLN
8	S6	15	THR
8	S6	16	PHE
8	S6	25	ARG
8	S6	44	GLU
8	S6	51	LYS
8	S6	52	ILE
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	81	VAL
8	S6	82	SER
8	S6	89	ASP
8	S6	109	LEU
8	S6	115	LYS

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Mol	Chain	Res	Type
8	S6	120	GLU
8	S6	125	THR
8	S6	128	THR
8	S6	133	LEU
8	S6	151	ASP
8	S6	155	ASP
8	S6	162	VAL
8	S6	168	THR
8	S6	169	TYR
8	S6	170	THR
8	S6	175	ILE
8	S6	177	ARG
8	S6	180	THR
8	S6	181	PRO
8	S6	193	LEU
8	S6	211	LEU
8	S6	212	LEU
8	S6	223	LYS
9	S7	7	LYS
9	S7	11	GLN
9	S7	15	GLU
9	S7	19	GLN
9	S7	28	GLU
9	S7	37	GLU
9	S7	38	LEU
9	S7	39	ARG
9	S7	49	ILE
9	S7	51	VAL
9	S7	60	ILE
9	S7	70	PHE
9	S7	71	HIS
9	S7	77	LEU
9	S7	79	ARG
9	S7	85	PHE
9	S7	92	PHE
9	S7	95	GLU
9	S7	97	ARG
9	S7	109	VAL
9	S7	114	ARG
9	S7	126	LEU
9	S7	129	LEU
9	S7	130	VAL

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Mol	Chain	Res	Type
9	S7	144	VAL
9	S7	147	ASN
9	S7	166	LEU
9	S7	167	GLU
9	S7	181	ILE
9	S7	185	ILE
10	S8	7	SER
10	S8	9	HIS
10	S8	14	THR
10	S8	21	PHE
10	S8	22	ARG
10	S8	25	ARG
10	S8	26	LYS
10	S8	29	LEU
10	S8	43	ILE
10	S8	45	SER
10	S8	46	VAL
10	S8	49	ARG
10	S8	58	LEU
10	S8	59	ARG
10	S8	66	SER
10	S8	72	ILE
10	S8	97	THR
10	S8	98	LYS
10	S8	103	GLN
10	S8	107	THR
10	S8	110	ARG
10	S8	138	ASN
10	S8	140	GLU
10	S8	152	ILE
10	S8	164	ARG
10	S8	187	GLU
10	S8	196	LEU
11	S9	3	ARG
11	S9	6	ARG
11	S9	7	THR
11	S9	14	THR
11	S9	17	ARG
11	S9	21	SER
11	S9	28	LEU
11	S9	36	LEU
11	S9	39	LYS

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Mol	Chain	Res	Type
11	S9	49	LEU
11	S9	63	ASP
11	S9	74	ASN
11	S9	77	ILE
11	S9	78	ARG
11	S9	79	ARG
11	S9	82	ARG
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	97	LEU
11	S9	99	LEU
11	S9	101	VAL
11	S9	105	LEU
11	S9	109	LEU
11	S9	110	GLN
11	S9	115	LYS
11	S9	118	LEU
11	S9	122	VAL
11	S9	126	ARG
11	S9	134	ILE
11	S9	138	LYS
11	S9	140	ILE
11	S9	149	ARG
11	S9	157	ASP
11	S9	168	ARG
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	182	GLU
12	C0	5	LYS
12	C0	8	ARG
12	C0	20	VAL
12	C0	25	LYS
12	C0	27	PHE
12	C0	28	ASN
12	C0	29	GLN
12	C0	31	LYS
12	C0	33	GLU
12	C0	46	LEU
12	C0	55	VAL
12	C0	56	LYS

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Mol	Chain	Res	Type
12	C0	71	GLU
12	C0	76	LEU
12	C0	79	TYR
12	C0	82	LEU
13	C1	18	HIS
13	C1	21	ASN
13	C1	29	LYS
13	C1	36	LYS
13	C1	40	LEU
13	C1	44	THR
13	C1	56	LYS
13	C1	67	ARG
13	C1	69	LYS
13	C1	72	THR
13	C1	75	VAL
13	C1	80	MET
13	C1	83	THR
13	C1	88	ARG
13	C1	90	TYR
13	C1	91	LEU
13	C1	94	ILE
13	C1	101	GLU
13	C1	105	LYS
13	C1	109	VAL
13	C1	123	VAL
13	C1	129	ARG
13	C1	131	ILE
13	C1	140	VAL
14	C2	43	ARG
14	C2	53	THR
14	C2	62	LEU
14	C2	63	VAL
14	C2	66	VAL
14	C2	71	ILE
14	C2	74	LEU
14	C2	81	ASP
14	C2	86	VAL
14	C2	89	ILE
14	C2	97	LEU
14	C2	103	LEU
14	C2	119	SER
14	C2	126	TRP

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Mol	Chain	Res	Type
14	C2	129	GLU
14	C2	132	GLU
14	C2	136	ILE
14	C2	139	HIS
14	C2	140	PHE
14	C2	141	SER
14	C2	143	GLN
15	C3	3	ARG
15	C3	11	ILE
15	C3	16	ILE
15	C3	27	LYS
15	C3	31	GLU
15	C3	32	SER
15	C3	35	GLU
15	C3	39	LYS
15	C3	61	THR
15	C3	64	ARG
15	C3	70	LYS
15	C3	72	MET
15	C3	76	LYS
15	C3	77	SER
15	C3	80	LEU
15	C3	83	GLU
15	C3	88	LEU
15	C3	99	ARG
15	C3	102	LEU
15	C3	103	GLU
15	C3	105	ASN
15	C3	106	ARG
15	C3	107	LYS
15	C3	109	LYS
15	C3	115	LEU
15	C3	120	SER
15	C3	125	LEU
15	C3	131	THR
15	C3	140	LYS
15	C3	141	TYR
15	C3	142	GLU
16	C4	14	PHE
16	C4	22	SER
16	C4	26	THR
16	C4	29	HIS

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Mol	Chain	Res	Type
16	C4	39	ILE
16	C4	42	VAL
16	C4	55	SER
16	C4	86	THR
16	C4	89	THR
16	C4	92	LYS
16	C4	103	ARG
16	C4	123	SER
16	C4	124	ASP
16	C4	137	LEU
17	C5	14	THR
17	C5	20	VAL
17	C5	22	LEU
17	C5	26	LEU
17	C5	28	MET
17	C5	29	SER
17	C5	31	GLU
17	C5	34	VAL
17	C5	35	LYS
17	C5	36	LEU
17	C5	40	ARG
17	C5	43	ARG
17	C5	89	MET
17	C5	90	ILE
17	C5	94	VAL
17	C5	98	ASN
17	C5	106	GLU
17	C5	110	GLU
17	C5	121	ILE
17	C5	124	THR
17	C5	128	HIS
17	C5	130	ARG
18	C6	4	VAL
18	C6	13	LYS
18	C6	19	VAL
18	C6	28	LEU
18	C6	45	ARG
18	C6	48	VAL
18	C6	50	GLU
18	C6	54	LEU
18	C6	57	LEU
18	C6	66	ARG

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Mol	Chain	Res	Type
18	C6	85	ILE
18	C6	89	LEU
18	C6	105	LEU
18	C6	109	PHE
18	C6	114	ARG
18	C6	121	SER
18	C6	123	ARG
18	C6	127	LYS
18	C6	128	LYS
18	C6	137	ARG
19	C7	3	ARG
19	C7	5	ARG
19	C7	6	THR
19	C7	7	LYS
19	C7	8	THR
19	C7	25	THR
19	C7	34	LEU
19	C7	38	ILE
19	C7	40	THR
19	C7	43	SER
19	C7	46	LEU
19	C7	49	LYS
19	C7	54	THR
19	C7	58	MET
19	C7	62	GLN
19	C7	69	ILE
19	C7	72	LYS
19	C7	78	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	88	VAL
19	C7	107	SER
19	C7	113	LEU
19	C7	115	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	6	GLN
20	C8	8	GLN
20	C8	10	SER
20	C8	11	PHE
20	C8	13	HIS
20	C8	14	ILE

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Mol	Chain	Res	Type
20	C8	15	LEU
20	C8	17	LEU
20	C8	20	THR
20	C8	32	LEU
20	C8	40	ARG
20	C8	47	CYS
20	C8	53	ASP
20	C8	54	LEU
20	C8	61	LEU
20	C8	71	GLN
20	C8	77	THR
20	C8	80	LYS
20	C8	82	PRO
20	C8	89	GLN
20	C8	92	ILE
20	C8	93	THR
20	C8	115	ARG
20	C8	119	ILE
20	C8	120	ARG
20	C8	132	ARG
20	C8	136	GLN
20	C8	138	THR
20	C8	141	THR
20	C8	143	ARG
20	C8	144	ARG
21	C9	6	VAL
21	C9	15	ILE
21	C9	18	TYR
21	C9	22	LEU
21	C9	25	GLN
21	C9	28	LEU
21	C9	30	VAL
21	C9	33	TYR
21	C9	34	VAL
21	C9	35	ASP
21	C9	36	ILE
21	C9	39	THR
21	C9	43	ASN
21	C9	57	ARG
21	C9	60	SER
21	C9	63	ARG
21	C9	67	MET

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Mol	Chain	Res	Type
21	C9	70	GLN
21	C9	71	VAL
21	C9	73	VAL
21	C9	76	LEU
21	C9	89	ARG
21	C9	115	GLU
21	C9	122	ARG
21	C9	124	ILE
21	C9	125	SER
21	C9	130	ARG
21	C9	139	THR
21	C9	143	ASP
22	D0	15	GLN
22	D0	21	LYS
22	D0	22	ILE
22	D0	23	ARG
22	D0	27	THR
22	D0	31	VAL
22	D0	46	GLU
22	D0	50	LEU
22	D0	51	VAL
22	D0	57	ARG
22	D0	60	THR
22	D0	64	LYS
22	D0	66	SER
22	D0	70	THR
22	D0	72	ASN
22	D0	74	GLU
22	D0	76	SER
22	D0	89	ARG
22	D0	97	VAL
22	D0	99	ILE
22	D0	103	ILE
22	D0	108	ILE
22	D0	109	GLU
22	D0	117	VAL
23	D1	1	MET
23	D1	2	GLU
23	D1	5	LYS
23	D1	11	LEU
23	D1	25	LYS
23	D1	32	VAL

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Mol	Chain	Res	Type
23	D1	49	GLU
23	D1	62	ARG
23	D1	69	LEU
23	D1	72	LEU
23	D1	78	LEU
23	D1	80	LYS
23	D1	87	ARG
24	D2	2	THR
24	D2	7	LEU
24	D2	12	ASN
24	D2	22	LYS
24	D2	23	ARG
24	D2	24	GLN
24	D2	26	LEU
24	D2	37	PHE
24	D2	53	ILE
24	D2	56	HIS
24	D2	65	LEU
24	D2	68	ARG
24	D2	76	SER
24	D2	86	ILE
24	D2	93	LEU
24	D2	97	ARG
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	121	VAL
25	D3	3	LYS
25	D3	7	ARG
25	D3	14	LYS
25	D3	16	ARG
25	D3	18	HIS
25	D3	19	ARG
25	D3	26	GLU
25	D3	28	ASN
25	D3	40	SER
25	D3	47	SER
25	D3	53	VAL
25	D3	66	SER
25	D3	69	ARG
25	D3	72	VAL
25	D3	75	GLN

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Mol	Chain	Res	Type
25	D3	84	THR
25	D3	96	VAL
25	D3	107	PHE
25	D3	109	ARG
25	D3	110	LYS
25	D3	114	LYS
25	D3	127	VAL
25	D3	132	LEU
25	D3	140	LYS
26	D4	13	ILE
26	D4	21	LYS
26	D4	24	VAL
26	D4	28	LEU
26	D4	32	ARG
26	D4	34	ASN
26	D4	35	VAL
26	D4	37	LYS
26	D4	51	GLU
26	D4	74	LEU
26	D4	88	THR
26	D4	98	GLU
26	D4	99	LYS
26	D4	102	LYS
26	D4	105	ARG
26	D4	123	LYS
26	D4	124	ARG
26	D4	125	LEU
26	D4	128	LYS
27	D5	37	GLN
27	D5	42	LEU
27	D5	50	ILE
27	D5	59	TYR
27	D5	60	VAL
27	D5	62	VAL
27	D5	67	ASP
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	92	ILE
27	D5	95	HIS
27	D5	97	LYS
27	D5	100	ILE

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Mol	Chain	Res	Type
27	D5	102	THR
28	D6	5	ARG
28	D6	12	LYS
28	D6	19	LYS
28	D6	21	VAL
28	D6	30	ILE
28	D6	36	ILE
28	D6	38	ARG
28	D6	41	ILE
28	D6	44	ILE
28	D6	45	VAL
28	D6	46	GLU
28	D6	61	GLU
28	D6	64	LEU
28	D6	66	LYS
28	D6	67	THR
28	D6	69	ASN
28	D6	82	ARG
28	D6	85	ARG
28	D6	86	VAL
28	D6	88	SER
28	D6	90	GLU
28	D6	91	ASP
29	D7	2	VAL
29	D7	3	LEU
29	D7	5	GLN
29	D7	20	LYS
29	D7	26	GLN
29	D7	33	LEU
29	D7	34	ASP
29	D7	41	LEU
29	D7	42	ASN
29	D7	63	LEU
29	D7	65	THR
30	D8	8	THR
30	D8	12	VAL
30	D8	13	ILE
30	D8	14	LYS
30	D8	15	VAL
30	D8	19	THR
30	D8	26	THR
30	D8	32	PHE

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Mol	Chain	Res	Type
30	D8	40	ILE
30	D8	52	ASP
30	D8	58	GLU
31	D9	5	ASN
31	D9	7	TRP
31	D9	21	CYS
31	D9	22	ARG
31	D9	30	LEU
31	D9	40	ARG
31	D9	42	CYS
32	E0	20	LYS
32	E0	22	GLU
32	E0	28	LYS
32	E0	41	THR
32	E0	42	ARG
32	E0	47	VAL
32	E0	49	LEU
32	E0	54	ARG
32	E0	56	MET
33	E1	84	VAL
33	E1	86	THR
33	E1	89	LYS
33	E1	93	HIS
33	E1	94	LYS
33	E1	97	LYS
33	E1	102	VAL
33	E1	107	LYS
33	E1	113	LYS
33	E1	115	THR
33	E1	116	LYS
33	E1	120	GLU
33	E1	146	SER
33	E1	147	VAL
34	SR	10	ARG
34	SR	14	GLU
34	SR	17	ASN
34	SR	37	SER
34	SR	48	THR
34	SR	50	ASP
34	SR	52	GLN
34	SR	66	HIS
34	SR	74	THR

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Mol	Chain	Res	Type
34	SR	76	ASP
34	SR	89	LEU
34	SR	94	VAL
34	SR	96	THR
34	SR	102	ARG
34	SR	113	VAL
34	SR	115	ILE
34	SR	117	LYS
34	SR	144	LEU
34	SR	149	ASP
34	SR	154	VAL
34	SR	164	ASP
34	SR	165	ASP
34	SR	188	ILE
34	SR	196	ASN
34	SR	199	ILE
34	SR	207	ASP
34	SR	221	MET
34	SR	231	MET
34	SR	238	ASP
34	SR	241	PHE
34	SR	248	ASN
34	SR	268	GLN
34	SR	269	TYR
34	SR	295	SER
34	SR	300	THR
34	SR	316	MET
34	SR	317	THR
35	SM	23	LYS
35	SM	24	GLU
35	SM	34	LYS
35	SM	45	SER
35	SM	46	LYS
35	SM	48	ARG
35	SM	51	ARG
35	SM	53	ARG
35	SM	61	ILE
35	SM	64	LYS
35	SM	68	ARG
35	SM	69	ARG
35	SM	84	LYS
35	SM	89	ARG

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Mol	Chain	Res	Type
35	SM	91	THR
35	SM	94	HIS
35	SM	100	THR
35	SM	101	ASP
35	SM	102	THR
35	SM	104	LYS
35	SM	105	LYS
35	SM	117	LEU
35	SM	121	LYS
35	SM	133	GLU
35	SM	139	GLU
39	L2	6	ARG
39	L2	19	HIS
39	L2	20	THR
39	L2	31	THR
39	L2	32	LEU
39	L2	33	ASP
39	L2	36	GLU
39	L2	41	ILE
39	L2	44	ILE
39	L2	45	VAL
39	L2	46	LYS
39	L2	48	ILE
39	L2	49	VAL
39	L2	52	SER
39	L2	61	VAL
39	L2	62	VAL
39	L2	70	ARG
39	L2	71	LEU
39	L2	73	GLU
39	L2	74	GLU
39	L2	84	THR
39	L2	97	ASN
39	L2	104	LEU
39	L2	107	VAL
39	L2	109	GLU
39	L2	114	SER
39	L2	116	VAL
39	L2	118	GLU
39	L2	143	GLU
39	L2	145	LYS
39	L2	157	VAL

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Mol	Chain	Res	Type
39	L2	165	VAL
39	L2	179	LEU
39	L2	180	LEU
39	L2	190	ARG
39	L2	192	LYS
39	L2	199	THR
39	L2	204	MET
39	L2	205	ASN
39	L2	206	PRO
39	L2	207	VAL
39	L2	218	HIS
39	L2	223	SER
39	L2	225	ILE
39	L2	226	SER
39	L2	227	ARG
39	L2	230	VAL
39	L2	238	ILE
39	L2	242	ARG
39	L2	247	ARG
40	L3	4	ARG
40	L3	7	GLU
40	L3	17	LEU
40	L3	19	ARG
40	L3	25	ILE
40	L3	30	LYS
40	L3	37	ARG
40	L3	39	LYS
40	L3	43	LEU
40	L3	45	SER
40	L3	55	THR
40	L3	61	ASP
40	L3	66	LYS
40	L3	73	VAL
40	L3	79	VAL
40	L3	85	VAL
40	L3	87	VAL
40	L3	100	ARG
40	L3	103	THR
40	L3	112	ASP
40	L3	114	VAL
40	L3	116	ARG
40	L3	120	LYS

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Mol	Chain	Res	Type
40	L3	124	LYS
40	L3	139	GLN
40	L3	146	ARG
40	L3	148	LEU
40	L3	150	ARG
40	L3	157	VAL
40	L3	159	ARG
40	L3	160	VAL
40	L3	168	LYS
40	L3	173	GLN
40	L3	178	LEU
40	L3	188	ILE
40	L3	196	ARG
40	L3	202	THR
40	L3	205	VAL
40	L3	208	VAL
40	L3	210	GLU
40	L3	226	PHE
40	L3	229	VAL
40	L3	238	LEU
40	L3	246	LEU
40	L3	252	ILE
40	L3	264	VAL
40	L3	284	ARG
40	L3	291	GLU
40	L3	293	ASN
40	L3	305	ILE
40	L3	306	THR
40	L3	317	ILE
40	L3	319	ASN
40	L3	320	ASP
40	L3	324	VAL
40	L3	328	ILE
40	L3	332	ARG
40	L3	338	LEU
40	L3	343	TYR
40	L3	344	THR
40	L3	347	SER
40	L3	352	GLU
40	L3	354	VAL
40	L3	356	LEU
41	L4	2	SER

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Mol	Chain	Res	Type
41	L4	25	VAL
41	L4	37	THR
41	L4	41	SER
41	L4	47	ARG
41	L4	60	THR
41	L4	69	ARG
41	L4	74	ILE
41	L4	92	ASN
41	L4	93	MET
41	L4	99	MET
41	L4	105	THR
41	L4	108	LYS
41	L4	112	LYS
41	L4	114	ASN
41	L4	120	TYR
41	L4	133	SER
41	L4	138	ARG
41	L4	142	VAL
41	L4	148	ILE
41	L4	150	LEU
41	L4	152	VAL
41	L4	156	LEU
41	L4	158	SER
41	L4	161	LYS
41	L4	169	LEU
41	L4	170	LYS
41	L4	176	SER
41	L4	179	LEU
41	L4	180	LYS
41	L4	185	LYS
41	L4	187	LEU
41	L4	193	LYS
41	L4	194	TYR
41	L4	196	ASN
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	250	TRP

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Mol	Chain	Res	Type
41	L4	256	THR
41	L4	258	LEU
41	L4	259	ASP
41	L4	265	GLU
41	L4	267	VAL
41	L4	272	VAL
41	L4	278	SER
41	L4	282	SER
41	L4	287	THR
41	L4	288	ARG
41	L4	295	ILE
41	L4	299	ILE
41	L4	300	ARG
41	L4	306	THR
41	L4	308	LYS
41	L4	313	LEU
41	L4	323	VAL
41	L4	338	LYS
41	L4	347	THR
41	L4	350	LYS
41	L4	354	VAL
41	L4	356	THR
42	L5	4	GLN
42	L5	5	LYS
42	L5	9	SER
42	L5	22	ARG
42	L5	23	ARG
42	L5	35	ARG
42	L5	41	LYS
42	L5	58	LYS
42	L5	66	SER
42	L5	69	ILE
42	L5	85	ARG
42	L5	88	ILE
42	L5	89	THR
42	L5	105	ILE
42	L5	109	THR
42	L5	112	LYS
42	L5	115	LEU
42	L5	122	VAL
42	L5	125	VAL
42	L5	131	LEU

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Mol	Chain	Res	Type
42	L5	132	THR
42	L5	140	ARG
42	L5	144	VAL
42	L5	146	LEU
42	L5	148	ILE
42	L5	151	GLN
42	L5	152	ARG
42	L5	154	THR
42	L5	155	THR
42	L5	163	LEU
42	L5	177	GLU
42	L5	181	PRO
42	L5	185	PHE
42	L5	187	THR
42	L5	188	GLU
42	L5	190	ILE
42	L5	194	LEU
42	L5	196	ARG
42	L5	197	SER
42	L5	203	HIS
42	L5	211	LEU
42	L5	217	GLU
42	L5	218	ARG
42	L5	222	LEU
42	L5	229	ASP
42	L5	235	SER
42	L5	257	GLU
42	L5	259	LYS
42	L5	263	GLU
42	L5	268	GLU
42	L5	277	LEU
42	L5	290	ILE
42	L5	293	LEU
43	L6	5	LYS
43	L6	9	TRP
43	L6	15	VAL
43	L6	21	THR
43	L6	28	GLN
43	L6	30	LEU
43	L6	35	VAL
43	L6	46	ARG
43	L6	52	VAL

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Mol	Chain	Res	Type
43	L6	64	LEU
43	L6	76	LEU
43	L6	77	ARG
43	L6	78	ARG
43	L6	85	ILE
43	L6	89	THR
43	L6	90	LYS
43	L6	100	LYS
43	L6	109	GLU
43	L6	129	GLU
43	L6	134	ARG
43	L6	140	VAL
43	L6	145	LEU
43	L6	152	THR
43	L6	154	LEU
43	L6	155	LEU
43	L6	156	LYS
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	30	ARG
44	L7	37	ASN
44	L7	46	GLU
44	L7	48	ASN
44	L7	53	LYS
44	L7	59	GLU
44	L7	60	ARG
44	L7	82	LYS
44	L7	83	LEU
44	L7	92	ILE
44	L7	93	ASN
44	L7	109	THR
44	L7	110	ARG
44	L7	111	ILE
44	L7	115	THR
44	L7	124	LEU
44	L7	129	LEU
44	L7	151	ARG
44	L7	153	PHE
44	L7	156	ILE
44	L7	158	LYS
44	L7	173	LEU

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Mol	Chain	Res	Type
44	L7	179	LEU
44	L7	180	SER
44	L7	181	ILE
44	L7	184	LEU
44	L7	190	THR
44	L7	238	LYS
44	L7	239	LEU
45	L8	26	LEU
45	L8	27	THR
45	L8	31	PRO
45	L8	38	GLN
45	L8	41	GLN
45	L8	47	SER
45	L8	50	VAL
45	L8	58	VAL
45	L8	63	LYS
45	L8	67	ILE
45	L8	69	LEU
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	82	LEU
45	L8	84	ARG
45	L8	106	LYS
45	L8	108	ARG
45	L8	118	GLU
45	L8	126	SER
45	L8	132	VAL
45	L8	136	LEU
45	L8	150	LEU
45	L8	156	ASP
45	L8	160	ILE
45	L8	163	VAL
45	L8	169	LEU
45	L8	172	LYS
45	L8	181	LYS
45	L8	185	ARG
45	L8	194	THR
45	L8	201	THR
45	L8	206	GLU
45	L8	211	LEU
45	L8	216	SER

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Mol	Chain	Res	Type
45	L8	232	HIS
45	L8	240	ASN
46	L9	1	MET
46	L9	4	ILE
46	L9	5	GLN
46	L9	9	GLN
46	L9	14	GLU
46	L9	16	VAL
46	L9	17	THR
46	L9	18	VAL
46	L9	19	SER
46	L9	20	ILE
46	L9	33	THR
46	L9	41	ILE
46	L9	44	THR
46	L9	46	THR
46	L9	47	LYS
46	L9	48	VAL
46	L9	49	ASN
46	L9	52	LEU
46	L9	62	ARG
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	73	SER
46	L9	79	ILE
46	L9	82	VAL
46	L9	83	THR
46	L9	84	LYS
46	L9	120	ASP
46	L9	126	VAL
46	L9	132	VAL
46	L9	138	THR
46	L9	139	ASN
46	L9	146	LEU
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	168	ARG

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Mol	Chain	Res	Type
46	L9	172	ILE
46	L9	174	LYS
46	L9	188	THR
46	L9	189	GLU
47	M0	3	ARG
47	M0	7	ARG
47	M0	15	LYS
47	M0	21	ARG
47	M0	26	VAL
47	M0	30	LYS
47	M0	32	ARG
47	M0	34	TYR
47	M0	39	LYS
47	M0	48	LEU
47	M0	52	LEU
47	M0	57	LEU
47	M0	66	GLU
47	M0	74	LYS
47	M0	82	ARG
47	M0	87	LEU
47	M0	90	ARG
47	M0	99	ILE
47	M0	102	MET
47	M0	116	ARG
47	M0	125	LEU
47	M0	128	ARG
47	M0	130	ASP
47	M0	138	VAL
47	M0	139	ARG
47	M0	144	ASN
47	M0	145	LYS
47	M0	146	ASP
47	M0	156	ARG
47	M0	163	GLN
47	M0	165	ILE
47	M0	166	ILE
47	M0	169	LYS
47	M0	176	LEU
47	M0	177	ASP
47	M0	184	LYS
47	M0	185	ARG
47	M0	189	GLU

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Mol	Chain	Res	Type
47	M0	203	LYS
47	M0	208	ASN
48	M1	9	MET
48	M1	10	ARG
48	M1	11	ASP
48	M1	12	LEU
48	M1	13	LYS
48	M1	16	LYS
48	M1	19	LEU
48	M1	23	VAL
48	M1	26	SER
48	M1	30	LEU
48	M1	34	SER
48	M1	44	THR
48	M1	46	VAL
48	M1	56	THR
48	M1	65	ILE
48	M1	71	VAL
48	M1	80	LEU
48	M1	82	ARG
48	M1	92	ARG
48	M1	94	ARG
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	115	LYS
48	M1	132	ASN
48	M1	133	ARG
48	M1	137	ARG
48	M1	138	VAL
48	M1	140	ARG
48	M1	143	ARG
48	M1	151	SER
48	M1	154	THR
48	M1	161	SER
48	M1	166	LYS
48	M1	171	VAL
49	M3	10	LEU
49	M3	11	LYS
49	M3	17	HIS
49	M3	23	LYS
49	M3	24	VAL

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Mol	Chain	Res	Type
49	M3	34	SER
49	M3	53	LEU
49	M3	54	LEU
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	79	GLU
49	M3	85	LEU
49	M3	97	VAL
49	M3	107	GLU
49	M3	108	ILE
49	M3	113	VAL
49	M3	121	SER
49	M3	124	ILE
49	M3	128	ARG
49	M3	131	LYS
49	M3	136	GLU
49	M3	144	THR
49	M3	164	GLU
49	M3	169	THR
49	M3	171	ARG
49	M3	175	SER
49	M3	190	LYS
49	M3	192	GLU
50	M4	3	THR
50	M4	5	SER
50	M4	8	LYS
50	M4	15	VAL
50	M4	25	LYS
50	M4	27	GLN
50	M4	38	ILE
50	M4	39	ILE
50	M4	44	VAL
50	M4	50	LYS
50	M4	53	VAL
50	M4	58	ILE
50	M4	63	VAL
50	M4	65	LEU
50	M4	69	THR

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Mol	Chain	Res	Type
50	M4	72	LEU
50	M4	82	SER
50	M4	90	VAL
50	M4	91	CYS
50	M4	102	LYS
50	M4	105	GLN
50	M4	107	GLU
51	M5	10	LEU
51	M5	13	LYS
51	M5	18	VAL
51	M5	19	LEU
51	M5	20	ARG
51	M5	22	LEU
51	M5	24	ARG
51	M5	33	LYS
51	M5	38	ARG
51	M5	41	ARG
51	M5	43	THR
51	M5	44	ARG
51	M5	49	ARG
51	M5	56	LYS
51	M5	62	TYR
51	M5	64	VAL
51	M5	68	ARG
51	M5	71	ARG
51	M5	75	VAL
51	M5	80	THR
51	M5	83	LYS
51	M5	86	ASN
51	M5	90	ASN
51	M5	93	LYS
51	M5	98	LEU
51	M5	104	GLU
51	M5	106	VAL
51	M5	109	ARG
51	M5	117	ASN
51	M5	133	ILE
51	M5	144	ARG
51	M5	151	ILE
51	M5	153	ASP
51	M5	157	LYS
51	M5	159	ARG

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Mol	Chain	Res	Type
51	M5	170	LYS
51	M5	182	ASN
51	M5	188	ARG
51	M5	190	THR
51	M5	195	ASN
51	M5	198	SER
51	M5	201	ARG
51	M5	204	LYS
52	M6	8	VAL
52	M6	22	VAL
52	M6	33	ILE
52	M6	34	VAL
52	M6	35	VAL
52	M6	41	LEU
52	M6	44	SER
52	M6	56	ASP
52	M6	57	PHE
52	M6	68	ARG
52	M6	74	ARG
52	M6	78	ARG
52	M6	79	ILE
52	M6	84	LEU
52	M6	85	ARG
52	M6	91	LYS
52	M6	101	ARG
52	M6	106	GLU
52	M6	117	ARG
52	M6	120	VAL
52	M6	122	GLN
52	M6	124	LEU
52	M6	126	VAL
52	M6	128	ARG
52	M6	134	LYS
52	M6	143	THR
52	M6	150	GLU
52	M6	151	ASP
52	M6	152	VAL
52	M6	155	LYS
52	M6	160	ARG
52	M6	164	SER
52	M6	170	LYS
52	M6	175	THR

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Mol	Chain	Res	Type
52	M6	182	ASN
52	M6	184	THR
52	M6	187	GLU
52	M6	188	SER
52	M6	190	VAL
53	M7	7	THR
53	M7	8	SER
53	M7	9	THR
53	M7	14	SER
53	M7	23	ARG
53	M7	30	ARG
53	M7	32	THR
53	M7	36	ILE
53	M7	49	GLU
53	M7	52	LEU
53	M7	53	ASP
53	M7	56	ARG
53	M7	69	ARG
53	M7	76	PHE
53	M7	78	VAL
53	M7	79	THR
53	M7	87	SER
53	M7	91	VAL
53	M7	94	LEU
53	M7	105	LYS
53	M7	115	SER
53	M7	126	ARG
53	M7	127	ARG
53	M7	128	ARG
53	M7	141	SER
53	M7	144	SER
53	M7	154	GLU
53	M7	168	LEU
53	M7	181	ARG
54	M8	3	ILE
54	M8	7	SER
54	M8	15	HIS
54	M8	17	THR
54	M8	22	ASP
54	M8	26	LEU
54	M8	30	VAL
54	M8	32	LEU

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Mol	Chain	Res	Type
54	M8	34	THR
54	M8	36	LEU
54	M8	39	ARG
54	M8	40	THR
54	M8	41	ASP
54	M8	50	LYS
54	M8	63	SER
54	M8	66	ARG
54	M8	67	ILE
54	M8	69	ARG
54	M8	74	GLU
54	M8	81	VAL
54	M8	86	THR
54	M8	95	GLU
54	M8	98	LYS
54	M8	111	ARG
54	M8	113	LYS
54	M8	129	VAL
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	146	SER
54	M8	171	LYS
54	M8	178	ARG
54	M8	179	ARG
54	M8	181	SER
55	M9	5	ARG
55	M9	7	GLN
55	M9	9	ARG
55	M9	41	ILE
55	M9	44	LEU
55	M9	51	VAL
55	M9	52	LYS
55	M9	55	VAL
55	M9	57	VAL
55	M9	60	LYS
55	M9	71	ARG
55	M9	74	ARG
55	M9	81	ARG
55	M9	85	ARG
55	M9	91	SER
55	M9	103	ARG

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Mol	Chain	Res	Type
55	M9	104	ARG
55	M9	106	LEU
55	M9	116	ASP
55	M9	128	LYS
55	M9	133	LYS
55	M9	134	HIS
55	M9	153	LYS
55	M9	155	LEU
55	M9	160	GLU
55	M9	164	LEU
55	M9	171	ASP
55	M9	176	ARG
55	M9	180	LYS
56	N0	1	MET
56	N0	3	HIS
56	N0	8	GLN
56	N0	16	THR
56	N0	23	LYS
56	N0	39	SER
56	N0	40	ARG
56	N0	45	LEU
56	N0	46	GLN
56	N0	51	VAL
56	N0	57	GLU
56	N0	61	ILE
56	N0	62	ASN
56	N0	71	LYS
56	N0	81	TYR
56	N0	87	THR
56	N0	104	GLU
56	N0	105	THR
56	N0	113	ARG
56	N0	115	ARG
56	N0	117	ARG
56	N0	122	HIS
56	N0	137	ARG
56	N0	138	GLN
56	N0	139	TYR
56	N0	145	THR
56	N0	155	ARG
56	N0	157	GLN
56	N0	158	LYS

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Mol	Chain	Res	Type
56	N0	160	THR
56	N0	162	THR
56	N0	167	ARG
56	N0	169	SER
56	N0	171	PHE
57	N1	9	SER
57	N1	12	ARG
57	N1	18	ASP
57	N1	27	LEU
57	N1	29	THR
57	N1	36	VAL
57	N1	38	ASP
57	N1	48	ILE
57	N1	52	MET
57	N1	60	LYS
57	N1	64	VAL
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	92	ARG
57	N1	97	LYS
57	N1	103	GLN
57	N1	104	GLU
57	N1	106	LEU
57	N1	122	GLN
57	N1	126	VAL
57	N1	128	LEU
57	N1	136	ARG
57	N1	139	ARG
57	N1	140	ILE
57	N1	141	VAL
57	N1	143	THR
57	N1	144	GLU
57	N1	149	GLN
57	N1	154	VAL
57	N1	158	THR
58	N2	10	LYS
58	N2	14	THR
58	N2	21	SER

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Mol	Chain	Res	Type
58	N2	37	LEU
58	N2	38	ILE
58	N2	43	VAL
58	N2	52	ASN
58	N2	63	VAL
58	N2	81	LYS
58	N2	88	GLN
58	N2	93	ILE
58	N2	95	PHE
58	N2	100	THR
58	N2	105	LEU
59	N3	13	ILE
59	N3	32	ARG
59	N3	33	ASN
59	N3	45	ARG
59	N3	58	VAL
59	N3	63	LYS
59	N3	69	LEU
59	N3	72	LYS
59	N3	74	MET
59	N3	78	VAL
59	N3	83	LYS
59	N3	91	VAL
59	N3	98	ASN
59	N3	102	ILE
59	N3	104	ASN
59	N3	106	LYS
59	N3	120	LYS
59	N3	125	LEU
59	N3	132	ASN
59	N3	136	VAL
60	N4	5	ILE
60	N4	7	SER
60	N4	19	THR
60	N4	27	LYS
60	N4	31	PHE
60	N4	45	ASN
60	N4	52	THR
60	N4	53	VAL
60	N4	54	LEU
60	N4	58	HIS
61	N5	27	ARG

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Mol	Chain	Res	Type
61	N5	33	ARG
61	N5	36	LYS
61	N5	38	LEU
61	N5	39	LYS
61	N5	42	ARG
61	N5	45	LYS
61	N5	48	SER
61	N5	49	LYS
61	N5	59	SER
61	N5	63	ILE
61	N5	71	THR
61	N5	73	MET
61	N5	75	LYS
61	N5	86	VAL
61	N5	92	LYS
61	N5	104	GLU
61	N5	115	ARG
61	N5	120	LYS
61	N5	125	ARG
61	N5	130	TYR
61	N5	134	ASP
61	N5	135	ILE
61	N5	138	ARG
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS
62	N6	6	LEU
62	N6	10	SER
62	N6	11	ASP
62	N6	13	ARG
62	N6	17	LYS
62	N6	37	LYS
62	N6	45	ILE
62	N6	48	LEU
62	N6	57	LEU
62	N6	58	VAL
62	N6	60	ARG
62	N6	71	SER
62	N6	74	TYR
62	N6	80	VAL
62	N6	88	GLU
62	N6	101	PRO

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Mol	Chain	Res	Type
62	N6	102	SER
62	N6	113	LYS
62	N6	115	ARG
62	N6	127	GLU
63	N7	9	LYS
63	N7	14	VAL
63	N7	21	LYS
63	N7	24	VAL
63	N7	33	SER
63	N7	34	LYS
63	N7	46	ILE
63	N7	53	VAL
63	N7	67	LYS
63	N7	72	ILE
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	87	LEU
63	N7	95	VAL
63	N7	99	GLU
63	N7	102	GLU
63	N7	103	GLN
63	N7	119	GLU
63	N7	127	ASN
63	N7	135	ARG
64	N8	4	ARG
64	N8	8	THR
64	N8	12	ARG
64	N8	24	LYS
64	N8	29	PRO
64	N8	34	MET
64	N8	43	ILE
64	N8	46	ASP
64	N8	47	LYS
64	N8	65	GLN
64	N8	78	LEU
64	N8	91	LEU
64	N8	115	LYS
64	N8	118	ILE
64	N8	120	ASN
64	N8	123	VAL
64	N8	124	ILE

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Mol	Chain	Res	Type
64	N8	130	VAL
64	N8	133	LEU
64	N8	137	LYS
65	N9	5	LYS
65	N9	8	THR
65	N9	13	THR
65	N9	14	ARG
65	N9	18	ARG
65	N9	25	LYS
65	N9	28	LYS
65	N9	36	ASP
65	N9	38	LYS
65	N9	42	ASN
65	N9	59	LYS
66	O0	14	LEU
66	O0	16	LEU
66	O0	18	ILE
66	O0	33	SER
66	O0	34	LEU
66	O0	36	GLN
66	O0	40	LYS
66	O0	42	ILE
66	O0	52	ARG
66	O0	61	MET
66	O0	75	ASN
66	O0	86	ARG
66	O0	99	ASP
66	O0	100	ILE
66	O0	102	THR
67	O1	6	ASP
67	O1	13	THR
67	O1	16	LEU
67	O1	26	LYS
67	O1	28	ARG
67	O1	31	ARG
67	O1	34	LYS
67	O1	42	LEU
67	O1	46	THR
67	O1	64	VAL
67	O1	65	LYS
67	O1	68	GLU
67	O1	71	LEU

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Mol	Chain	Res	Type
67	O1	73	LEU
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	98	VAL
67	O1	100	SER
67	O1	106	THR
68	O2	10	VAL
68	O2	19	ARG
68	O2	27	ARG
68	O2	34	LYS
68	O2	41	VAL
68	O2	51	SER
68	O2	54	LYS
68	O2	59	SER
68	O2	61	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	79	VAL
68	O2	82	LEU
68	O2	84	THR
68	O2	87	MET
68	O2	99	ASN
68	O2	101	SER
68	O2	103	LYS
68	O2	105	ARG
68	O2	109	LEU
68	O2	123	LYS
68	O2	125	ARG
69	O3	4	SER
69	O3	15	SER
69	O3	21	ARG
69	O3	29	LEU
69	O3	31	LYS
69	O3	37	THR
69	O3	45	LEU
69	O3	47	LYS
69	O3	48	ARG
69	O3	49	ILE

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Mol	Chain	Res	Type
69	O3	59	VAL
69	O3	70	LYS
69	O3	77	ASN
69	O3	80	VAL
69	O3	81	VAL
69	O3	88	ASN
69	O3	93	THR
69	O3	98	VAL
69	O3	106	ASN
70	O4	5	VAL
70	O4	7	PHE
70	O4	8	ARG
70	O4	16	ARG
70	O4	20	ILE
70	O4	21	LYS
70	O4	29	ILE
70	O4	36	LYS
70	O4	38	LEU
70	O4	51	LEU
70	O4	52	GLN
70	O4	58	ARG
70	O4	65	VAL
70	O4	71	THR
70	O4	74	ARG
70	O4	81	CYS
70	O4	86	LYS
70	O4	88	ARG
70	O4	103	LYS
70	O4	104	VAL
71	O5	13	SER
71	O5	21	LEU
71	O5	27	GLU
71	O5	28	LEU
71	O5	31	LEU
71	O5	44	ILE
71	O5	45	LYS
71	O5	46	THR
71	O5	49	LYS
71	O5	62	GLN
71	O5	69	LEU
71	O5	71	LYS
71	O5	73	LYS

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Mol	Chain	Res	Type
71	O5	89	ARG
71	O5	90	ARG
71	O5	96	GLU
71	O5	101	THR
71	O5	102	GLU
71	O5	103	LYS
71	O5	115	LYS
71	O5	119	LYS
72	O6	9	ILE
72	O6	20	MET
72	O6	21	THR
72	O6	25	LYS
72	O6	26	ILE
72	O6	28	TYR
72	O6	30	LYS
72	O6	44	VAL
72	O6	45	ARG
72	O6	46	GLU
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	64	SER
72	O6	67	LYS
72	O6	68	ARG
72	O6	70	ARG
72	O6	74	LYS
72	O6	76	ARG
72	O6	81	THR
72	O6	82	ARG
72	O6	84	LYS
72	O6	88	GLU
72	O6	90	MET
72	O6	98	ARG
73	O7	15	SER
73	O7	18	LEU
73	O7	19	CYS
73	O7	21	ARG
73	O7	24	ARG
73	O7	25	ARG
73	O7	34	CYS
73	O7	36	SER
73	O7	44	THR

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Mol	Chain	Res	Type
73	O7	55	ARG
73	O7	58	THR
73	O7	59	THR
73	O7	67	LEU
73	O7	76	ASN
73	O7	87	SER
74	O8	5	ILE
74	O8	6	THR
74	O8	28	ASN
74	O8	31	LEU
74	O8	32	ASN
74	O8	39	ARG
74	O8	46	ARG
74	O8	48	SER
74	O8	50	SER
74	O8	51	LEU
74	O8	53	THR
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	69	LEU
74	O8	72	THR
74	O8	73	LEU
74	O8	77	ARG
75	O9	5	LYS
75	O9	21	ARG
75	O9	23	LEU
75	O9	25	GLN
75	O9	51	ILE
76	Q0	78	ILE
76	Q0	79	GLU
76	Q0	92	ASP
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	127	LEU
77	Q1	2	ARG
77	Q1	5	TRP
77	Q1	10	THR
77	Q1	11	ARG
77	Q1	13	LEU
77	Q1	15	ARG
77	Q1	16	LYS

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Mol	Chain	Res	Type
78	Q2	6	LYS
78	Q2	9	LYS
78	Q2	13	LYS
78	Q2	20	HIS
78	Q2	28	TYR
78	Q2	29	LYS
78	Q2	32	LYS
78	Q2	35	LEU
78	Q2	38	GLN
78	Q2	45	ARG
78	Q2	61	LYS
78	Q2	66	LYS
78	Q2	71	ARG
78	Q2	78	LYS
78	Q2	80	ARG
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	86	LYS
78	Q2	88	CYS
78	Q2	93	LEU
78	Q2	100	LYS
78	Q2	104	LEU
79	Q3	11	THR
79	Q3	28	LYS
79	Q3	32	GLN
79	Q3	33	GLN
79	Q3	38	ASP
79	Q3	40	SER
79	Q3	45	LYS
79	Q3	57	CYS
79	Q3	59	CYS
79	Q3	60	CYS
79	Q3	64	VAL
79	Q3	71	VAL
79	Q3	78	THR
79	Q3	84	ARG
79	Q3	90	VAL
79	Q3	91	GLU
2	s0	9	LEU
2	s0	10	THR
2	s0	27	ARG

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Mol	Chain	Res	Type
2	s0	30	GLN
2	s0	32	HIS
2	s0	41	ARG
2	s0	45	VAL
2	s0	50	VAL
2	s0	59	LEU
2	s0	72	ASP
2	s0	80	THR
2	s0	83	GLN
2	s0	87	LEU
2	s0	88	LYS
2	s0	96	THR
2	s0	101	ARG
2	s0	114	SER
2	s0	141	ILE
2	s0	154	GLU
2	s0	162	CYS
2	s0	164	ASN
2	s0	165	ARG
2	s0	168	HIS
2	s0	172	LEU
2	s0	177	LEU
2	s0	183	ARG
2	s0	189	VAL
2	s0	200	ASP
2	s0	202	TYR
2	s0	203	PHE
3	s1	21	VAL
3	s1	25	THR
3	s1	47	LEU
3	s1	48	VAL
3	s1	51	SER
3	s1	54	LEU
3	s1	58	SER
3	s1	62	LYS
3	s1	64	ARG
3	s1	68	VAL
3	s1	70	LEU
3	s1	72	ASP
3	s1	73	LEU
3	s1	78	ASP
3	s1	81	PHE

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Mol	Chain	Res	Type
3	s1	82	ARG
3	s1	90	GLU
3	s1	97	LEU
3	s1	105	PHE
3	s1	111	ARG
3	s1	115	ARG
3	s1	125	VAL
3	s1	126	THR
3	s1	129	THR
3	s1	135	LEU
3	s1	151	LYS
3	s1	154	SER
3	s1	159	SER
3	s1	169	SER
3	s1	173	THR
3	s1	175	GLU
3	s1	177	GLN
3	s1	179	SER
3	s1	180	THR
3	s1	181	LEU
3	s1	183	GLN
3	s1	186	SER
3	s1	189	ILE
3	s1	203	ASP
3	s1	204	ILE
3	s1	205	PHE
3	s1	212	VAL
3	s1	217	LEU
3	s1	223	PHE
3	s1	225	VAL
4	s2	41	LEU
4	s2	44	LEU
4	s2	51	THR
4	s2	52	THR
4	s2	53	ILE
4	s2	54	GLU
4	s2	55	GLU
4	s2	58	LEU
4	s2	60	SER
4	s2	65	GLU
4	s2	69	ILE
4	s2	70	ASP

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Mol	Chain	Res	Type
4	s2	72	LEU
4	s2	76	LEU
4	s2	77	GLN
4	s2	83	ILE
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	95	ARG
4	s2	97	ARG
4	s2	101	VAL
4	s2	111	VAL
4	s2	113	LEU
4	s2	116	LYS
4	s2	117	THR
4	s2	125	ILE
4	s2	134	LEU
4	s2	137	ILE
4	s2	141	ARG
4	s2	148	LEU
4	s2	158	THR
4	s2	165	VAL
4	s2	169	LEU
4	s2	174	ARG
4	s2	178	ILE
4	s2	181	SER
4	s2	194	GLU
4	s2	198	THR
4	s2	210	THR
4	s2	222	TYR
4	s2	226	THR
4	s2	228	ASN
4	s2	232	GLU
4	s2	237	VAL
4	s2	240	LEU
4	s2	246	GLU
4	s2	250	GLN
5	s3	7	LYS
5	s3	11	LEU
5	s3	21	LEU
5	s3	26	THR
5	s3	39	VAL
5	s3	40	ARG

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Mol	Chain	Res	Type
5	s3	42	THR
5	s3	44	THR
5	s3	57	ASP
5	s3	61	GLU
5	s3	70	THR
5	s3	72	LEU
5	s3	84	ILE
5	s3	86	LEU
5	s3	90	ARG
5	s3	93	ASP
5	s3	96	LEU
5	s3	115	ILE
5	s3	127	MET
5	s3	128	GLU
5	s3	134	CYS
5	s3	142	LEU
5	s3	143	ARG
5	s3	157	LEU
5	s3	158	ILE
5	s3	162	GLN
5	s3	164	VAL
5	s3	168	ILE
5	s3	169	ASP
5	s3	172	THR
5	s3	176	LEU
5	s3	185	LYS
5	s3	195	SER
5	s3	196	ARG
5	s3	202	LEU
5	s3	204	ASP
5	s3	206	VAL
5	s3	210	GLU
5	s3	212	LYS
5	s3	213	GLU
5	s3	217	ILE
5	s3	224	ASP
6	s4	6	LYS
6	s4	9	LEU
6	s4	11	ARG
6	s4	22	LYS
6	s4	38	LEU
6	s4	39	ARG

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Mol	Chain	Res	Type
6	s4	40	GLU
6	s4	42	LEU
6	s4	45	ILE
6	s4	47	PHE
6	s4	48	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	67	GLN
6	s4	70	VAL
6	s4	76	VAL
6	s4	78	THR
6	s4	80	THR
6	s4	92	LEU
6	s4	97	GLU
6	s4	98	ASN
6	s4	115	THR
6	s4	116	ASP
6	s4	123	LEU
6	s4	126	VAL
6	s4	131	LEU
6	s4	143	ASP
6	s4	146	THR
6	s4	147	ILE
6	s4	148	ARG
6	s4	164	LEU
6	s4	176	ASP
6	s4	180	LEU
6	s4	182	TYR
6	s4	194	THR
6	s4	195	ILE
6	s4	208	VAL
6	s4	219	VAL
6	s4	221	ARG
6	s4	222	LEU
6	s4	226	PHE
6	s4	227	VAL
6	s4	228	ILE
6	s4	235	TYR
6	s4	236	ILE
6	s4	246	LEU
6	s4	247	SER
6	s4	252	ARG

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Mol	Chain	Res	Type
7	s5	24	VAL
7	s5	25	LEU
7	s5	31	GLU
7	s5	38	THR
7	s5	39	GLU
7	s5	41	LYS
7	s5	45	LYS
7	s5	59	VAL
7	s5	63	GLN
7	s5	66	GLN
7	s5	68	ILE
7	s5	72	HIS
7	s5	83	ARG
7	s5	89	ILE
7	s5	92	ARG
7	s5	93	LEU
7	s5	104	ASN
7	s5	108	LEU
7	s5	112	ARG
7	s5	125	THR
7	s5	130	ILE
7	s5	140	THR
7	s5	148	ARG
7	s5	149	VAL
7	s5	156	ARG
7	s5	157	ARG
7	s5	160	VAL
7	s5	162	VAL
7	s5	163	SER
7	s5	166	ARG
7	s5	167	ARG
7	s5	190	ILE
7	s5	194	LEU
7	s5	196	GLU
7	s5	216	GLU
7	s5	217	LEU
7	s5	219	ARG
8	s6	25	ARG
8	s6	68	LEU
8	s6	69	LEU
8	s6	93	LYS
8	s6	96	SER

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Mol	Chain	Res	Type
8	s6	109	LEU
8	s6	112	VAL
8	s6	120	GLU
8	s6	121	LEU
8	s6	122	GLU
8	s6	124	LEU
8	s6	125	THR
8	s6	126	ASP
8	s6	127	THR
8	s6	129	VAL
8	s6	133	LEU
8	s6	143	LYS
8	s6	151	ASP
8	s6	153	VAL
8	s6	157	VAL
8	s6	162	VAL
8	s6	163	THR
8	s6	167	LYS
8	s6	168	THR
8	s6	170	THR
8	s6	177	ARG
8	s6	179	VAL
8	s6	180	THR
8	s6	182	GLN
8	s6	208	TYR
8	s6	212	LEU
8	s6	215	ARG
8	s6	216	LEU
8	s6	218	GLU
9	s7	10	SER
9	s7	17	GLU
9	s7	22	GLN
9	s7	27	LEU
9	s7	28	GLU
9	s7	30	SER
9	s7	33	GLU
9	s7	35	LYS
9	s7	39	ARG
9	s7	42	GLN
9	s7	50	ASP
9	s7	62	VAL
9	s7	67	LEU

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Mol	Chain	Res	Type
9	s7	75	THR
9	s7	76	LYS
9	s7	78	THR
9	s7	88	ARG
9	s7	93	LEU
9	s7	97	ARG
9	s7	106	SER
9	s7	107	ARG
9	s7	108	GLN
9	s7	110	GLN
9	s7	114	ARG
9	s7	116	ARG
9	s7	118	LEU
9	s7	122	HIS
9	s7	123	ASP
9	s7	143	LEU
9	s7	144	VAL
9	s7	149	ILE
9	s7	160	GLN
9	s7	161	GLN
9	s7	166	LEU
9	s7	185	ILE
10	s8	6	ASP
10	s8	20	GLN
10	s8	22	ARG
10	s8	24	LYS
10	s8	25	ARG
10	s8	29	LEU
10	s8	32	GLN
10	s8	48	THR
10	s8	58	LEU
10	s8	59	ARG
10	s8	60	ILE
10	s8	76	THR
10	s8	95	THR
10	s8	97	THR
10	s8	120	THR
10	s8	152	ILE
10	s8	155	SER
10	s8	172	ARG
10	s8	175	GLN
10	s8	182	TYR

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Mol	Chain	Res	Type
10	s8	184	LEU
10	s8	185	GLU
10	s8	199	LYS
11	s9	3	ARG
11	s9	6	ARG
11	s9	7	THR
11	s9	16	LYS
11	s9	20	GLU
11	s9	21	SER
11	s9	28	LEU
11	s9	33	GLU
11	s9	36	LEU
11	s9	39	LYS
11	s9	46	SER
11	s9	81	VAL
11	s9	82	ARG
11	s9	93	LEU
11	s9	96	VAL
11	s9	110	GLN
11	s9	114	TYR
11	s9	122	VAL
11	s9	126	ARG
11	s9	130	THR
11	s9	132	ARG
11	s9	134	ILE
11	s9	150	LEU
11	s9	152	SER
11	s9	161	THR
11	s9	162	SER
11	s9	168	ARG
11	s9	171	ARG
11	s9	172	VAL
11	s9	182	GLU
12	c0	2	LEU
12	c0	6	GLU
12	c0	12	HIS
12	c0	15	LEU
12	c0	27	PHE
12	c0	36	ASP
12	c0	40	LEU
12	c0	47	GLN
12	c0	55	VAL

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Mol	Chain	Res	Type
12	c0	57	THR
12	c0	67	THR
12	c0	70	GLU
12	c0	77	ARG
13	c1	5	LEU
13	c1	9	SER
13	c1	10	GLU
13	c1	14	GLN
13	c1	26	LYS
13	c1	27	THR
13	c1	31	THR
13	c1	33	ARG
13	c1	44	THR
13	c1	49	ILE
13	c1	60	PHE
13	c1	67	ARG
13	c1	72	THR
13	c1	74	THR
13	c1	80	MET
13	c1	82	ARG
13	c1	83	THR
13	c1	99	ARG
13	c1	109	VAL
13	c1	123	VAL
13	c1	141	LYS
14	c2	28	LEU
14	c2	52	LEU
14	c2	53	THR
14	c2	58	LEU
14	c2	61	VAL
14	c2	62	LEU
14	c2	71	ILE
14	c2	74	LEU
14	c2	83	GLU
14	c2	85	LYS
14	c2	89	ILE
14	c2	93	ASP
14	c2	95	LYS
14	c2	103	LEU
14	c2	126	TRP
14	c2	132	GLU
14	c2	140	PHE

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Mol	Chain	Res	Type
15	c3	4	MET
15	c3	6	SER
15	c3	11	ILE
15	c3	16	ILE
15	c3	21	ASN
15	c3	35	GLU
15	c3	36	GLN
15	c3	39	LYS
15	c3	43	LYS
15	c3	64	ARG
15	c3	66	ILE
15	c3	70	LYS
15	c3	72	MET
15	c3	80	LEU
15	c3	83	GLU
15	c3	84	ILE
15	c3	87	ASP
15	c3	97	SER
15	c3	102	LEU
15	c3	104	ARG
15	c3	119	GLU
15	c3	125	LEU
15	c3	131	THR
15	c3	134	VAL
15	c3	149	LEU
16	c4	14	PHE
16	c4	26	THR
16	c4	28	VAL
16	c4	31	THR
16	c4	38	THR
16	c4	61	MET
16	c4	65	GLN
16	c4	77	THR
16	c4	79	VAL
16	c4	81	VAL
16	c4	103	ARG
16	c4	107	ARG
16	c4	108	SER
16	c4	111	ARG
16	c4	114	ARG
16	c4	121	VAL
16	c4	123	SER

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Mol	Chain	Res	Type
16	c4	125	SER
16	c4	129	LYS
16	c4	132	ARG
16	c4	136	ARG
17	c5	12	PHE
17	c5	21	ASP
17	c5	24	LYS
17	c5	26	LEU
17	c5	27	GLU
17	c5	29	SER
17	c5	34	VAL
17	c5	36	LEU
17	c5	43	ARG
17	c5	61	ARG
17	c5	69	GLU
17	c5	72	LYS
17	c5	94	VAL
17	c5	107	ILE
17	c5	122	THR
17	c5	123	TYR
17	c5	124	THR
17	c5	126	VAL
18	c6	15	SER
18	c6	17	THR
18	c6	23	LYS
18	c6	28	LEU
18	c6	31	VAL
18	c6	37	THR
18	c6	42	GLU
18	c6	43	ILE
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	83	GLN
18	c6	94	GLN
18	c6	98	ASP
18	c6	105	LEU
18	c6	110	THR
18	c6	114	ARG

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Mol	Chain	Res	Type
18	c6	117	LEU
18	c6	137	ARG
19	c7	3	ARG
19	c7	6	THR
19	c7	8	THR
19	c7	25	THR
19	c7	26	LEU
19	c7	29	GLN
19	c7	34	LEU
19	c7	35	CYS
19	c7	38	ILE
19	c7	44	LYS
19	c7	46	LEU
19	c7	47	ARG
19	c7	49	LYS
19	c7	55	THR
19	c7	62	GLN
19	c7	69	ILE
19	c7	72	LYS
19	c7	85	VAL
19	c7	88	VAL
19	c7	110	VAL
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	13	HIS
20	c8	15	LEU
20	c8	20	THR
20	c8	25	ASN
20	c8	26	ILE
20	c8	27	LYS
20	c8	28	ILE
20	c8	29	VAL
20	c8	33	THR
20	c8	34	THR
20	c8	36	LYS
20	c8	40	ARG
20	c8	41	ARG
20	c8	54	LEU
20	c8	55	HIS
20	c8	63	GLN

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Mol	Chain	Res	Type
20	c8	66	LEU
20	c8	85	PHE
20	c8	86	LEU
20	c8	94	ASP
20	c8	103	ASN
20	c8	110	ARG
20	c8	112	ASP
20	c8	113	LEU
20	c8	119	ILE
20	c8	138	THR
20	c8	140	THR
20	c8	141	THR
20	c8	144	ARG
20	c8	145	ARG
21	c9	6	VAL
21	c9	9	VAL
21	c9	20	SER
21	c9	27	LYS
21	c9	28	LEU
21	c9	38	LYS
21	c9	68	ARG
21	c9	70	GLN
21	c9	86	ARG
21	c9	89	ARG
21	c9	111	ILE
21	c9	116	ILE
21	c9	117	SER
21	c9	123	ARG
21	c9	139	THR
21	c9	140	LEU
21	c9	141	GLU
21	c9	142	GLU
21	c9	144	GLU
22	d0	15	GLN
22	d0	16	GLN
22	d0	20	ILE
22	d0	23	ARG
22	d0	27	THR
22	d0	31	VAL
22	d0	34	LEU
22	d0	39	SER
22	d0	44	ASN

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Mol	Chain	Res	Type
22	d0	49	ASN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	61	LYS
22	d0	62	VAL
22	d0	66	SER
22	d0	70	THR
22	d0	72	ASN
22	d0	74	GLU
22	d0	76	SER
22	d0	77	LYS
22	d0	81	THR
22	d0	88	LYS
22	d0	92	ASP
22	d0	97	VAL
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	105	GLN
22	d0	108	ILE
22	d0	114	VAL
23	d1	2	GLU
23	d1	5	LYS
23	d1	12	TYR
23	d1	13	VAL
23	d1	18	SER
23	d1	24	ILE
23	d1	31	SER
23	d1	32	VAL
23	d1	34	ILE
23	d1	39	VAL
23	d1	41	GLU
23	d1	50	TYR
23	d1	52	THR
23	d1	68	SER
23	d1	78	LEU
23	d1	85	TYR
24	d2	2	THR
24	d2	6	VAL
24	d2	7	LEU
24	d2	16	ASN

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Mol	Chain	Res	Type
24	d2	23	ARG
24	d2	24	GLN
24	d2	25	VAL
24	d2	26	LEU
24	d2	37	PHE
24	d2	49	GLU
24	d2	56	HIS
24	d2	65	LEU
24	d2	74	VAL
24	d2	93	LEU
24	d2	97	ARG
24	d2	98	GLN
24	d2	103	ILE
24	d2	117	ARG
24	d2	118	ARG
24	d2	126	LEU
24	d2	129	VAL
25	d3	7	ARG
25	d3	13	ARG
25	d3	18	HIS
25	d3	20	ARG
25	d3	22	ASN
25	d3	23	ARG
25	d3	28	ASN
25	d3	29	TYR
25	d3	36	THR
25	d3	41	SER
25	d3	46	SER
25	d3	52	ILE
25	d3	62	LYS
25	d3	72	VAL
25	d3	73	ARG
25	d3	78	LYS
25	d3	83	VAL
25	d3	84	THR
25	d3	99	ASN
25	d3	103	LEU
25	d3	107	PHE
25	d3	109	ARG
25	d3	117	ILE
25	d3	125	VAL
25	d3	130	VAL

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Mol	Chain	Res	Type
25	d3	132	LEU
25	d3	133	LEU
25	d3	138	GLU
26	d4	2	SER
26	d4	6	THR
26	d4	9	THR
26	d4	13	ILE
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	52	LYS
26	d4	62	THR
26	d4	83	LYS
26	d4	88	THR
26	d4	92	VAL
26	d4	96	LEU
26	d4	118	ILE
26	d4	127	LYS
26	d4	133	ASN
27	d5	41	ILE
27	d5	43	ASP
27	d5	45	GLU
27	d5	49	ARG
27	d5	51	LEU
27	d5	57	TYR
27	d5	60	VAL
27	d5	68	ARG
27	d5	71	ILE
27	d5	81	ARG
27	d5	96	SER
27	d5	102	THR
27	d5	103	ARG
28	d6	5	ARG
28	d6	8	ASN
28	d6	10	ARG
28	d6	12	LYS
28	d6	15	ARG
28	d6	18	VAL
28	d6	25	ASN

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Mol	Chain	Res	Type
28	d6	27	SER
28	d6	38	ARG
28	d6	42	ARG
28	d6	43	ASN
28	d6	44	ILE
28	d6	46	GLU
28	d6	51	ARG
28	d6	55	GLU
28	d6	61	GLU
28	d6	82	ARG
28	d6	85	ARG
29	d7	3	LEU
29	d7	9	HIS
29	d7	17	ARG
29	d7	34	ASP
29	d7	38	PRO
29	d7	43	ILE
29	d7	45	THR
29	d7	46	VAL
29	d7	52	THR
29	d7	56	CYS
29	d7	65	THR
29	d7	72	LYS
29	d7	77	THR
29	d7	78	SER
29	d7	81	ARG
30	d8	13	ILE
30	d8	16	LEU
30	d8	19	THR
30	d8	22	ARG
30	d8	32	PHE
30	d8	33	LEU
30	d8	38	ARG
30	d8	48	VAL
30	d8	58	GLU
30	d8	62	GLU
30	d8	64	ARG
30	d8	65	ARG
30	d8	66	LEU
31	d9	6	VAL
31	d9	10	HIS
31	d9	14	TYR

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Mol	Chain	Res	Type
31	d9	32	ARG
31	d9	36	LEU
31	d9	38	ILE
31	d9	42	CYS
31	d9	44	ARG
31	d9	45	GLU
31	d9	49	ASP
31	d9	54	LYS
80	e0	13	LYS
80	e0	14	VAL
80	e0	16	SER
80	e0	24	THR
80	e0	25	GLU
80	e0	26	LYS
80	e0	29	LYS
80	e0	31	LYS
80	e0	39	LEU
80	e0	41	THR
80	e0	45	VAL
80	e0	46	ASN
80	e0	49	LEU
80	e0	51	ASN
80	e0	54	ARG
33	e1	80	ARG
33	e1	82	LYS
33	e1	86	THR
33	e1	90	LYS
33	e1	91	ILE
33	e1	96	LYS
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	109	ASP
33	e1	113	LYS
33	e1	118	ARG
33	e1	135	HIS
33	e1	137	ASP
33	e1	147	VAL
33	e1	148	TYR
33	e1	150	VAL
34	sR	4	ASN
34	sR	6	VAL

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Mol	Chain	Res	Type
34	sR	9	LEU
34	sR	17	ASN
34	sR	21	THR
34	sR	29	GLN
34	sR	46	LYS
34	sR	53	LYS
34	sR	58	VAL
34	sR	64	HIS
34	sR	66	HIS
34	sR	70	ASP
34	sR	72	THR
34	sR	76	ASP
34	sR	84	SER
34	sR	87	LYS
34	sR	96	THR
34	sR	100	TYR
34	sR	102	ARG
34	sR	108	SER
34	sR	130	THR
34	sR	145	LEU
34	sR	149	ASP
34	sR	159	ASN
34	sR	167	VAL
34	sR	176	LYS
34	sR	178	VAL
34	sR	191	ASP
34	sR	207	ASP
34	sR	210	LEU
34	sR	228	LYS
34	sR	232	TYR
34	sR	235	SER
34	sR	286	GLU
34	sR	297	ASP
34	sR	299	GLN
34	sR	314	GLN
34	sR	317	THR
35	sM	41	SER
35	sM	43	ASP
35	sM	61	ILE
35	sM	69	ARG
35	sM	71	ASN
35	sM	74	LYS

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Mol	Chain	Res	Type
35	sM	75	ASP
35	sM	76	VAL
35	sM	81	THR
39	l2	30	ARG
39	l2	31	THR
39	l2	32	LEU
39	l2	36	GLU
39	l2	42	ARG
39	l2	44	ILE
39	l2	45	VAL
39	l2	46	LYS
39	l2	48	ILE
39	l2	49	VAL
39	l2	61	VAL
39	l2	62	VAL
39	l2	70	ARG
39	l2	71	LEU
39	l2	75	ILE
39	l2	77	ILE
39	l2	79	ASN
39	l2	80	GLU
39	l2	82	VAL
39	l2	101	VAL
39	l2	119	LYS
39	l2	122	ASP
39	l2	128	ARG
39	l2	130	SER
39	l2	132	ASN
39	l2	137	ILE
39	l2	144	ASN
39	l2	147	ARG
39	l2	148	VAL
39	l2	149	ARG
39	l2	157	VAL
39	l2	158	ILE
39	l2	165	VAL
39	l2	169	ILE
39	l2	179	LEU
39	l2	184	ARG
39	l2	191	LEU
39	l2	192	LYS
39	l2	193	ARG

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Mol	Chain	Res	Type
39	12	202	VAL
39	12	204	MET
39	12	218	HIS
39	12	224	THR
39	12	227	ARG
39	12	230	VAL
39	12	238	ILE
39	12	243	THR
39	12	246	LEU
40	13	3	HIS
40	13	4	ARG
40	13	5	LYS
40	13	7	GLU
40	13	10	ARG
40	13	17	LEU
40	13	19	ARG
40	13	25	ILE
40	13	37	ARG
40	13	44	THR
40	13	45	SER
40	13	47	LEU
40	13	50	LYS
40	13	55	THR
40	13	69	LYS
40	13	73	VAL
40	13	77	THR
40	13	81	THR
40	13	85	VAL
40	13	95	THR
40	13	101	SER
40	13	104	THR
40	13	114	VAL
40	13	120	LYS
40	13	127	LYS
40	13	140	ASP
40	13	146	ARG
40	13	148	LEU
40	13	150	ARG
40	13	161	LEU
40	13	164	THR
40	13	167	ARG
40	13	169	THR

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Mol	Chain	Res	Type
40	l3	178	LEU
40	l3	184	ASN
40	l3	188	ILE
40	l3	205	VAL
40	l3	208	VAL
40	l3	212	ASN
40	l3	221	THR
40	l3	222	LYS
40	l3	232	ARG
40	l3	238	LEU
40	l3	242	THR
40	l3	244	ARG
40	l3	249	VAL
40	l3	252	ILE
40	l3	256	HIS
40	l3	261	MET
40	l3	264	VAL
40	l3	266	ARG
40	l3	274	SER
40	l3	278	ILE
40	l3	282	ILE
40	l3	287	LYS
40	l3	299	ASP
40	l3	300	ARG
40	l3	304	THR
40	l3	318	LYS
40	l3	319	ASN
40	l3	322	ILE
40	l3	328	ILE
40	l3	331	ASN
40	l3	332	ARG
40	l3	340	LYS
40	l3	342	LEU
40	l3	346	THR
40	l3	354	VAL
40	l3	356	LEU
40	l3	359	ILE
40	l3	364	LYS
40	l3	380	MET
41	l4	3	ARG
41	l4	12	THR
41	l4	14	GLU

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Mol	Chain	Res	Type
41	14	22	LEU
41	14	37	THR
41	14	42	VAL
41	14	52	VAL
41	14	55	LYS
41	14	63	GLU
41	14	67	THR
41	14	73	ARG
41	14	76	ARG
41	14	84	ARG
41	14	90	PHE
41	14	93	MET
41	14	105	THR
41	14	131	VAL
41	14	136	LEU
41	14	144	LYS
41	14	145	ILE
41	14	150	LEU
41	14	151	VAL
41	14	152	VAL
41	14	176	SER
41	14	178	LEU
41	14	179	LEU
41	14	182	LEU
41	14	186	LYS
41	14	187	LEU
41	14	203	ARG
41	14	206	LEU
41	14	217	LYS
41	14	222	VAL
41	14	226	GLU
41	14	230	VAL
41	14	246	ARG
41	14	249	ILE
41	14	256	THR
41	14	258	LEU
41	14	265	GLU
41	14	276	LEU
41	14	278	SER
41	14	286	VAL
41	14	287	THR
41	14	289	ILE

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Mol	Chain	Res	Type
41	14	292	SER
41	14	304	GLN
41	14	306	THR
41	14	307	GLN
41	14	310	THR
41	14	313	LEU
41	14	319	LYS
41	14	323	VAL
41	14	327	LEU
41	14	345	GLU
41	14	346	LYS
41	14	349	THR
41	14	354	VAL
41	14	357	GLU
42	15	34	LYS
42	15	37	VAL
42	15	41	LYS
42	15	51	LEU
42	15	66	SER
42	15	70	THR
42	15	89	THR
42	15	92	LEU
42	15	101	THR
42	15	110	LEU
42	15	115	LEU
42	15	116	ASP
42	15	118	THR
42	15	122	VAL
42	15	125	VAL
42	15	128	GLU
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	152	ARG
42	15	154	THR
42	15	158	ARG
42	15	173	VAL
42	15	176	SER

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Mol	Chain	Res	Type
42	15	177	GLU
42	15	185	PHE
42	15	194	LEU
42	15	196	ARG
42	15	222	LEU
42	15	234	ASP
42	15	235	SER
42	15	241	THR
42	15	245	GLU
42	15	247	ILE
42	15	254	LYS
42	15	259	LYS
42	15	268	GLU
42	15	273	ARG
42	15	276	LYS
42	15	286	VAL
42	15	293	LEU
43	16	8	LYS
43	16	9	TRP
43	16	12	SER
43	16	14	ASP
43	16	21	THR
43	16	28	GLN
43	16	31	ARG
43	16	35	VAL
43	16	46	ARG
43	16	50	LYS
43	16	52	VAL
43	16	56	LYS
43	16	64	LEU
43	16	65	ILE
43	16	74	VAL
43	16	78	ARG
43	16	79	VAL
43	16	82	ARG
43	16	88	SER
43	16	89	THR
43	16	90	LYS
43	16	91	VAL
43	16	103	VAL
43	16	104	GLU
43	16	108	LYS

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Mol	Chain	Res	Type
43	16	109	GLU
43	16	131	LYS
43	16	152	THR
43	16	155	LEU
43	16	164	SER
43	16	169	ASP
43	16	170	LYS
43	16	174	LEU
44	17	22	THR
44	17	26	VAL
44	17	33	ARG
44	17	38	LYS
44	17	41	ARG
44	17	54	GLU
44	17	59	GLU
44	17	60	ARG
44	17	61	ASN
44	17	77	VAL
44	17	88	ARG
44	17	93	ASN
44	17	98	LYS
44	17	101	LYS
44	17	111	ILE
44	17	115	THR
44	17	119	VAL
44	17	124	LEU
44	17	129	LEU
44	17	130	ILE
44	17	142	SER
44	17	156	ILE
44	17	158	LYS
44	17	173	LEU
44	17	175	LYS
44	17	176	TYR
44	17	179	LEU
44	17	181	ILE
44	17	184	LEU
44	17	193	PRO
44	17	206	LYS
44	17	208	SER
44	17	224	ILE
44	17	229	PHE

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Mol	Chain	Res	Type
44	17	239	LEU
45	18	26	LEU
45	18	38	GLN
45	18	41	GLN
45	18	50	VAL
45	18	68	ARG
45	18	71	VAL
45	18	74	THR
45	18	77	GLN
45	18	79	GLN
45	18	83	ASP
45	18	85	ASN
45	18	91	PHE
45	18	93	LEU
45	18	95	ASN
45	18	111	LYS
45	18	134	TYR
45	18	136	LEU
45	18	146	LYS
45	18	149	LYS
45	18	150	LEU
45	18	153	ILE
45	18	156	ASP
45	18	157	VAL
45	18	160	ILE
45	18	183	LYS
45	18	185	ARG
45	18	191	ASN
45	18	203	VAL
45	18	211	LEU
45	18	213	LYS
45	18	217	THR
45	18	224	ASP
45	18	230	LYS
45	18	231	LYS
45	18	245	LYS
45	18	248	LYS
46	19	1	MET
46	19	5	GLN
46	19	6	THR
46	19	16	VAL
46	19	17	THR

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Mol	Chain	Res	Type
46	19	18	VAL
46	19	19	SER
46	19	31	ARG
46	19	33	THR
46	19	39	LYS
46	19	46	THR
46	19	52	LEU
46	19	55	VAL
46	19	68	LEU
46	19	70	THR
46	19	72	LYS
46	19	76	ASP
46	19	77	ASN
46	19	82	VAL
46	19	87	LYS
46	19	91	ARG
46	19	92	TYR
46	19	96	HIS
46	19	102	ASN
46	19	105	GLU
46	19	106	LYS
46	19	107	ASP
46	19	113	GLU
46	19	115	ARG
46	19	118	LEU
46	19	121	LYS
46	19	132	VAL
46	19	133	THR
46	19	138	THR
46	19	144	ILE
46	19	146	LEU
46	19	151	VAL
46	19	157	ASN
46	19	161	LEU
46	19	162	GLN
46	19	166	ARG
46	19	175	PHE
46	19	181	VAL
47	m0	3	ARG
47	m0	4	ARG
47	m0	19	LYS
47	m0	24	ARG

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Mol	Chain	Res	Type
47	m0	29	SER
47	m0	35	ASP
47	m0	39	LYS
47	m0	42	THR
47	m0	44	ASP
47	m0	48	LEU
47	m0	52	LEU
47	m0	57	LEU
47	m0	58	GLU
47	m0	61	SER
47	m0	71	CYS
47	m0	80	SER
47	m0	91	VAL
47	m0	121	LYS
47	m0	125	LEU
47	m0	133	GLN
47	m0	139	ARG
47	m0	143	SER
47	m0	158	LYS
47	m0	163	GLN
47	m0	169	LYS
47	m0	176	LEU
47	m0	177	ASP
47	m0	184	LYS
47	m0	197	VAL
47	m0	206	LEU
47	m0	208	ASN
47	m0	210	ILE
47	m0	212	GLU
47	m0	215	GLU
47	m0	217	PHE
48	m1	7	ASN
48	m1	9	MET
48	m1	10	ARG
48	m1	12	LEU
48	m1	13	LYS
48	m1	16	LYS
48	m1	19	LEU
48	m1	35	LYS
48	m1	40	LEU
48	m1	55	ARG
48	m1	57	PHE

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Mol	Chain	Res	Type
48	m1	59	ILE
48	m1	60	ARG
48	m1	77	GLU
48	m1	78	GLU
48	m1	80	LEU
48	m1	82	ARG
48	m1	85	LYS
48	m1	97	SER
48	m1	99	THR
48	m1	106	ILE
48	m1	107	ASP
48	m1	110	ILE
48	m1	112	LEU
48	m1	127	PHE
48	m1	130	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	143	ARG
48	m1	148	VAL
48	m1	150	ASN
48	m1	152	HIS
48	m1	154	THR
48	m1	157	GLU
48	m1	160	VAL
48	m1	171	VAL
49	m3	4	SER
49	m3	16	LYS
49	m3	42	ARG
49	m3	46	ILE
49	m3	53	LEU
49	m3	54	LEU
49	m3	58	VAL
49	m3	62	THR
49	m3	67	ARG
49	m3	69	VAL
49	m3	73	ARG
49	m3	76	THR
49	m3	80	VAL
49	m3	86	THR
49	m3	92	THR
49	m3	104	ARG
49	m3	113	VAL

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Mol	Chain	Res	Type
49	m3	118	GLU
49	m3	123	ILE
49	m3	124	ILE
49	m3	131	LYS
49	m3	137	GLN
49	m3	150	PRO
49	m3	152	THR
49	m3	153	ASP
49	m3	154	VAL
49	m3	155	GLU
49	m3	157	ARG
49	m3	162	ASN
49	m3	164	GLU
49	m3	165	SER
49	m3	183	ARG
49	m3	184	GLU
49	m3	189	GLU
50	m4	3	THR
50	m4	8	LYS
50	m4	13	ARG
50	m4	16	GLU
50	m4	20	VAL
50	m4	24	LYS
50	m4	46	ILE
50	m4	53	VAL
50	m4	62	GLN
50	m4	63	VAL
50	m4	64	VAL
50	m4	66	THR
50	m4	72	LEU
50	m4	80	THR
50	m4	82	SER
50	m4	90	VAL
50	m4	106	ARG
50	m4	108	ARG
50	m4	119	GLN
50	m4	124	ARG
50	m4	126	GLN
50	m4	128	ARG
51	m5	5	LYS
51	m5	10	LEU
51	m5	12	ARG

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Mol	Chain	Res	Type
51	m5	14	LYS
51	m5	16	SER
51	m5	20	ARG
51	m5	22	LEU
51	m5	24	ARG
51	m5	25	VAL
51	m5	32	GLN
51	m5	36	ILE
51	m5	49	ARG
51	m5	67	ARG
51	m5	80	THR
51	m5	90	ASN
51	m5	92	LEU
51	m5	96	ARG
51	m5	108	ARG
51	m5	109	ARG
51	m5	112	ASN
51	m5	116	LEU
51	m5	151	ILE
51	m5	153	ASP
51	m5	155	VAL
51	m5	159	ARG
51	m5	171	SER
51	m5	174	ILE
51	m5	175	ASN
51	m5	176	LYS
51	m5	188	ARG
51	m5	189	LYS
51	m5	190	THR
51	m5	194	GLN
51	m5	204	LYS
52	m6	4	GLU
52	m6	12	LYS
52	m6	15	LEU
52	m6	34	VAL
52	m6	41	LEU
52	m6	42	ASN
52	m6	46	GLU
52	m6	57	PHE
52	m6	59	ARG
52	m6	60	LYS
52	m6	66	LYS

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Mol	Chain	Res	Type
52	m6	68	ARG
52	m6	74	ARG
52	m6	78	ARG
52	m6	82	LYS
52	m6	84	LEU
52	m6	85	ARG
52	m6	88	VAL
52	m6	89	SER
52	m6	100	GLU
52	m6	104	VAL
52	m6	106	GLU
52	m6	108	ILE
52	m6	115	LYS
52	m6	117	ARG
52	m6	124	LEU
52	m6	126	VAL
52	m6	129	LEU
52	m6	133	ARG
52	m6	143	THR
52	m6	145	VAL
52	m6	160	ARG
52	m6	167	TYR
52	m6	177	LYS
52	m6	182	ASN
52	m6	187	GLU
52	m6	190	VAL
52	m6	192	LYS
52	m6	194	LEU
52	m6	197	LEU
53	m7	3	ARG
53	m7	7	THR
53	m7	9	THR
53	m7	31	GLU
53	m7	32	THR
53	m7	52	LEU
53	m7	56	ARG
53	m7	69	ARG
53	m7	70	THR
53	m7	80	LYS
53	m7	86	LYS
53	m7	89	LYS
53	m7	96	GLN

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Mol	Chain	Res	Type
53	m7	103	GLU
53	m7	112	LEU
53	m7	114	VAL
53	m7	119	VAL
53	m7	120	ASN
53	m7	127	ARG
53	m7	128	ARG
53	m7	133	HIS
53	m7	136	ILE
53	m7	142	SER
53	m7	148	LEU
54	m8	3	ILE
54	m8	7	SER
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	49	LEU
54	m8	53	PHE
54	m8	55	SER
54	m8	57	ILE
54	m8	66	ARG
54	m8	69	ARG
54	m8	80	THR
54	m8	81	VAL
54	m8	86	THR
54	m8	93	ILE
54	m8	111	ARG
54	m8	113	LYS
54	m8	135	GLN
54	m8	136	ASN
54	m8	138	LEU
54	m8	144	ARG
54	m8	145	ASN
54	m8	150	VAL
54	m8	161	LYS
54	m8	165	ILE
54	m8	166	LEU
54	m8	170	ARG

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Mol	Chain	Res	Type
54	m8	176	ARG
54	m8	178	ARG
54	m8	182	LYS
55	m9	4	LEU
55	m9	5	ARG
55	m9	7	GLN
55	m9	10	LEU
55	m9	20	ARG
55	m9	31	GLU
55	m9	34	GLN
55	m9	37	SER
55	m9	56	THR
55	m9	57	VAL
55	m9	61	SER
55	m9	74	ARG
55	m9	81	ARG
55	m9	85	ARG
55	m9	88	ARG
55	m9	98	ARG
55	m9	99	LEU
55	m9	105	LEU
55	m9	106	LEU
55	m9	127	SER
55	m9	138	LEU
55	m9	152	GLU
55	m9	153	LYS
55	m9	164	LEU
55	m9	170	ARG
55	m9	173	ARG
55	m9	177	VAL
55	m9	182	ASP
56	n0	1	MET
56	n0	16	THR
56	n0	32	SER
56	n0	45	LEU
56	n0	47	LYS
56	n0	52	LYS
56	n0	62	ASN
56	n0	73	LYS
56	n0	80	ARG
56	n0	89	ASN
56	n0	92	LYS

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Mol	Chain	Res	Type
56	n0	95	ARG
56	n0	96	ASP
56	n0	97	VAL
56	n0	100	VAL
56	n0	107	TYR
56	n0	115	ARG
56	n0	117	ARG
56	n0	125	LYS
56	n0	130	GLU
56	n0	137	ARG
56	n0	138	GLN
56	n0	145	THR
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	164	SER
56	n0	167	ARG
56	n0	171	PHE
56	n0	172	TYR
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	28	SER
57	n1	35	LYS
57	n1	47	SER
57	n1	60	LYS
57	n1	68	THR
57	n1	72	VAL
57	n1	78	LYS
57	n1	80	VAL
57	n1	88	ARG
57	n1	89	LEU
57	n1	102	ARG
57	n1	104	GLU
57	n1	112	ASN
57	n1	118	GLU
57	n1	126	VAL
57	n1	127	GLN

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Mol	Chain	Res	Type
57	n1	128	LEU
57	n1	131	GLN
57	n1	134	GLN
57	n1	138	SER
57	n1	140	ILE
57	n1	143	THR
57	n1	149	GLN
57	n1	150	THR
57	n1	151	LEU
57	n1	157	GLU
58	n2	13	LYS
58	n2	16	THR
58	n2	19	VAL
58	n2	27	VAL
58	n2	38	ILE
58	n2	39	ASP
58	n2	43	VAL
58	n2	47	VAL
58	n2	49	ASN
58	n2	54	VAL
58	n2	57	THR
58	n2	58	GLU
58	n2	59	ASP
58	n2	63	VAL
58	n2	64	THR
58	n2	66	VAL
58	n2	68	THR
58	n2	74	LYS
58	n2	75	TYR
58	n2	80	THR
58	n2	88	GLN
58	n2	90	ARG
58	n2	93	ILE
58	n2	95	PHE
58	n2	96	VAL
58	n2	98	THR
58	n2	100	THR
59	n3	4	ASN
59	n3	7	GLN
59	n3	9	THR
59	n3	10	LYS
59	n3	14	SER

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Mol	Chain	Res	Type
59	n3	22	ILE
59	n3	23	MET
59	n3	61	THR
59	n3	69	LEU
59	n3	70	ARG
59	n3	73	VAL
59	n3	74	MET
59	n3	83	LYS
59	n3	88	ARG
59	n3	91	VAL
59	n3	93	LEU
59	n3	104	ASN
59	n3	112	SER
59	n3	120	LYS
60	n4	1	MET
60	n4	2	LYS
60	n4	7	SER
60	n4	9	SER
60	n4	19	THR
60	n4	30	ARG
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	100	VAL
60	n4	105	ARG
60	n4	107	GLU
60	n4	112	ASN
60	n4	114	GLU
60	n4	119	GLU
60	n4	127	LYS
60	n4	134	GLN
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	37	THR
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE

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Mol	Chain	Res	Type
61	n5	71	THR
61	n5	86	VAL
61	n5	87	SER
61	n5	108	LEU
61	n5	109	LYS
61	n5	115	ARG
61	n5	119	THR
61	n5	124	VAL
61	n5	125	ARG
61	n5	126	LEU
61	n5	133	LEU
61	n5	135	ILE
62	n6	3	LYS
62	n6	6	LEU
62	n6	12	ARG
62	n6	17	LYS
62	n6	28	ARG
62	n6	32	SER
62	n6	35	LEU
62	n6	36	SER
62	n6	37	LYS
62	n6	39	LEU
62	n6	50	ILE
62	n6	51	ARG
62	n6	55	GLU
62	n6	56	VAL
62	n6	66	GLN
62	n6	74	TYR
62	n6	95	VAL
62	n6	105	VAL
62	n6	106	ILE
62	n6	113	LYS
62	n6	115	ARG
62	n6	120	GLN
62	n6	126	LEU
62	n6	127	GLU
63	n7	3	LYS
63	n7	5	LEU
63	n7	14	VAL
63	n7	17	ARG
63	n7	24	VAL
63	n7	27	LYS

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Mol	Chain	Res	Type
63	n7	28	PRO
63	n7	33	SER
63	n7	34	LYS
63	n7	51	LEU
63	n7	52	LYS
63	n7	67	LYS
63	n7	72	ILE
63	n7	73	LYS
63	n7	75	VAL
63	n7	81	LEU
63	n7	83	THR
63	n7	85	TYR
63	n7	87	LEU
63	n7	93	LYS
63	n7	94	SER
63	n7	99	GLU
63	n7	100	THR
63	n7	102	GLU
63	n7	103	GLN
63	n7	128	GLN
63	n7	134	LEU
63	n7	135	ARG
64	n8	3	SER
64	n8	6	THR
64	n8	8	THR
64	n8	9	ARG
64	n8	10	LYS
64	n8	12	ARG
64	n8	15	VAL
64	n8	22	ILE
64	n8	24	LYS
64	n8	25	HIS
64	n8	26	ARG
64	n8	27	LYS
64	n8	43	ILE
64	n8	47	LYS
64	n8	56	VAL
64	n8	60	TYR
64	n8	65	GLN
64	n8	70	LYS
64	n8	73	LEU
64	n8	88	ASP

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Mol	Chain	Res	Type
64	n8	91	LEU
64	n8	97	GLU
64	n8	117	ARG
64	n8	128	ARG
64	n8	132	LYS
64	n8	133	LEU
64	n8	139	ARG
65	n9	3	LYS
65	n9	4	SER
65	n9	7	HIS
65	n9	8	THR
65	n9	13	THR
65	n9	14	ARG
65	n9	15	LYS
65	n9	17	HIS
65	n9	19	ASN
65	n9	21	ILE
65	n9	22	LYS
65	n9	26	THR
65	n9	31	SER
65	n9	38	LYS
65	n9	58	LYS
65	n9	59	LYS
66	o0	8	GLU
66	o0	13	LYS
66	o0	19	LYS
66	o0	32	LYS
66	o0	33	SER
66	o0	34	LEU
66	o0	51	LEU
66	o0	61	MET
66	o0	71	GLN
66	o0	74	ASN
66	o0	84	LEU
66	o0	86	ARG
66	o0	87	VAL
66	o0	101	LEU
66	o0	103	THR
67	o1	6	ASP
67	o1	13	THR
67	o1	16	LEU
67	o1	24	SER

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Mol	Chain	Res	Type
67	o1	26	LYS
67	o1	28	ARG
67	o1	31	ARG
67	o1	42	LEU
67	o1	44	MET
67	o1	46	THR
67	o1	55	LEU
67	o1	64	VAL
67	o1	67	VAL
67	o1	68	GLU
67	o1	71	LEU
67	o1	73	LEU
67	o1	75	ILE
67	o1	76	SER
67	o1	83	GLU
67	o1	87	ASN
67	o1	90	PHE
67	o1	91	SER
67	o1	93	VAL
67	o1	96	VAL
67	o1	97	LEU
67	o1	100	SER
67	o1	102	LYS
67	o1	104	LEU
67	o1	106	THR
67	o1	107	VAL
67	o1	110	GLU
68	o2	4	LEU
68	o2	6	HIS
68	o2	8	LYS
68	o2	10	VAL
68	o2	14	THR
68	o2	19	ARG
68	o2	21	HIS
68	o2	24	ARG
68	o2	27	ARG
68	o2	33	ARG
68	o2	35	GLN
68	o2	40	SER
68	o2	41	VAL
68	o2	44	ARG
68	o2	45	ARG

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Mol	Chain	Res	Type
68	o2	51	SER
68	o2	59	SER
68	o2	61	LYS
68	o2	67	SER
68	o2	73	THR
68	o2	75	LEU
68	o2	91	THR
68	o2	105	ARG
68	o2	109	LEU
68	o2	119	VAL
68	o2	120	THR
68	o2	125	ARG
68	o2	126	LEU
69	o3	9	VAL
69	o3	22	VAL
69	o3	31	LYS
69	o3	37	THR
69	o3	42	GLN
69	o3	57	LYS
69	o3	58	GLU
69	o3	59	VAL
69	o3	60	ARG
69	o3	70	LYS
69	o3	73	ARG
69	o3	74	THR
69	o3	93	THR
69	o3	97	SER
69	o3	98	VAL
70	o4	4	ARG
70	o4	10	ARG
70	o4	17	SER
70	o4	22	VAL
70	o4	25	THR
70	o4	30	LEU
70	o4	47	CYS
70	o4	58	ARG
70	o4	66	SER
70	o4	79	SER
70	o4	86	LYS
70	o4	98	GLN
70	o4	104	VAL
71	o5	4	VAL

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Mol	Chain	Res	Type
71	o5	5	LYS
71	o5	20	GLN
71	o5	21	LEU
71	o5	26	LYS
71	o5	27	GLU
71	o5	28	LEU
71	o5	30	GLU
71	o5	31	LEU
71	o5	37	SER
71	o5	38	ARG
71	o5	46	THR
71	o5	47	VAL
71	o5	48	ARG
71	o5	57	VAL
71	o5	62	GLN
71	o5	68	GLN
71	o5	69	LEU
71	o5	76	GLN
71	o5	81	ARG
71	o5	84	LYS
71	o5	89	ARG
71	o5	90	ARG
71	o5	93	THR
71	o5	107	LYS
71	o5	108	GLN
71	o5	113	GLN
72	o6	7	ILE
72	o6	9	ILE
72	o6	13	LYS
72	o6	17	VAL
72	o6	20	MET
72	o6	21	THR
72	o6	27	SER
72	o6	29	LYS
72	o6	35	ASN
72	o6	36	ARG
72	o6	37	THR
72	o6	42	SER
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE

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Mol	Chain	Res	Type
72	o6	60	LEU
72	o6	68	ARG
72	o6	70	ARG
72	o6	74	LYS
72	o6	75	LYS
72	o6	76	ARG
72	o6	79	SER
72	o6	81	THR
72	o6	94	ILE
72	o6	98	ARG
72	o6	99	ARG
73	o7	15	SER
73	o7	17	THR
73	o7	21	ARG
73	o7	24	ARG
73	o7	25	ARG
73	o7	33	THR
73	o7	36	SER
73	o7	46	SER
73	o7	54	LYS
73	o7	55	ARG
73	o7	59	THR
73	o7	64	MET
73	o7	65	ARG
73	o7	67	LEU
73	o7	73	ARG
73	o7	75	LYS
73	o7	76	ASN
73	o7	85	LYS
74	o8	8	ILE
74	o8	12	LEU
74	o8	15	THR
74	o8	16	ARG
74	o8	17	ARG
74	o8	19	ASP
74	o8	24	THR
74	o8	27	ILE
74	o8	41	THR
74	o8	46	ARG
74	o8	48	SER
74	o8	53	THR
74	o8	55	VAL

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Mol	Chain	Res	Type
74	o8	61	LYS
74	o8	63	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	72	THR
75	o9	4	GLN
75	o9	9	ILE
75	o9	11	GLN
75	o9	15	LYS
75	o9	19	GLN
75	o9	21	ARG
75	o9	23	LEU
75	o9	28	ARG
75	o9	29	LEU
75	o9	36	ARG
75	o9	45	ARG
75	o9	48	LYS
76	q0	77	ILE
76	q0	78	ILE
76	q0	79	GLU
76	q0	85	LEU
76	q0	91	CYS
76	q0	93	LYS
76	q0	94	SER
76	q0	95	VAL
76	q0	98	LYS
76	q0	99	CYS
76	q0	106	ARG
76	q0	108	THR
76	q0	112	LYS
76	q0	114	LYS
76	q0	127	LEU
77	q1	1	MET
77	q1	2	ARG
77	q1	6	ARG
77	q1	9	ARG
77	q1	14	LYS
77	q1	18	ARG
77	q1	20	VAL
77	q1	21	ARG
77	q1	23	ARG
78	q2	7	THR

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Mol	Chain	Res	Type
78	q2	8	ARG
78	q2	28	TYR
78	q2	38	GLN
78	q2	45	ARG
78	q2	61	LYS
78	q2	71	ARG
78	q2	72	LEU
78	q2	79	THR
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	89	LYS
78	q2	92	GLU
78	q2	93	LEU
78	q2	98	LYS
78	q2	100	LYS
78	q2	104	LEU
78	q2	105	GLN
78	q2	106	PHE
79	q3	3	LYS
79	q3	8	VAL
79	q3	10	ILE
79	q3	20	SER
79	q3	21	SER
79	q3	33	GLN
79	q3	40	SER
79	q3	42	CYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	58	SER
79	q3	59	CYS
79	q3	64	VAL
79	q3	70	THR
79	q3	78	THR
79	q3	85	ARG
81	p0	4	ILE
81	p0	5	ARG
81	p0	30	VAL
81	p0	43	LYS
81	p0	48	ARG
81	p0	51	VAL

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Mol	Chain	Res	Type
81	p0	57	THR
81	p0	67	LEU
81	p0	68	SER
81	p0	69	ASP
81	p0	70	LEU
81	p0	72	ASP
81	p0	81	LYS
81	p0	84	VAL
81	p0	89	THR
81	p0	93	LEU
81	p0	95	GLU
81	p0	97	LYS
81	p0	104	ARG
81	p0	192	ASP
81	p0	193	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
2	S0	32	HIS
5	S3	111	ASN
5	S3	179	GLN
6	S4	17	HIS
6	S4	50	ASN
6	S4	98	ASN
7	S5	103	ASN
9	S7	5	GLN
9	S7	71	HIS
10	S8	9	HIS
13	C1	104	HIS
15	C3	5	HIS
15	C3	105	ASN
17	C5	82	ASN
18	C6	83	GLN
20	C8	89	GLN
24	D2	24	GLN
24	D2	56	HIS
29	D7	5	GLN
31	D9	48	ASN
34	SR	153	GLN
39	L2	209	HIS
40	L3	256	HIS

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Mol	Chain	Res	Type
41	L4	5	GLN
44	L7	64	GLN
45	L8	45	ASN
46	L9	49	ASN
46	L9	59	ASN
46	L9	116	ASN
47	M0	12	GLN
49	M3	25	HIS
52	M6	29	ASN
54	M8	145	ASN
58	N2	52	ASN
59	N3	33	ASN
59	N3	98	ASN
63	N7	57	HIS
64	N8	74	ASN
65	N9	45	HIS
70	O4	18	ASN
72	O6	91	ASN
2	s0	39	ASN
2	s0	46	HIS
3	s1	148	ASN
3	s1	149	GLN
8	s6	210	GLN
11	s9	124	HIS
12	c0	32	HIS
12	c0	39	ASN
19	c7	29	GLN
20	c8	90	ASN
21	c9	101	ASN
22	d0	48	HIS
25	d3	10	ASN
25	d3	18	HIS
26	d4	77	ASN
28	d6	43	ASN
33	e1	151	ASN
34	sR	198	ASN
35	sM	71	ASN
41	l4	221	ASN
45	l8	41	GLN
47	m0	12	GLN
51	m5	178	HIS
53	m7	137	ASN

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Mol	Chain	Res	Type
57	n1	98	HIS
61	n5	55	ASN
62	n6	66	GLN
63	n7	123	GLN
64	n8	28	HIS
69	o3	88	ASN
70	o4	18	ASN
78	q2	38	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	541 (30%)	51 (2%)
1	6	1793/1800 (99%)	494 (27%)	48 (2%)
36	1	3145/3396 (92%)	774 (24%)	86 (2%)
36	5	3145/3396 (92%)	801 (25%)	77 (2%)
37	3	120/121 (99%)	20 (16%)	0
37	7	120/121 (99%)	28 (23%)	2 (1%)
38	4	157/158 (99%)	42 (26%)	3 (1%)
38	8	157/158 (99%)	44 (28%)	2 (1%)
All	All	10384/10950 (94%)	2744 (26%)	269 (2%)

All (2744) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	10	G
1	2	25	C
1	2	26	A
1	2	27	U
1	2	31	C
1	2	34	G
1	2	45	U
1	2	46	A
1	2	47	A
1	2	54	C
1	2	57	G
1	2	60	U
1	2	66	U
1	2	68	A

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Mol	Chain	Res	Type
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	80	A
1	2	104	A
1	2	114	C
1	2	116	U
1	2	128	U
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	151	G
1	2	153	G
1	2	158	U
1	2	159	U
1	2	161	U
1	2	166	C
1	2	167	U
1	2	169	A
1	2	176	C
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U

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Mol	Chain	Res	Type
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	200	A
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	226	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	231	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	236	A
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	242	U
1	2	246	G
1	2	249	U
1	2	250	C
1	2	260	U
1	2	261	U
1	2	265	A
1	2	270	C
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	284	G

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Mol	Chain	Res	Type
1	2	285	G
1	2	288	A
1	2	290	G
1	2	299	A
1	2	302	U
1	2	308	C
1	2	309	C
1	2	313	U
1	2	314	C
1	2	316	A
1	2	319	U
1	2	321	C
1	2	322	G
1	2	337	G
1	2	338	C
1	2	339	C
1	2	346	G
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	393	C
1	2	397	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	416	A
1	2	418	G
1	2	419	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	430	G
1	2	434	G
1	2	437	A
1	2	439	U
1	2	444	C
1	2	446	A

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Mol	Chain	Res	Type
1	2	448	C
1	2	454	U
1	2	455	C
1	2	459	G
1	2	468	A
1	2	470	A
1	2	473	A
1	2	475	A
1	2	477	A
1	2	480	G
1	2	483	A
1	2	484	C
1	2	485	A
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G
1	2	511	A
1	2	512	A
1	2	513	U
1	2	514	G
1	2	515	A
1	2	516	G
1	2	527	A
1	2	532	U
1	2	533	U
1	2	536	C
1	2	538	A
1	2	539	G

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Mol	Chain	Res	Type
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	546	U
1	2	548	G
1	2	554	C
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	579	A
1	2	580	A
1	2	582	U
1	2	585	A
1	2	594	A
1	2	595	G
1	2	597	G
1	2	598	U
1	2	611	U
1	2	619	A
1	2	620	A
1	2	621	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	630	A
1	2	631	G
1	2	639	U
1	2	640	U
1	2	650	U
1	2	652	G
1	2	653	C
1	2	654	C
1	2	656	G
1	2	658	C
1	2	677	G
1	2	680	U
1	2	682	C

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Mol	Chain	Res	Type
1	2	684	A
1	2	685	A
1	2	686	C
1	2	692	C
1	2	694	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	699	U
1	2	700	C
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	707	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	711	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	716	C
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	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

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Mol	Chain	Res	Type
1	2	742	U
1	2	745	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	771	A
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	787	G
1	2	789	A
1	2	793	A
1	2	794	U
1	2	795	U
1	2	796	A
1	2	806	A
1	2	807	A
1	2	811	A
1	2	812	A
1	2	814	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	823	G
1	2	824	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	833	U
1	2	846	G
1	2	848	C
1	2	852	C

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Mol	Chain	Res	Type
1	2	855	A
1	2	856	A
1	2	862	A
1	2	863	A
1	2	876	G
1	2	886	U
1	2	892	A
1	2	897	C
1	2	898	A
1	2	908	U
1	2	912	U
1	2	913	G
1	2	914	G
1	2	915	A
1	2	916	U
1	2	921	U
1	2	933	A
1	2	935	U
1	2	942	G
1	2	952	A
1	2	960	U
1	2	964	U
1	2	966	A
1	2	975	C
1	2	977	A
1	2	988	A
1	2	991	G
1	2	992	A
1	2	993	A
1	2	995	A
1	2	997	G
1	2	1001	A
1	2	1002	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1011	G
1	2	1014	G
1	2	1026	A
1	2	1028	C
1	2	1032	G
1	2	1039	A

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Mol	Chain	Res	Type
1	2	1040	G
1	2	1043	A
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1064	G
1	2	1074	G
1	2	1076	A
1	2	1079	U
1	2	1080	U
1	2	1082	C
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1093	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1109	G
1	2	1138	A
1	2	1139	A
1	2	1141	G
1	2	1143	A
1	2	1146	G
1	2	1150	G
1	2	1151	A
1	2	1155	G
1	2	1157	A
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1167	G
1	2	1168	U
1	2	1185	U
1	2	1187	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
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	1217	A
1	2	1218	G
1	2	1226	A
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1235	C
1	2	1238	A
1	2	1241	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1258	U
1	2	1273	G
1	2	1276	U
1	2	1284	C
1	2	1285	U
1	2	1286	U
1	2	1288	G
1	2	1307	U
1	2	1314	U
1	2	1315	U
1	2	1320	U
1	2	1321	A
1	2	1332	C
1	2	1337	A
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1354	G
1	2	1355	C
1	2	1363	U
1	2	1364	G
1	2	1370	U

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Mol	Chain	Res	Type
1	2	1371	A
1	2	1372	U
1	2	1379	C
1	2	1384	A
1	2	1388	A
1	2	1390	U
1	2	1391	A
1	2	1395	G
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	1415	U
1	2	1418	G
1	2	1427	A
1	2	1428	G
1	2	1432	U
1	2	1433	G
1	2	1445	G
1	2	1446	A
1	2	1447	C
1	2	1448	G
1	2	1457	C
1	2	1458	G
1	2	1459	C
1	2	1460	A
1	2	1461	C
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1478	G
1	2	1482	C
1	2	1483	A
1	2	1487	A
1	2	1488	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A

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Mol	Chain	Res	Type
1	2	1499	G
1	2	1501	C
1	2	1506	G
1	2	1514	U
1	2	1515	A
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	1533	C
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1539	G
1	2	1542	G
1	2	1555	A
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1573	A
1	2	1574	G
1	2	1576	A
1	2	1584	G
1	2	1590	G
1	2	1596	C
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1619	C
1	2	1624	C
1	2	1626	U
1	2	1631	A
1	2	1634	C
1	2	1637	C
1	2	1650	U
1	2	1657	U
1	2	1658	G
1	2	1666	U
1	2	1682	U

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Mol	Chain	Res	Type
1	2	1683	C
1	2	1684	U
1	2	1731	A
1	2	1750	A
1	2	1754	A
1	2	1755	A
1	2	1756	A
1	2	1760	G
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	1789	G
1	2	1790	A
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1796	C
36	1	6	A
36	1	14	U
36	1	26	A
36	1	39	A
36	1	40	A
36	1	43	A
36	1	49	A
36	1	55	G
36	1	57	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	76	G
36	1	77	A
36	1	83	U
36	1	92	G
36	1	93	C
36	1	97	U
36	1	99	A
36	1	102	C

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Mol	Chain	Res	Type
36	1	109	A
36	1	110	G
36	1	111	C
36	1	114	A
36	1	115	A
36	1	116	A
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	139	G
36	1	156	G
36	1	157	A
36	1	160	G
36	1	165	A
36	1	166	C
36	1	169	U
36	1	170	G
36	1	177	U
36	1	187	A
36	1	188	U
36	1	190	U
36	1	191	U
36	1	201	A
36	1	202	G
36	1	210	U
36	1	213	A
36	1	218	G
36	1	219	A
36	1	220	G
36	1	224	C
36	1	227	G
36	1	239	G
36	1	240	U
36	1	241	G
36	1	243	G
36	1	245	U
36	1	246	U
36	1	247	C
36	1	249	U
36	1	250	U

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Mol	Chain	Res	Type
36	1	251	G
36	1	252	U
36	1	269	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	315	C
36	1	316	U
36	1	323	A
36	1	326	U
36	1	329	U
36	1	339	C
36	1	350	C
36	1	352	A
36	1	374	A
36	1	375	A
36	1	376	G
36	1	398	A
36	1	399	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	404	G
36	1	421	G
36	1	422	A
36	1	424	G
36	1	438	A
36	1	439	C
36	1	440	A
36	1	495	G
36	1	497	C
36	1	503	C
36	1	510	G
36	1	518	G
36	1	520	U
36	1	521	A
36	1	529	A
36	1	531	G
36	1	535	G
36	1	544	C
36	1	546	C

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Mol	Chain	Res	Type
36	1	547	G
36	1	548	G
36	1	550	A
36	1	551	A
36	1	552	G
36	1	553	U
36	1	555	U
36	1	557	A
36	1	558	U
36	1	559	A
36	1	572	A
36	1	578	A
36	1	579	G
36	1	581	U
36	1	592	A
36	1	594	U
36	1	596	C
36	1	599	C
36	1	600	G
36	1	601	U
36	1	604	G
36	1	609	G
36	1	611	A
36	1	618	C
36	1	619	A
36	1	620	U
36	1	621	A
36	1	624	G
36	1	636	C
36	1	637	C
36	1	638	C
36	1	642	U
36	1	644	G
36	1	648	C
36	1	649	A
36	1	651	G
36	1	657	A
36	1	660	A
36	1	661	G
36	1	662	U
36	1	675	C
36	1	677	A

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Mol	Chain	Res	Type
36	1	681	U
36	1	683	U
36	1	685	G
36	1	691	A
36	1	705	A
36	1	708	G
36	1	709	A
36	1	711	A
36	1	712	G
36	1	715	A
36	1	716	A
36	1	717	C
36	1	719	U
36	1	762	U
36	1	764	U
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	780	A
36	1	781	G
36	1	785	G
36	1	786	A
36	1	790	U
36	1	792	G
36	1	798	G
36	1	803	C
36	1	806	A
36	1	817	A
36	1	825	U
36	1	830	A
36	1	837	A
36	1	845	G
36	1	861	C
36	1	867	G
36	1	869	G
36	1	871	U
36	1	872	U
36	1	874	U
36	1	875	G
36	1	879	U
36	1	880	G

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Mol	Chain	Res	Type
36	1	890	C
36	1	896	A
36	1	907	G
36	1	908	G
36	1	910	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	919	U
36	1	923	C
36	1	924	G
36	1	930	U
36	1	937	G
36	1	944	C
36	1	953	G
36	1	959	C
36	1	960	U
36	1	963	G
36	1	969	C
36	1	979	U
36	1	981	U
36	1	982	C
36	1	984	G
36	1	991	G
36	1	993	G
36	1	994	G
36	1	995	U
36	1	1000	C
36	1	1001	G
36	1	1002	A
36	1	1003	A
36	1	1004	U
36	1	1010	G
36	1	1017	C
36	1	1018	G
36	1	1019	G
36	1	1020	G
36	1	1021	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1034	U

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Mol	Chain	Res	Type
36	1	1036	A
36	1	1037	C
36	1	1041	U
36	1	1042	U
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1053	A
36	1	1063	G
36	1	1064	A
36	1	1065	A
36	1	1068	C
36	1	1072	G
36	1	1081	U
36	1	1082	U
36	1	1087	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1129	A
36	1	1131	G
36	1	1153	A
36	1	1159	A
36	1	1160	C
36	1	1178	G
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1191	U
36	1	1192	C
36	1	1200	A
36	1	1201	C
36	1	1202	A
36	1	1209	G
36	1	1212	A
36	1	1213	G

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Mol	Chain	Res	Type
36	1	1217	A
36	1	1222	G
36	1	1225	A
36	1	1226	G
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1236	G
36	1	1237	G
36	1	1241	U
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1251	A
36	1	1253	U
36	1	1254	C
36	1	1257	C
36	1	1258	U
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
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	1276	U
36	1	1278	A
36	1	1279	C
36	1	1285	G
36	1	1287	A
36	1	1292	C
36	1	1305	U
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1312	C
36	1	1313	G
36	1	1318	A

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Mol	Chain	Res	Type
36	1	1325	U
36	1	1330	A
36	1	1331	U
36	1	1339	C
36	1	1348	U
36	1	1349	G
36	1	1350	A
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1373	A
36	1	1386	A
36	1	1392	G
36	1	1397	C
36	1	1399	A
36	1	1400	G
36	1	1405	U
36	1	1406	A
36	1	1417	G
36	1	1418	A
36	1	1419	A
36	1	1429	G
36	1	1431	G
36	1	1433	A
36	1	1434	G
36	1	1435	A
36	1	1437	C
36	1	1446	A
36	1	1450	G
36	1	1468	A
36	1	1471	U
36	1	1472	U
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1508	C
36	1	1511	U
36	1	1527	C
36	1	1533	U

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Mol	Chain	Res	Type
36	1	1535	A
36	1	1548	C
36	1	1555	U
36	1	1556	C
36	1	1557	A
36	1	1560	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1572	U
36	1	1578	C
36	1	1579	C
36	1	1580	A
36	1	1581	C
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1593	A
36	1	1594	A
36	1	1605	A
36	1	1607	U
36	1	1608	C
36	1	1620	U
36	1	1621	A
36	1	1624	G
36	1	1629	U
36	1	1633	C
36	1	1639	C
36	1	1641	U
36	1	1643	A
36	1	1645	U
36	1	1656	A
36	1	1657	C
36	1	1668	G
36	1	1679	A
36	1	1683	A

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Mol	Chain	Res	Type
36	1	1687	U
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1725	C
36	1	1731	A
36	1	1736	G
36	1	1741	A
36	1	1742	U
36	1	1750	A
36	1	1751	G
36	1	1756	C
36	1	1761	C
36	1	1764	U
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1770	G
36	1	1773	C
36	1	1775	G
36	1	1780	G
36	1	1782	U
36	1	1793	C
36	1	1797	A
36	1	1810	A
36	1	1814	A
36	1	1815	U
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1835	A
36	1	1839	A
36	1	1842	A
36	1	1845	G
36	1	1846	C
36	1	1849	C
36	1	1858	A
36	1	1866	C
36	1	1871	U
36	1	1879	A

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Mol	Chain	Res	Type
36	1	1880	U
36	1	1886	A
36	1	1901	A
36	1	1906	G
36	1	1908	A
36	1	1920	U
36	1	1951	C
36	1	1952	G
36	1	1953	G
36	1	1954	G
36	1	2101	C
36	1	2102	U
36	1	2106	A
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2114	C
36	1	2116	G
36	1	2121	G
36	1	2122	G
36	1	2127	U
36	1	2131	A
36	1	2134	G
36	1	2139	A
36	1	2140	U
36	1	2149	A
36	1	2156	C
36	1	2158	A
36	1	2169	G
36	1	2187	G
36	1	2198	A
36	1	2205	U
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2213	A
36	1	2223	A
36	1	2225	U
36	1	2228	A
36	1	2229	A
36	1	2239	G
36	1	2244	A

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Mol	Chain	Res	Type
36	1	2245	C
36	1	2246	G
36	1	2247	G
36	1	2249	G
36	1	2250	G
36	1	2252	A
36	1	2255	A
36	1	2256	A
36	1	2262	A
36	1	2266	U
36	1	2272	G
36	1	2273	G
36	1	2276	G
36	1	2281	A
36	1	2282	U
36	1	2283	G
36	1	2284	C
36	1	2288	G
36	1	2295	A
36	1	2303	A
36	1	2306	C
36	1	2307	G
36	1	2308	C
36	1	2309	A
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2318	U
36	1	2319	U
36	1	2324	A
36	1	2334	U
36	1	2336	U
36	1	2350	C
36	1	2352	A
36	1	2361	A
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2375	G
36	1	2382	G
36	1	2385	G

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Mol	Chain	Res	Type
36	1	2388	U
36	1	2393	G
36	1	2394	G
36	1	2397	A
36	1	2402	A
36	1	2403	G
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2427	U
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	2530	G
36	1	2531	C
36	1	2532	U
36	1	2533	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2544	U
36	1	2545	C
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

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Mol	Chain	Res	Type
36	1	2572	C
36	1	2573	G
36	1	2581	U
36	1	2582	C
36	1	2585	G
36	1	2593	A
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2626	A
36	1	2629	U
36	1	2637	A
36	1	2638	C
36	1	2652	U
36	1	2656	A
36	1	2657	A
36	1	2660	G
36	1	2672	G
36	1	2674	A
36	1	2675	C
36	1	2677	G
36	1	2681	U
36	1	2689	A
36	1	2690	G
36	1	2691	A
36	1	2694	A
36	1	2696	A
36	1	2705	A
36	1	2714	G
36	1	2725	U
36	1	2727	A
36	1	2728	G
36	1	2729	U
36	1	2739	A
36	1	2740	A
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

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Mol	Chain	Res	Type
36	1	2779	A
36	1	2796	G
36	1	2797	C
36	1	2800	G
36	1	2801	A
36	1	2802	A
36	1	2810	C
36	1	2814	G
36	1	2816	G
36	1	2817	A
36	1	2818	U
36	1	2821	C
36	1	2822	U
36	1	2827	U
36	1	2829	U
36	1	2839	G
36	1	2842	U
36	1	2844	C
36	1	2845	A
36	1	2847	A
36	1	2849	C
36	1	2855	U
36	1	2860	U
36	1	2862	U
36	1	2863	G
36	1	2865	U
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2884	C
36	1	2887	A
36	1	2889	C
36	1	2893	C
36	1	2897	A
36	1	2898	G
36	1	2899	C
36	1	2911	A
36	1	2917	G
36	1	2923	U
36	1	2933	A
36	1	2935	U
36	1	2936	A

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Mol	Chain	Res	Type
36	1	2942	C
36	1	2945	G
36	1	2947	G
36	1	2954	U
36	1	2971	A
36	1	2973	G
36	1	2974	U
36	1	2977	G
36	1	2979	U
36	1	2982	A
36	1	2983	C
36	1	2990	G
36	1	2996	U
36	1	2997	G
36	1	3012	A
36	1	3021	A
36	1	3030	G
36	1	3041	U
36	1	3049	A
36	1	3056	U
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3080	G
36	1	3085	G
36	1	3086	A
36	1	3087	A
36	1	3092	C
36	1	3093	C
36	1	3113	A
36	1	3120	C
36	1	3122	A
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

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Mol	Chain	Res	Type
36	1	3156	U
36	1	3157	U
36	1	3158	G
36	1	3164	C
36	1	3165	A
36	1	3167	A
36	1	3168	A
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3187	A
36	1	3195	U
36	1	3196	U
36	1	3198	U
36	1	3199	G
36	1	3204	C
36	1	3206	C
36	1	3207	U
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3228	C
36	1	3229	G
36	1	3243	A
36	1	3244	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3249	C
36	1	3253	G
36	1	3259	U
36	1	3262	U
36	1	3263	G
36	1	3269	U
36	1	3270	U
36	1	3273	A
36	1	3276	G
36	1	3279	A

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Mol	Chain	Res	Type
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3288	G
36	1	3289	G
36	1	3290	G
36	1	3293	U
36	1	3294	A
36	1	3295	A
36	1	3304	U
36	1	3309	G
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	3363	U
36	1	3369	G
36	1	3372	A
36	1	3375	A
36	1	3376	A
36	1	3378	C
36	1	3382	U
36	1	3389	U
36	1	3390	G
36	1	3396	U
37	3	7	G
37	3	9	C
37	3	21	G

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Mol	Chain	Res	Type
37	3	22	A
37	3	25	G
37	3	27	A
37	3	44	C
37	3	45	A
37	3	51	A
37	3	54	U
37	3	60	G
37	3	65	G
37	3	74	C
37	3	76	A
37	3	92	A
37	3	93	C
37	3	102	A
37	3	106	U
37	3	112	G
37	3	121	U
38	4	2	A
38	4	17	A
38	4	20	U
38	4	23	U
38	4	26	U
38	4	34	U
38	4	35	C
38	4	43	A
38	4	50	C
38	4	51	G
38	4	52	A
38	4	54	A
38	4	58	G
38	4	59	A
38	4	62	C
38	4	63	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

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Mol	Chain	Res	Type
38	4	95	G
38	4	96	A
38	4	97	A
38	4	104	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	114	G
38	4	125	U
38	4	126	A
38	4	128	U
38	4	134	G
38	4	138	A
38	4	152	G
38	4	155	A
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	6	G
1	6	11	A
1	6	17	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	38	C
1	6	45	U
1	6	46	A
1	6	47	A
1	6	50	C
1	6	57	G
1	6	61	A
1	6	66	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	78	A

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Mol	Chain	Res	Type
1	6	101	U
1	6	104	A
1	6	105	A
1	6	111	U
1	6	114	C
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	142	G
1	6	143	G
1	6	144	U
1	6	145	A
1	6	146	U
1	6	153	G
1	6	158	U
1	6	159	U
1	6	171	A
1	6	176	C
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	196	G
1	6	199	G
1	6	200	A
1	6	214	G
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

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Mol	Chain	Res	Type
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	271	A
1	6	272	U
1	6	273	G
1	6	275	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	281	G
1	6	287	G
1	6	292	U
1	6	299	A
1	6	302	U
1	6	308	C
1	6	314	C
1	6	316	A
1	6	320	U
1	6	321	C
1	6	322	G
1	6	337	G
1	6	338	C
1	6	341	A
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	370	A
1	6	381	C
1	6	386	G
1	6	390	G
1	6	400	A

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Mol	Chain	Res	Type
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	418	G
1	6	419	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	429	G
1	6	434	G
1	6	437	A
1	6	439	U
1	6	444	C
1	6	448	C
1	6	470	A
1	6	475	A
1	6	477	A
1	6	484	C
1	6	485	A
1	6	486	G
1	6	487	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U
1	6	496	G
1	6	499	U
1	6	500	C
1	6	501	U
1	6	502	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

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Mol	Chain	Res	Type
1	6	515	A
1	6	518	A
1	6	519	C
1	6	527	A
1	6	536	C
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	554	C
1	6	557	G
1	6	558	U
1	6	559	C
1	6	565	C
1	6	570	A
1	6	574	G
1	6	575	C
1	6	578	U
1	6	579	A
1	6	580	A
1	6	582	U
1	6	584	C
1	6	588	U
1	6	594	A
1	6	595	G
1	6	611	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	634	G
1	6	635	A
1	6	637	C
1	6	639	U
1	6	650	U
1	6	651	G
1	6	652	G
1	6	653	C
1	6	655	G

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Mol	Chain	Res	Type
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
1	6	669	G
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	680	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	691	C
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	726	C
1	6	730	G
1	6	741	C
1	6	742	U
1	6	744	U
1	6	751	G
1	6	752	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

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Mol	Chain	Res	Type
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	811	A
1	6	812	A
1	6	814	A
1	6	815	G
1	6	816	G
1	6	820	U
1	6	821	U
1	6	823	G
1	6	824	G
1	6	825	U
1	6	826	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	856	A
1	6	860	U
1	6	862	A
1	6	863	A
1	6	868	G
1	6	873	U
1	6	875	G
1	6	898	A
1	6	906	A
1	6	912	U
1	6	913	G
1	6	914	G
1	6	915	A
1	6	916	U
1	6	925	G
1	6	931	C
1	6	933	A

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Mol	Chain	Res	Type
1	6	935	U
1	6	940	A
1	6	942	G
1	6	944	A
1	6	945	U
1	6	954	G
1	6	959	U
1	6	960	U
1	6	966	A
1	6	969	C
1	6	971	A
1	6	983	A
1	6	992	A
1	6	993	A
1	6	996	U
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1021	C
1	6	1026	A
1	6	1028	C
1	6	1029	U
1	6	1039	A
1	6	1040	G
1	6	1041	G
1	6	1042	G
1	6	1043	A
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	1071	U
1	6	1074	G
1	6	1080	U
1	6	1081	A
1	6	1082	C
1	6	1092	A
1	6	1096	C
1	6	1097	U
1	6	1098	U

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Mol	Chain	Res	Type
1	6	1100	G
1	6	1109	G
1	6	1121	C
1	6	1138	A
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1161	C
1	6	1167	G
1	6	1185	U
1	6	1194	A
1	6	1196	A
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1217	A
1	6	1218	G
1	6	1219	A
1	6	1220	C
1	6	1221	A
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1236	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	1248	C
1	6	1252	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1259	U
1	6	1275	A
1	6	1285	U

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Mol	Chain	Res	Type
1	6	1286	U
1	6	1288	G
1	6	1293	U
1	6	1307	U
1	6	1312	A
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1319	A
1	6	1320	U
1	6	1321	A
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1354	G
1	6	1355	C
1	6	1360	A
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1370	U
1	6	1371	A
1	6	1373	C
1	6	1382	A
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1412	G
1	6	1413	U
1	6	1415	U
1	6	1422	A
1	6	1427	A
1	6	1428	G
1	6	1431	C
1	6	1433	G
1	6	1445	G
1	6	1446	A

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Mol	Chain	Res	Type
1	6	1447	C
1	6	1448	G
1	6	1459	C
1	6	1461	C
1	6	1471	A
1	6	1481	C
1	6	1482	C
1	6	1483	A
1	6	1486	G
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	1514	U
1	6	1515	A
1	6	1516	A
1	6	1517	U
1	6	1519	U
1	6	1520	U
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	1526	A
1	6	1531	G
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	1550	A
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1560	U
1	6	1569	A
1	6	1573	A
1	6	1574	G
1	6	1575	G

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Mol	Chain	Res	Type
1	6	1584	G
1	6	1590	G
1	6	1596	C
1	6	1600	A
1	6	1601	G
1	6	1619	C
1	6	1620	C
1	6	1621	U
1	6	1634	C
1	6	1637	C
1	6	1638	G
1	6	1641	C
1	6	1657	U
1	6	1658	G
1	6	1682	U
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	1703	C
1	6	1712	A
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1727	G
1	6	1731	A
1	6	1735	U
1	6	1736	G
1	6	1742	U
1	6	1747	G
1	6	1760	G
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A
1	6	1783	C
1	6	1788	G

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Mol	Chain	Res	Type
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1796	C
1	6	1798	U
1	6	1799	U
1	6	1800	A
36	5	15	C
36	5	16	A
36	5	26	A
36	5	40	A
36	5	43	A
36	5	44	U
36	5	49	A
36	5	58	G
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	73	C
36	5	76	G
36	5	85	A
36	5	92	G
36	5	94	G
36	5	96	G
36	5	102	C
36	5	108	A
36	5	109	A
36	5	110	G
36	5	111	C
36	5	116	A
36	5	120	G
36	5	121	A
36	5	122	A
36	5	130	A
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G
36	5	152	U
36	5	156	G
36	5	157	A

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Mol	Chain	Res	Type
36	5	165	A
36	5	169	U
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	187	A
36	5	190	U
36	5	191	U
36	5	200	C
36	5	203	G
36	5	204	A
36	5	206	G
36	5	210	U
36	5	211	A
36	5	213	A
36	5	218	G
36	5	219	A
36	5	220	G
36	5	221	A
36	5	222	A
36	5	227	G
36	5	231	G
36	5	234	G
36	5	236	G
36	5	239	G
36	5	240	U
36	5	244	G
36	5	247	C
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	259	C
36	5	269	G
36	5	284	A

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Mol	Chain	Res	Type
36	5	286	U
36	5	294	U
36	5	295	A
36	5	311	C
36	5	321	C
36	5	322	U
36	5	323	A
36	5	328	U
36	5	329	U
36	5	333	G
36	5	334	A
36	5	338	A
36	5	339	C
36	5	349	A
36	5	350	C
36	5	351	A
36	5	361	A
36	5	366	A
36	5	376	G
36	5	377	A
36	5	384	A
36	5	395	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	404	G
36	5	417	A
36	5	419	G
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	492	U
36	5	507	U
36	5	520	U
36	5	521	A

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Mol	Chain	Res	Type
36	5	525	C
36	5	531	G
36	5	535	G
36	5	538	G
36	5	539	C
36	5	542	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	553	U
36	5	555	U
36	5	557	A
36	5	558	U
36	5	559	A
36	5	569	A
36	5	578	A
36	5	579	G
36	5	582	G
36	5	592	A
36	5	604	G
36	5	609	G
36	5	611	A
36	5	612	U
36	5	619	A
36	5	621	A
36	5	636	C
36	5	648	C
36	5	649	A
36	5	660	A
36	5	662	U
36	5	677	A
36	5	681	U
36	5	692	A
36	5	699	A
36	5	705	A
36	5	712	G
36	5	715	A
36	5	716	A
36	5	719	U
36	5	724	U
36	5	725	G
36	5	726	G

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Mol	Chain	Res	Type
36	5	727	G
36	5	744	A
36	5	762	U
36	5	765	C
36	5	766	U
36	5	767	U
36	5	768	C
36	5	776	U
36	5	777	U
36	5	780	A
36	5	781	G
36	5	784	A
36	5	785	G
36	5	786	A
36	5	805	G
36	5	806	A
36	5	817	A
36	5	821	U
36	5	829	U
36	5	830	A
36	5	831	G
36	5	837	A
36	5	842	G
36	5	857	G
36	5	861	C
36	5	869	G
36	5	874	U
36	5	876	A
36	5	879	U
36	5	882	A
36	5	890	C
36	5	891	G
36	5	896	A
36	5	897	U
36	5	898	U
36	5	907	G
36	5	908	G
36	5	909	G
36	5	910	G
36	5	913	A
36	5	914	A
36	5	916	G

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Mol	Chain	Res	Type
36	5	917	A
36	5	921	A
36	5	923	C
36	5	924	G
36	5	929	A
36	5	931	C
36	5	932	U
36	5	937	G
36	5	944	C
36	5	948	C
36	5	959	C
36	5	960	U
36	5	964	G
36	5	979	U
36	5	980	A
36	5	981	U
36	5	994	G
36	5	1001	G
36	5	1002	A
36	5	1006	A
36	5	1010	G
36	5	1014	U
36	5	1015	U
36	5	1017	C
36	5	1019	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1028	U
36	5	1029	G
36	5	1032	C
36	5	1035	G
36	5	1047	A
36	5	1049	C
36	5	1057	A
36	5	1059	G
36	5	1063	G
36	5	1064	A
36	5	1065	A
36	5	1072	G
36	5	1081	U

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Mol	Chain	Res	Type
36	5	1082	U
36	5	1083	G
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1106	G
36	5	1112	A
36	5	1115	G
36	5	1117	G
36	5	1129	A
36	5	1131	G
36	5	1143	A
36	5	1152	G
36	5	1153	A
36	5	1155	C
36	5	1159	A
36	5	1161	G
36	5	1162	U
36	5	1169	A
36	5	1178	G
36	5	1179	A
36	5	1180	A
36	5	1181	U
36	5	1190	A
36	5	1191	U
36	5	1192	C
36	5	1193	A
36	5	1201	C
36	5	1206	G
36	5	1209	G
36	5	1220	U
36	5	1222	G
36	5	1232	C
36	5	1235	U
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U

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Mol	Chain	Res	Type
36	5	1242	G
36	5	1244	A
36	5	1245	A
36	5	1246	G
36	5	1252	A
36	5	1258	U
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1266	G
36	5	1268	G
36	5	1269	U
36	5	1275	C
36	5	1281	G
36	5	1284	C
36	5	1285	G
36	5	1292	C
36	5	1305	U
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1314	C
36	5	1324	U
36	5	1330	A
36	5	1331	U
36	5	1332	A
36	5	1347	U
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
36	5	1365	G
36	5	1368	U
36	5	1370	G
36	5	1372	C
36	5	1377	G
36	5	1379	G

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Mol	Chain	Res	Type
36	5	1380	G
36	5	1385	C
36	5	1386	A
36	5	1391	C
36	5	1392	G
36	5	1398	U
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	1440	G
36	5	1441	G
36	5	1450	G
36	5	1456	A
36	5	1465	A
36	5	1466	G
36	5	1481	A
36	5	1482	A
36	5	1483	G
36	5	1495	U
36	5	1502	C
36	5	1508	C
36	5	1511	U
36	5	1519	G
36	5	1533	U
36	5	1536	G
36	5	1549	U
36	5	1552	G
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1557	A
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1564	U

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Mol	Chain	Res	Type
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	1577	G
36	5	1578	C
36	5	1579	C
36	5	1581	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1598	G
36	5	1600	U
36	5	1605	A
36	5	1607	U
36	5	1608	C
36	5	1619	A
36	5	1620	U
36	5	1629	U
36	5	1639	C
36	5	1641	U
36	5	1642	A
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1666	G
36	5	1683	A
36	5	1684	U
36	5	1686	U
36	5	1687	U
36	5	1688	U
36	5	1713	G
36	5	1714	A
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1729	A
36	5	1733	G

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Mol	Chain	Res	Type
36	5	1736	G
36	5	1750	A
36	5	1751	G
36	5	1760	A
36	5	1761	C
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1767	C
36	5	1769	G
36	5	1770	G
36	5	1775	G
36	5	1780	G
36	5	1793	C
36	5	1795	U
36	5	1797	A
36	5	1810	A
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1821	U
36	5	1839	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1849	C
36	5	1866	C
36	5	1871	U
36	5	1876	U
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1881	A
36	5	1885	U
36	5	1886	A
36	5	1891	A
36	5	1893	A
36	5	1901	A
36	5	1903	U

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Mol	Chain	Res	Type
36	5	1904	C
36	5	1906	G
36	5	1922	A
36	5	1944	U
36	5	1948	G
36	5	2100	A
36	5	2101	C
36	5	2102	U
36	5	2111	G
36	5	2112	U
36	5	2113	A
36	5	2114	C
36	5	2121	G
36	5	2122	G
36	5	2131	A
36	5	2154	U
36	5	2158	A
36	5	2169	G
36	5	2176	U
36	5	2187	G
36	5	2192	C
36	5	2198	A
36	5	2205	U
36	5	2209	U
36	5	2210	G
36	5	2223	A
36	5	2225	U
36	5	2228	A
36	5	2231	C
36	5	2234	G
36	5	2244	A
36	5	2250	G
36	5	2252	A
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2264	U
36	5	2270	A
36	5	2272	G
36	5	2273	G
36	5	2276	G
36	5	2281	A

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Mol	Chain	Res	Type
36	5	2282	U
36	5	2283	G
36	5	2287	C
36	5	2288	G
36	5	2291	A
36	5	2298	U
36	5	2307	G
36	5	2309	A
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2362	C
36	5	2365	C
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2379	U
36	5	2385	G
36	5	2388	U
36	5	2392	C
36	5	2393	G
36	5	2394	G
36	5	2397	A
36	5	2398	A
36	5	2401	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2410	U
36	5	2411	U
36	5	2412	G
36	5	2413	A
36	5	2414	G
36	5	2418	G
36	5	2420	C
36	5	2435	G
36	5	2437	G
36	5	2438	A

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Mol	Chain	Res	Type
36	5	2439	A
36	5	2441	A
36	5	2443	A
36	5	2444	C
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	2513	U
36	5	2514	U
36	5	2515	A
36	5	2523	A
36	5	2524	A
36	5	2525	G
36	5	2526	C
36	5	2530	G
36	5	2531	C
36	5	2535	A
36	5	2537	U
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2545	C
36	5	2547	A
36	5	2549	G
36	5	2552	C
36	5	2554	A
36	5	2555	G
36	5	2557	A
36	5	2560	C
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

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Mol	Chain	Res	Type
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2578	U
36	5	2584	G
36	5	2585	G
36	5	2586	G
36	5	2589	G
36	5	2593	A
36	5	2598	G
36	5	2600	C
36	5	2606	G
36	5	2607	G
36	5	2609	A
36	5	2614	G
36	5	2618	G
36	5	2629	U
36	5	2637	A
36	5	2638	C
36	5	2642	A
36	5	2652	U
36	5	2653	C
36	5	2656	A
36	5	2667	A
36	5	2670	G
36	5	2674	A
36	5	2675	C
36	5	2677	G
36	5	2681	U
36	5	2689	A
36	5	2690	G
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2705	A
36	5	2706	G
36	5	2707	C
36	5	2714	G
36	5	2725	U
36	5	2727	A
36	5	2728	G
36	5	2729	U

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Mol	Chain	Res	Type
36	5	2740	A
36	5	2752	U
36	5	2753	G
36	5	2755	C
36	5	2762	A
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2779	A
36	5	2782	U
36	5	2783	U
36	5	2788	C
36	5	2796	G
36	5	2797	C
36	5	2800	G
36	5	2801	A
36	5	2802	A
36	5	2810	C
36	5	2814	G
36	5	2817	A
36	5	2818	U
36	5	2819	A
36	5	2837	A
36	5	2839	G
36	5	2842	U
36	5	2843	U
36	5	2844	C
36	5	2845	A
36	5	2847	A
36	5	2849	C
36	5	2853	A
36	5	2870	C
36	5	2871	G
36	5	2872	A
36	5	2873	U
36	5	2875	U
36	5	2876	C
36	5	2880	U
36	5	2887	A
36	5	2896	A
36	5	2899	C

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Mol	Chain	Res	Type
36	5	2900	A
36	5	2911	A
36	5	2921	U
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2941	A
36	5	2942	C
36	5	2943	G
36	5	2947	G
36	5	2954	U
36	5	2960	C
36	5	2964	G
36	5	2971	A
36	5	2972	G
36	5	2973	G
36	5	2974	U
36	5	2979	U
36	5	2980	U
36	5	2983	C
36	5	2988	C
36	5	2989	U
36	5	2990	G
36	5	2996	U
36	5	2997	G
36	5	3006	A
36	5	3012	A
36	5	3025	C
36	5	3030	G
36	5	3034	C
36	5	3049	A
36	5	3056	U
36	5	3057	U
36	5	3058	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3081	C
36	5	3086	A
36	5	3092	C
36	5	3098	G
36	5	3104	U

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Mol	Chain	Res	Type
36	5	3115	C
36	5	3119	U
36	5	3122	A
36	5	3123	A
36	5	3127	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3148	U
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	3166	C
36	5	3171	U
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3180	A
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3206	C
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3224	G
36	5	3227	A
36	5	3228	C
36	5	3229	G
36	5	3234	A
36	5	3238	G
36	5	3239	G
36	5	3244	A

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Mol	Chain	Res	Type
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	3268	A
36	5	3270	U
36	5	3273	A
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3282	U
36	5	3283	U
36	5	3284	G
36	5	3285	C
36	5	3286	G
36	5	3287	U
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3303	G
36	5	3304	U
36	5	3313	U
36	5	3316	A
36	5	3317	U
36	5	3318	G
36	5	3319	U
36	5	3320	A
36	5	3324	C
36	5	3330	A
36	5	3331	U
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3350	C
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3356	G
36	5	3358	U

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Mol	Chain	Res	Type
36	5	3360	C
36	5	3368	U
36	5	3369	G
36	5	3376	A
36	5	3378	C
36	5	3382	U
36	5	3383	G
36	5	3389	U
36	5	3390	G
36	5	3396	U
37	7	2	G
37	7	7	G
37	7	9	C
37	7	22	A
37	7	29	C
37	7	38	U
37	7	39	C
37	7	41	G
37	7	49	G
37	7	51	A
37	7	53	U
37	7	54	U
37	7	55	A
37	7	57	G
37	7	60	G
37	7	65	G
37	7	73	C
37	7	74	C
37	7	76	A
37	7	84	A
37	7	92	A
37	7	93	C
37	7	102	A
37	7	104	A
37	7	110	G
37	7	112	G
37	7	114	U
37	7	121	U
38	8	13	A
38	8	21	C
38	8	23	U
38	8	34	U

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Mol	Chain	Res	Type
38	8	35	C
38	8	48	A
38	8	50	C
38	8	51	G
38	8	53	A
38	8	59	A
38	8	62	C
38	8	63	G
38	8	64	U
38	8	71	A
38	8	80	A
38	8	81	U
38	8	82	U
38	8	83	C
38	8	84	C
38	8	85	G
38	8	86	U
38	8	87	G
38	8	88	A
38	8	90	U
38	8	95	G
38	8	96	A
38	8	97	A
38	8	104	A
38	8	105	A
38	8	106	C
38	8	110	C
38	8	111	A
38	8	113	U
38	8	114	G
38	8	116	G
38	8	122	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	138	A
38	8	148	G
38	8	152	G
38	8	157	U
38	8	158	U

All (269) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	25	C
1	2	45	U
1	2	73	U
1	2	130	C
1	2	131	C
1	2	136	C
1	2	139	C
1	2	158	U
1	2	187	G
1	2	192	U
1	2	218	A
1	2	240	U
1	2	278	U
1	2	280	U
1	2	321	C
1	2	400	A
1	2	417	A
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	545	A
1	2	555	A
1	2	558	U
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	755	A
1	2	794	U
1	2	829	A
1	2	913	G
1	2	1058	U
1	2	1081	A
1	2	1157	A
1	2	1226	A
1	2	1234	A
1	2	1244	A
1	2	1250	U
1	2	1344	A
1	2	1370	U
1	2	1481	C

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Mol	Chain	Res	Type
1	2	1489	U
1	2	1568	C
1	2	1573	A
1	2	1600	A
1	2	1615	C
1	2	1657	U
1	2	1761	U
1	2	1793	G
36	1	40	A
36	1	65	A
36	1	169	U
36	1	210	U
36	1	223	U
36	1	239	G
36	1	282	G
36	1	374	A
36	1	518	G
36	1	547	G
36	1	594	U
36	1	637	C
36	1	763	G
36	1	816	A
36	1	896	A
36	1	916	G
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1181	U
36	1	1190	A
36	1	1196	C
36	1	1268	G
36	1	1273	A
36	1	1307	G
36	1	1329	U
36	1	1331	U
36	1	1352	A
36	1	1355	A
36	1	1484	U
36	1	1514	G

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Mol	Chain	Res	Type
36	1	1554	U
36	1	1562	C
36	1	1589	A
36	1	1607	U
36	1	1716	U
36	1	1724	U
36	1	1820	U
36	1	2101	C
36	1	2111	G
36	1	2112	U
36	1	2121	G
36	1	2209	U
36	1	2249	G
36	1	2281	A
36	1	2282	U
36	1	2307	G
36	1	2323	G
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2418	G
36	1	2513	U
36	1	2537	U
36	1	2539	C
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2656	A
36	1	2704	A
36	1	2728	G
36	1	2772	C
36	1	2801	A
36	1	2817	A
36	1	2818	U
36	1	2859	U
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3157	U
36	1	3195	U
36	1	3218	A
36	1	3228	C

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Mol	Chain	Res	Type
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
36	1	3382	U
38	4	82	U
38	4	85	G
38	4	125	U
1	6	25	C
1	6	66	U
1	6	76	A
1	6	114	C
1	6	136	C
1	6	139	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	272	U
1	6	400	A
1	6	417	A
1	6	512	A
1	6	539	G
1	6	542	A
1	6	557	G
1	6	558	U
1	6	651	G
1	6	697	C
1	6	717	C
1	6	720	G
1	6	755	A
1	6	779	U
1	6	815	G
1	6	829	A
1	6	834	G
1	6	944	A

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Mol	Chain	Res	Type
1	6	1051	G
1	6	1058	U
1	6	1097	U
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1431	C
1	6	1481	C
1	6	1491	U
1	6	1535	U
1	6	1568	C
1	6	1573	A
1	6	1600	A
1	6	1620	C
1	6	1637	C
1	6	1657	U
1	6	1696	G
1	6	1698	G
1	6	1700	C
36	5	43	A
36	5	151	A
36	5	210	U
36	5	238	A
36	5	588	G
36	5	594	U
36	5	715	A
36	5	719	U
36	5	765	C
36	5	805	G
36	5	896	A
36	5	916	G
36	5	993	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1154	A
36	5	1160	C
36	5	1192	C
36	5	1238	C
36	5	1241	U
36	5	1284	C

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Mol	Chain	Res	Type
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1367	G
36	5	1481	A
36	5	1507	G
36	5	1514	G
36	5	1560	G
36	5	1574	C
36	5	1580	A
36	5	1607	U
36	5	1687	U
36	5	1716	U
36	5	1792	C
36	5	1816	A
36	5	1878	G
36	5	2101	C
36	5	2111	G
36	5	2112	U
36	5	2116	G
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2281	A
36	5	2372	A
36	5	2374	C
36	5	2440	G
36	5	2504	U
36	5	2507	C
36	5	2513	U
36	5	2539	C
36	5	2689	A
36	5	2728	G
36	5	2772	C
36	5	2818	U
36	5	2887	A
36	5	2971	A
36	5	3056	U
36	5	3078	U
36	5	3154	C

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Mol	Chain	Res	Type
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3244	A
36	5	3269	U
36	5	3275	U
36	5	3289	G
36	5	3330	A
36	5	3340	G
36	5	3341	U
36	5	3354	U
36	5	3357	U
37	7	49	G
37	7	111	U
38	8	113	U
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 2557 ligands modelled in this entry, 1423 are monoatomic - leaving 1134 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	4156	-	0,6,6	0.00	-	-		
86	OHX	3	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	1	4045	-	0,6,6	0.00	-	-		
86	OHX	1	4062	-	0,6,6	0.00	-	-		
86	OHX	2	2118	-	0,6,6	0.00	-	-		
86	OHX	6	2054	-	0,6,6	0.00	-	-		
86	OHX	5	4146	-	0,6,6	0.00	-	-		
86	OHX	6	2108	-	0,6,6	0.00	-	-		
86	OHX	2	2093	-	0,6,6	0.00	-	-		
86	OHX	6	2121	-	0,6,6	0.00	-	-		
86	OHX	1	4197	-	0,6,6	0.00	-	-		
86	OHX	2	2081	-	0,6,6	0.00	-	-		
86	OHX	1	4002	-	0,6,6	0.00	-	-		
86	OHX	2	2084	-	0,6,6	0.00	-	-		
86	OHX	2	2114	-	0,6,6	0.00	-	-		
86	OHX	6	2138	-	0,6,6	0.00	-	-		
86	OHX	1	4128	-	0,6,6	0.00	-	-		
86	OHX	5	4191	-	0,6,6	0.00	-	-		
86	OHX	6	2190	-	0,6,6	0.00	-	-		
86	OHX	O7	104	-	0,6,6	0.00	-	-		
86	OHX	6	2189	-	0,6,6	0.00	-	-		
86	OHX	2	2060	-	0,6,6	0.00	-	-		
86	OHX	2	2132	-	0,6,6	0.00	-	-		
86	OHX	6	2073	-	0,6,6	0.00	-	-		
86	OHX	6	2053	-	0,6,6	0.00	-	-		
86	OHX	5	4233	-	0,6,6	0.00	-	-		
86	OHX	N9	101	-	0,6,6	0.00	-	-		
86	OHX	2	2074	-	0,6,6	0.00	-	-		
86	OHX	1	3947	-	0,6,6	0.00	-	-		
86	OHX	5	4132	-	0,6,6	0.00	-	-		
86	OHX	6	2194	-	0,6,6	0.00	-	-		
86	OHX	1	4106	-	0,6,6	0.00	-	-		
86	OHX	5	4147	-	0,6,6	0.00	-	-		
86	OHX	1	4056	-	0,6,6	0.00	-	-		
86	OHX	1	4054	-	0,6,6	0.00	-	-		
86	OHX	5	4230	-	0,6,6	0.00	-	-		
86	OHX	5	4047	-	0,6,6	0.00	-	-		
86	OHX	5	4083	-	0,6,6	0.00	-	-		
86	OHX	14	403	-	0,6,6	0.00	-	-		
86	OHX	5	3989	-	0,6,6	0.00	-	-		
86	OHX	2	2103	-	0,6,6	0.00	-	-		
86	OHX	1	4182	-	0,6,6	0.00	-	-		
86	OHX	5	4099	-	0,6,6	0.00	-	-		
86	OHX	5	4231	-	0,6,6	0.00	-	-		
86	OHX	5	4153	-	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	4024	-	0,6,6	0.00	-	-		
86	OHX	5	3941	-	0,6,6	0.00	-	-		
86	OHX	5	4246	-	0,6,6	0.00	-	-		
86	OHX	C5	201	-	0,6,6	0.00	-	-		
86	OHX	6	2185	-	0,6,6	0.00	-	-		
86	OHX	1	4031	-	0,6,6	0.00	-	-		
86	OHX	5	4039	-	0,6,6	0.00	-	-		
86	OHX	2	2099	-	0,6,6	0.00	-	-		
86	OHX	6	2061	-	0,6,6	0.00	-	-		
86	OHX	5	4050	-	0,6,6	0.00	-	-		
86	OHX	1	3881	-	0,6,6	0.00	-	-		
86	OHX	6	2154	-	0,6,6	0.00	-	-		
86	OHX	6	2173	-	0,6,6	0.00	-	-		
86	OHX	5	4211	-	0,6,6	0.00	-	-		
86	OHX	2	2037	-	0,6,6	0.00	-	-		
86	OHX	6	2133	-	0,6,6	0.00	-	-		
86	OHX	5	4130	-	0,6,6	0.00	-	-		
86	OHX	6	2149	-	0,6,6	0.00	-	-		
86	OHX	5	4017	-	0,6,6	0.00	-	-		
86	OHX	1	4102	-	0,6,6	0.00	-	-		
86	OHX	5	4074	-	0,6,6	0.00	-	-		
86	OHX	5	4101	-	0,6,6	0.00	-	-		
86	OHX	6	2203	-	0,6,6	0.00	-	-		
86	OHX	3	224	-	0,6,6	0.00	-	-		
86	OHX	5	4223	-	0,6,6	0.00	-	-		
86	OHX	1	4068	-	0,6,6	0.00	-	-		
86	OHX	5	4216	-	0,6,6	0.00	-	-		
86	OHX	5	3974	-	0,6,6	0.00	-	-		
86	OHX	1	4103	-	0,6,6	0.00	-	-		
86	OHX	O1	202	-	0,6,6	0.00	-	-		
86	OHX	1	4015	-	0,6,6	0.00	-	-		
86	OHX	5	3958	-	0,6,6	0.00	-	-		
86	OHX	1	3936	-	0,6,6	0.00	-	-		
86	OHX	5	4178	-	0,6,6	0.00	-	-		
86	OHX	5	4166	-	0,6,6	0.00	-	-		
86	OHX	4	224	-	0,6,6	0.00	-	-		
86	OHX	2	2157	-	0,6,6	0.00	-	-		
86	OHX	5	3911	-	0,6,6	0.00	-	-		
86	OHX	3	221	-	0,6,6	0.00	-	-		
86	OHX	1	3894	-	0,6,6	0.00	-	-		
86	OHX	2	2026	-	0,6,6	0.00	-	-		
86	OHX	5	3988	-	0,6,6	0.00	-	-		
86	OHX	5	4125	-	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	4114	-	0,6,6	0.00	-	-		
86	OHX	5	4104	-	0,6,6	0.00	-	-		
86	OHX	1	3979	-	0,6,6	0.00	-	-		
86	OHX	1	3865	-	0,6,6	0.00	-	-		
86	OHX	2	2053	-	0,6,6	0.00	-	-		
86	OHX	1	4057	-	0,6,6	0.00	-	-		
86	OHX	1	4133	-	0,6,6	0.00	-	-		
86	OHX	5	3923	-	0,6,6	0.00	-	-		
86	OHX	5	4127	-	0,6,6	0.00	-	-		
86	OHX	1	3916	-	0,6,6	0.00	-	-		
86	OHX	5	4048	-	0,6,6	0.00	-	-		
86	OHX	1	4032	-	0,6,6	0.00	-	-		
86	OHX	5	4116	-	0,6,6	0.00	-	-		
86	OHX	1	4118	-	0,6,6	0.00	-	-		
86	OHX	5	4187	-	0,6,6	0.00	-	-		
86	OHX	1	3882	-	0,6,6	0.00	-	-		
86	OHX	2	2160	-	0,6,6	0.00	-	-		
86	OHX	m5	306	-	0,6,6	0.00	-	-		
86	OHX	5	3925	-	0,6,6	0.00	-	-		
86	OHX	5	3893	-	0,6,6	0.00	-	-		
86	OHX	1	4097	-	0,6,6	0.00	-	-		
86	OHX	2	2150	-	0,6,6	0.00	-	-		
86	OHX	1	4080	-	0,6,6	0.00	-	-		
86	OHX	6	2143	-	0,6,6	0.00	-	-		
86	OHX	7	223	-	0,6,6	0.00	-	-		
86	OHX	6	2200	-	0,6,6	0.00	-	-		
86	OHX	2	2122	-	0,6,6	0.00	-	-		
86	OHX	2	2062	-	0,6,6	0.00	-	-		
86	OHX	6	2050	-	0,6,6	0.00	-	-		
86	OHX	1	4055	-	0,6,6	0.00	-	-		
86	OHX	1	3907	-	0,6,6	0.00	-	-		
86	OHX	2	2124	-	0,6,6	0.00	-	-		
86	OHX	5	3930	-	0,6,6	0.00	-	-		
86	OHX	5	3975	-	0,6,6	0.00	-	-		
86	OHX	6	2164	-	0,6,6	0.00	-	-		
86	OHX	D3	202	-	0,6,6	0.00	-	-		
86	OHX	5	3948	-	0,6,6	0.00	-	-		
86	OHX	1	4190	-	0,6,6	0.00	-	-		
86	OHX	1	4063	-	0,6,6	0.00	-	-		
86	OHX	n3	202	-	0,6,6	0.00	-	-		
86	OHX	1	4003	-	0,6,6	0.00	-	-		
86	OHX	5	4092	-	0,6,6	0.00	-	-		
86	OHX	6	2144	-	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	4082	-	0,6,6	0.00	-	-		
86	OHX	6	2163	-	0,6,6	0.00	-	-		
86	OHX	1	4209	-	0,6,6	0.00	-	-		
86	OHX	6	2106	-	0,6,6	0.00	-	-		
86	OHX	6	2109	-	0,6,6	0.00	-	-		
86	OHX	5	4077	-	0,6,6	0.00	-	-		
86	OHX	6	2046	-	0,6,6	0.00	-	-		
86	OHX	5	4005	-	0,6,6	0.00	-	-		
86	OHX	1	3966	-	0,6,6	0.00	-	-		
86	OHX	7	224	-	0,6,6	0.00	-	-		
86	OHX	5	3955	-	0,6,6	0.00	-	-		
86	OHX	2	2048	-	0,6,6	0.00	-	-		
86	OHX	1	4160	-	0,6,6	0.00	-	-		
86	OHX	5	4094	-	0,6,6	0.00	-	-		
86	OHX	1	4207	-	0,6,6	0.00	-	-		
86	OHX	2	2168	-	0,6,6	0.00	-	-		
86	OHX	1	4093	-	0,6,6	0.00	-	-		
86	OHX	5	4063	-	0,6,6	0.00	-	-		
86	OHX	5	4025	-	0,6,6	0.00	-	-		
86	OHX	7	228	-	0,6,6	0.00	-	-		
86	OHX	2	2171	-	0,6,6	0.00	-	-		
86	OHX	2	2059	-	0,6,6	0.00	-	-		
86	OHX	1	4060	-	0,6,6	0.00	-	-		
86	OHX	6	2049	-	0,6,6	0.00	-	-		
86	OHX	1	4201	-	0,6,6	0.00	-	-		
86	OHX	1	4142	-	0,6,6	0.00	-	-		
86	OHX	6	2077	-	0,6,6	0.00	-	-		
86	OHX	1	3897	-	0,6,6	0.00	-	-		
86	OHX	2	2091	-	0,6,6	0.00	-	-		
86	OHX	2	2134	-	0,6,6	0.00	-	-		
86	OHX	6	2091	-	0,6,6	0.00	-	-		
86	OHX	5	4081	-	0,6,6	0.00	-	-		
86	OHX	6	2157	-	0,6,6	0.00	-	-		
86	OHX	1	3879	-	0,6,6	0.00	-	-		
86	OHX	5	4031	-	0,6,6	0.00	-	-		
86	OHX	2	2061	-	0,6,6	0.00	-	-		
86	OHX	5	3995	-	0,6,6	0.00	-	-		
86	OHX	1	4050	-	0,6,6	0.00	-	-		
86	OHX	2	2106	-	0,6,6	0.00	-	-		
86	OHX	5	4131	-	0,6,6	0.00	-	-		
86	OHX	6	2056	-	0,6,6	0.00	-	-		
86	OHX	1	4151	-	0,6,6	0.00	-	-		
86	OHX	6	2179	-	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	2176	-	0,6,6	0.00	-	-		
86	OHX	5	4194	-	0,6,6	0.00	-	-		
86	OHX	1	4189	-	0,6,6	0.00	-	-		
86	OHX	5	4072	-	0,6,6	0.00	-	-		
86	OHX	1	4017	-	0,6,6	0.00	-	-		
86	OHX	5	4103	-	0,6,6	0.00	-	-		
86	OHX	1	4175	-	0,6,6	0.00	-	-		
86	OHX	5	4205	-	0,6,6	0.00	-	-		
86	OHX	6	2097	-	0,6,6	0.00	-	-		
86	OHX	5	3971	-	0,6,6	0.00	-	-		
86	OHX	1	3969	-	0,6,6	0.00	-	-		
86	OHX	8	224	-	0,6,6	0.00	-	-		
86	OHX	1	3896	-	0,6,6	0.00	-	-		
86	OHX	6	2103	-	0,6,6	0.00	-	-		
86	OHX	5	4038	-	0,6,6	0.00	-	-		
86	OHX	5	4220	-	0,6,6	0.00	-	-		
86	OHX	6	2064	-	0,6,6	0.00	-	-		
86	OHX	1	3934	-	0,6,6	0.00	-	-		
86	OHX	1	3954	-	0,6,6	0.00	-	-		
86	OHX	4	238	-	0,6,6	0.00	-	-		
86	OHX	5	3913	-	0,6,6	0.00	-	-		
86	OHX	1	4147	-	0,6,6	0.00	-	-		
86	OHX	2	2075	-	0,6,6	0.00	-	-		
86	OHX	O3	201	-	0,6,6	0.00	-	-		
86	OHX	q2	502	-	0,6,6	0.00	-	-		
86	OHX	5	3964	-	0,6,6	0.00	-	-		
86	OHX	1	3940	-	0,6,6	0.00	-	-		
86	OHX	6	2086	-	0,6,6	0.00	-	-		
86	OHX	2	2082	-	0,6,6	0.00	-	-		
86	OHX	6	2082	-	0,6,6	0.00	-	-		
86	OHX	5	4126	-	0,6,6	0.00	-	-		
86	OHX	2	2046	-	0,6,6	0.00	-	-		
86	OHX	5	3933	-	0,6,6	0.00	-	-		
86	OHX	1	4065	-	0,6,6	0.00	-	-		
86	OHX	m0	302	-	0,6,6	0.00	-	-		
86	OHX	m0	303	-	0,6,6	0.00	-	-		
86	OHX	1	4117	-	0,6,6	0.00	-	-		
86	OHX	1	4064	-	0,6,6	0.00	-	-		
86	OHX	1	4071	-	0,6,6	0.00	-	-		
86	OHX	2	2024	-	0,6,6	0.00	-	-		
86	OHX	7	222	-	0,6,6	0.00	-	-		
86	OHX	2	2169	-	0,6,6	0.00	-	-		
86	OHX	5	3942	-	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	1	3873	-	0,6,6	0.00	-	-		
86	OHX	5	4096	-	0,6,6	0.00	-	-		
86	OHX	5	3957	-	0,6,6	0.00	-	-		
86	OHX	5	4238	-	0,6,6	0.00	-	-		
86	OHX	1	4022	-	0,6,6	0.00	-	-		
86	OHX	2	2055	-	0,6,6	0.00	-	-		
86	OHX	5	4235	-	0,6,6	0.00	-	-		
86	OHX	1	3933	-	0,6,6	0.00	-	-		
86	OHX	6	2080	-	0,6,6	0.00	-	-		
86	OHX	2	2126	-	0,6,6	0.00	-	-		
86	OHX	1	4094	-	0,6,6	0.00	-	-		
86	OHX	5	4046	-	0,6,6	0.00	-	-		
86	OHX	5	4229	-	0,6,6	0.00	-	-		
86	OHX	5	4043	-	0,6,6	0.00	-	-		
86	OHX	5	4093	-	0,6,6	0.00	-	-		
86	OHX	1	3978	-	0,6,6	0.00	-	-		
86	OHX	1	4152	-	0,6,6	0.00	-	-		
86	OHX	1	3928	-	0,6,6	0.00	-	-		
86	OHX	1	3880	-	0,6,6	0.00	-	-		
86	OHX	6	2171	-	0,6,6	0.00	-	-		
86	OHX	6	2153	-	0,6,6	0.00	-	-		
86	OHX	1	3875	-	0,6,6	0.00	-	-		
86	OHX	8	227	-	0,6,6	0.00	-	-		
86	OHX	5	4119	-	0,6,6	0.00	-	-		
86	OHX	1	4132	-	0,6,6	0.00	-	-		
86	OHX	1	4179	-	0,6,6	0.00	-	-		
86	OHX	1	4206	-	0,6,6	0.00	-	-		
86	OHX	6	2176	-	0,6,6	0.00	-	-		
86	OHX	1	3956	-	0,6,6	0.00	-	-		
86	OHX	1	3886	-	0,6,6	0.00	-	-		
86	OHX	5	3932	-	0,6,6	0.00	-	-		
86	OHX	6	2183	-	0,6,6	0.00	-	-		
86	OHX	5	3956	-	0,6,6	0.00	-	-		
86	OHX	6	2104	-	0,6,6	0.00	-	-		
86	OHX	1	3943	-	0,6,6	0.00	-	-		
86	OHX	5	4032	-	0,6,6	0.00	-	-		
86	OHX	c3	201	-	0,6,6	0.00	-	-		
86	OHX	4	232	-	0,6,6	0.00	-	-		
86	OHX	1	4150	-	0,6,6	0.00	-	-		
86	OHX	1	3888	-	0,6,6	0.00	-	-		
86	OHX	5	3935	-	0,6,6	0.00	-	-		
86	OHX	2	2043	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	C8	201	-	0,6,6	0.00	-	-		
86	OHX	6	2168	-	0,6,6	0.00	-	-		
86	OHX	1	3924	-	0,6,6	0.00	-	-		
86	OHX	6	2161	-	0,6,6	0.00	-	-		
86	OHX	2	2136	-	0,6,6	0.00	-	-		
86	OHX	5	4080	-	0,6,6	0.00	-	-		
86	OHX	5	4002	-	0,6,6	0.00	-	-		
86	OHX	6	2187	-	0,6,6	0.00	-	-		
86	OHX	5	4214	-	0,6,6	0.00	-	-		
86	OHX	1	3944	-	0,6,6	0.00	-	-		
86	OHX	5	3972	-	0,6,6	0.00	-	-		
86	OHX	1	3923	-	0,6,6	0.00	-	-		
86	OHX	6	2170	-	0,6,6	0.00	-	-		
86	OHX	1	3955	-	0,6,6	0.00	-	-		
86	OHX	6	2065	-	0,6,6	0.00	-	-		
86	OHX	1	3909	-	0,6,6	0.00	-	-		
86	OHX	1	4029	-	0,6,6	0.00	-	-		
86	OHX	5	4217	-	0,6,6	0.00	-	-		
86	OHX	n1	201	-	0,6,6	0.00	-	-		
86	OHX	1	4202	-	0,6,6	0.00	-	-		
86	OHX	2	2110	-	0,6,6	0.00	-	-		
86	OHX	5	3985	-	0,6,6	0.00	-	-		
86	OHX	5	4174	-	0,6,6	0.00	-	-		
86	OHX	1	4058	-	0,6,6	0.00	-	-		
86	OHX	5	3928	-	0,6,6	0.00	-	-		
86	OHX	1	4203	-	0,6,6	0.00	-	-		
86	OHX	6	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4204	-	0,6,6	0.00	-	-		
86	OHX	1	3938	-	0,6,6	0.00	-	-		
86	OHX	1	4004	-	0,6,6	0.00	-	-		
86	OHX	4	236	-	0,6,6	0.00	-	-		
86	OHX	s8	302	-	0,6,6	0.00	-	-		
86	OHX	7	221	-	0,6,6	0.00	-	-		
86	OHX	1	3972	-	0,6,6	0.00	-	-		
86	OHX	2	2152	-	0,6,6	0.00	-	-		
86	OHX	5	4184	-	0,6,6	0.00	-	-		
86	OHX	5	3983	-	0,6,6	0.00	-	-		
86	OHX	6	2177	-	0,6,6	0.00	-	-		
86	OHX	d9	102	-	0,6,6	0.00	-	-		
86	OHX	1	3997	-	0,6,6	0.00	-	-		
86	OHX	5	4236	-	0,6,6	0.00	-	-		
86	OHX	1	4174	-	0,6,6	0.00	-	-		
86	OHX	1	4052	-	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	3957	-	0,6,6	0.00	-	-		
86	OHX	1	4181	-	0,6,6	0.00	-	-		
86	OHX	6	2058	-	0,6,6	0.00	-	-		
86	OHX	6	2175	-	0,6,6	0.00	-	-		
86	OHX	6	2115	-	0,6,6	0.00	-	-		
86	OHX	1	3994	-	0,6,6	0.00	-	-		
86	OHX	2	2146	-	0,6,6	0.00	-	-		
86	OHX	6	2122	-	0,6,6	0.00	-	-		
86	OHX	2	2064	-	0,6,6	0.00	-	-		
86	OHX	1	4154	-	0,6,6	0.00	-	-		
86	OHX	o7	103	-	0,6,6	0.00	-	-		
86	OHX	1	4198	-	0,6,6	0.00	-	-		
86	OHX	5	3977	-	0,6,6	0.00	-	-		
86	OHX	5	3978	-	0,6,6	0.00	-	-		
86	OHX	1	3939	-	0,6,6	0.00	-	-		
86	OHX	7	226	-	0,6,6	0.00	-	-		
86	OHX	2	2151	-	0,6,6	0.00	-	-		
86	OHX	2	2080	-	0,6,6	0.00	-	-		
86	OHX	1	3932	-	0,6,6	0.00	-	-		
86	OHX	5	4137	-	0,6,6	0.00	-	-		
86	OHX	1	3995	-	0,6,6	0.00	-	-		
86	OHX	6	2193	-	0,6,6	0.00	-	-		
86	OHX	2	2087	-	0,6,6	0.00	-	-		
86	OHX	1	3901	-	0,6,6	0.00	-	-		
86	OHX	1	4176	-	0,6,6	0.00	-	-		
86	OHX	1	4112	-	0,6,6	0.00	-	-		
86	OHX	L3	405	-	0,6,6	0.00	-	-		
86	OHX	5	4218	-	0,6,6	0.00	-	-		
86	OHX	1	3990	-	0,6,6	0.00	-	-		
86	OHX	1	3942	-	0,6,6	0.00	-	-		
86	OHX	5	3970	-	0,6,6	0.00	-	-		
86	OHX	2	2131	-	0,6,6	0.00	-	-		
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	1	4086	-	0,6,6	0.00	-	-		
86	OHX	2	2045	-	0,6,6	0.00	-	-		
86	OHX	4	233	-	0,6,6	0.00	-	-		
86	OHX	5	4108	-	0,6,6	0.00	-	-		
86	OHX	2	2162	-	0,6,6	0.00	-	-		
86	OHX	1	3876	-	0,6,6	0.00	-	-		
86	OHX	5	4221	-	0,6,6	0.00	-	-		
86	OHX	5	4190	-	0,6,6	0.00	-	-		
86	OHX	5	3991	-	0,6,6	0.00	-	-		
86	OHX	1	4081	-	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	2096	-	0,6,6	0.00	-	-		
86	OHX	3	217	-	0,6,6	0.00	-	-		
86	OHX	6	2160	-	0,6,6	0.00	-	-		
86	OHX	2	2049	-	0,6,6	0.00	-	-		
86	OHX	6	2139	-	0,6,6	0.00	-	-		
86	OHX	5	4029	-	0,6,6	0.00	-	-		
86	OHX	2	2063	-	0,6,6	0.00	-	-		
86	OHX	5	3915	-	0,6,6	0.00	-	-		
86	OHX	3	216	-	0,6,6	0.00	-	-		
86	OHX	5	4057	-	0,6,6	0.00	-	-		
86	OHX	5	3929	-	0,6,6	0.00	-	-		
86	OHX	5	4222	-	0,6,6	0.00	-	-		
86	OHX	2	2125	-	0,6,6	0.00	-	-		
86	OHX	5	4209	-	0,6,6	0.00	-	-		
86	OHX	1	3977	-	0,6,6	0.00	-	-		
86	OHX	2	2112	-	0,6,6	0.00	-	-		
86	OHX	3	220	-	0,6,6	0.00	-	-		
86	OHX	1	4105	-	0,6,6	0.00	-	-		
86	OHX	6	2078	-	0,6,6	0.00	-	-		
86	OHX	2	2109	-	0,6,6	0.00	-	-		
86	OHX	n9	103	-	0,6,6	0.00	-	-		
86	OHX	1	4194	-	0,6,6	0.00	-	-		
86	OHX	6	2110	-	0,6,6	0.00	-	-		
86	OHX	1	3911	-	0,6,6	0.00	-	-		
86	OHX	1	3914	-	0,6,6	0.00	-	-		
86	OHX	2	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4138	-	0,6,6	0.00	-	-		
86	OHX	5	4011	-	0,6,6	0.00	-	-		
86	OHX	1	4139	-	0,6,6	0.00	-	-		
86	OHX	1	4014	-	0,6,6	0.00	-	-		
86	OHX	1	3931	-	0,6,6	0.00	-	-		
86	OHX	1	4092	-	0,6,6	0.00	-	-		
86	OHX	2	2180	-	0,6,6	0.00	-	-		
86	OHX	1	4119	-	0,6,6	0.00	-	-		
86	OHX	1	3993	-	0,6,6	0.00	-	-		
86	OHX	1	3941	-	0,6,6	0.00	-	-		
86	OHX	6	2066	-	0,6,6	0.00	-	-		
86	OHX	4	229	-	0,6,6	0.00	-	-		
86	OHX	2	2161	-	0,6,6	0.00	-	-		
86	OHX	6	2195	-	0,6,6	0.00	-	-		
86	OHX	6	2048	-	0,6,6	0.00	-	-		
86	OHX	5	4019	-	0,6,6	0.00	-	-		
86	OHX	5	4168	-	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	4167	-	0,6,6	0.00	-	-		
86	OHX	2	2177	-	0,6,6	0.00	-	-		
86	OHX	5	3897	-	0,6,6	0.00	-	-		
86	OHX	5	4156	-	0,6,6	0.00	-	-		
86	OHX	1	3860	-	0,6,6	0.00	-	-		
86	OHX	1	4155	-	0,6,6	0.00	-	-		
86	OHX	5	4175	-	0,6,6	0.00	-	-		
86	OHX	1	3918	-	0,6,6	0.00	-	-		
86	OHX	sR	401	-	0,6,6	0.00	-	-		
86	OHX	5	3944	-	0,6,6	0.00	-	-		
86	OHX	6	2093	-	0,6,6	0.00	-	-		
86	OHX	5	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4016	-	0,6,6	0.00	-	-		
86	OHX	5	4027	-	0,6,6	0.00	-	-		
86	OHX	5	4136	-	0,6,6	0.00	-	-		
86	OHX	5	4177	-	0,6,6	0.00	-	-		
86	OHX	5	3919	-	0,6,6	0.00	-	-		
86	OHX	5	4203	-	0,6,6	0.00	-	-		
86	OHX	2	2104	-	0,6,6	0.00	-	-		
86	OHX	6	2172	-	0,6,6	0.00	-	-		
86	OHX	1	3985	-	0,6,6	0.00	-	-		
86	OHX	5	3916	-	0,6,6	0.00	-	-		
86	OHX	1	3867	-	0,6,6	0.00	-	-		
86	OHX	2	2031	-	0,6,6	0.00	-	-		
86	OHX	1	3945	-	0,6,6	0.00	-	-		
86	OHX	5	3998	-	0,6,6	0.00	-	-		
86	OHX	l3	404	-	0,6,6	0.00	-	-		
86	OHX	5	4105	-	0,6,6	0.00	-	-		
86	OHX	2	2119	-	0,6,6	0.00	-	-		
86	OHX	4	234	-	0,6,6	0.00	-	-		
86	OHX	5	4158	-	0,6,6	0.00	-	-		
86	OHX	5	4090	-	0,6,6	0.00	-	-		
86	OHX	1	4161	-	0,6,6	0.00	-	-		
86	OHX	5	3952	-	0,6,6	0.00	-	-		
86	OHX	5	3980	-	0,6,6	0.00	-	-		
86	OHX	5	3910	-	0,6,6	0.00	-	-		
86	OHX	1	4146	-	0,6,6	0.00	-	-		
86	OHX	1	3926	-	0,6,6	0.00	-	-		
86	OHX	2	2143	-	0,6,6	0.00	-	-		
86	OHX	5	4163	-	0,6,6	0.00	-	-		
86	OHX	6	2150	-	0,6,6	0.00	-	-		
86	OHX	6	2180	-	0,6,6	0.00	-	-		
86	OHX	2	2086	-	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	2181	-	0,6,6	0.00	-	-		
86	OHX	1	3895	-	0,6,6	0.00	-	-		
86	OHX	2	2054	-	0,6,6	0.00	-	-		
86	OHX	1	4101	-	0,6,6	0.00	-	-		
86	OHX	5	3999	-	0,6,6	0.00	-	-		
86	OHX	5	4143	-	0,6,6	0.00	-	-		
86	OHX	6	2072	-	0,6,6	0.00	-	-		
86	OHX	c8	202	-	0,6,6	0.00	-	-		
86	OHX	6	2128	-	0,6,6	0.00	-	-		
86	OHX	6	2147	-	0,6,6	0.00	-	-		
86	OHX	1	3905	-	0,6,6	0.00	-	-		
86	OHX	5	3926	-	0,6,6	0.00	-	-		
86	OHX	1	4010	-	0,6,6	0.00	-	-		
86	OHX	6	2124	-	0,6,6	0.00	-	-		
86	OHX	5	3905	-	0,6,6	0.00	-	-		
86	OHX	8	226	-	0,6,6	0.00	-	-		
86	OHX	5	3973	-	0,6,6	0.00	-	-		
86	OHX	5	4067	-	0,6,6	0.00	-	-		
86	OHX	5	4164	-	0,6,6	0.00	-	-		
86	OHX	5	3976	-	0,6,6	0.00	-	-		
86	OHX	1	3915	-	0,6,6	0.00	-	-		
86	OHX	6	2156	-	0,6,6	0.00	-	-		
86	OHX	2	2139	-	0,6,6	0.00	-	-		
86	OHX	5	3992	-	0,6,6	0.00	-	-		
86	OHX	5	3946	-	0,6,6	0.00	-	-		
86	OHX	1	4078	-	0,6,6	0.00	-	-		
86	OHX	3	218	-	0,6,6	0.00	-	-		
86	OHX	2	2028	-	0,6,6	0.00	-	-		
86	OHX	6	2199	-	0,6,6	0.00	-	-		
86	OHX	1	4184	-	0,6,6	0.00	-	-		
86	OHX	5	4087	-	0,6,6	0.00	-	-		
86	OHX	6	2202	-	0,6,6	0.00	-	-		
86	OHX	1	4125	-	0,6,6	0.00	-	-		
86	OHX	6	2057	-	0,6,6	0.00	-	-		
86	OHX	1	3890	-	0,6,6	0.00	-	-		
86	OHX	5	4056	-	0,6,6	0.00	-	-		
86	OHX	5	4088	-	0,6,6	0.00	-	-		
86	OHX	5	4115	-	0,6,6	0.00	-	-		
86	OHX	1	3884	-	0,6,6	0.00	-	-		
86	OHX	1	4016	-	0,6,6	0.00	-	-		
86	OHX	1	3982	-	0,6,6	0.00	-	-		
86	OHX	5	4140	-	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	1	3998	-	0,6,6	0.00	-	-		
88	BLS	5	4248	-	25,31,31	1.46	2 (8%)	23,43,43	1.75	3 (13%)
86	OHX	5	4055	-	0,6,6	0.00	-	-		
86	OHX	1	4083	-	0,6,6	0.00	-	-		
86	OHX	5	4225	-	0,6,6	0.00	-	-		
86	OHX	1	4191	-	0,6,6	0.00	-	-		
86	OHX	7	219	-	0,6,6	0.00	-	-		
86	OHX	2	2172	-	0,6,6	0.00	-	-		
86	OHX	5	3894	-	0,6,6	0.00	-	-		
86	OHX	6	2068	-	0,6,6	0.00	-	-		
86	OHX	2	2144	-	0,6,6	0.00	-	-		
86	OHX	M7	206	-	0,6,6	0.00	-	-		
86	OHX	1	4025	-	0,6,6	0.00	-	-		
86	OHX	1	3920	-	0,6,6	0.00	-	-		
86	OHX	5	4026	-	0,6,6	0.00	-	-		
86	OHX	6	2174	-	0,6,6	0.00	-	-		
86	OHX	1	4019	-	0,6,6	0.00	-	-		
86	OHX	5	4151	-	0,6,6	0.00	-	-		
86	OHX	1	4138	-	0,6,6	0.00	-	-		
86	OHX	1	4109	-	0,6,6	0.00	-	-		
86	OHX	2	2073	-	0,6,6	0.00	-	-		
86	OHX	6	2123	-	0,6,6	0.00	-	-		
86	OHX	1	3900	-	0,6,6	0.00	-	-		
86	OHX	6	2074	-	0,6,6	0.00	-	-		
86	OHX	2	2047	-	0,6,6	0.00	-	-		
86	OHX	5	4045	-	0,6,6	0.00	-	-		
86	OHX	2	2149	-	0,6,6	0.00	-	-		
86	OHX	5	4036	-	0,6,6	0.00	-	-		
86	OHX	5	4198	-	0,6,6	0.00	-	-		
86	OHX	1	3858	-	0,6,6	0.00	-	-		
86	OHX	5	3909	-	0,6,6	0.00	-	-		
86	OHX	6	2151	-	0,6,6	0.00	-	-		
86	OHX	1	4023	-	0,6,6	0.00	-	-		
86	OHX	L3	406	-	0,6,6	0.00	-	-		
86	OHX	1	4116	-	0,6,6	0.00	-	-		
86	OHX	5	4023	-	0,6,6	0.00	-	-		
86	OHX	1	4145	-	0,6,6	0.00	-	-		
86	OHX	5	3917	-	0,6,6	0.00	-	-		
86	OHX	1	4013	-	0,6,6	0.00	-	-		
86	OHX	s1	302	-	0,6,6	0.00	-	-		
86	OHX	1	4183	-	0,6,6	0.00	-	-		
86	OHX	5	3982	-	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	1	3874	-	0,6,6	0.00	-	-		
86	OHX	1	3935	-	0,6,6	0.00	-	-		
86	OHX	5	3898	-	0,6,6	0.00	-	-		
86	OHX	6	2116	-	0,6,6	0.00	-	-		
86	OHX	5	4240	-	0,6,6	0.00	-	-		
86	OHX	5	4244	-	0,6,6	0.00	-	-		
86	OHX	6	2076	-	0,6,6	0.00	-	-		
86	OHX	2	2101	-	0,6,6	0.00	-	-		
86	OHX	2	2097	-	0,6,6	0.00	-	-		
86	OHX	5	4035	-	0,6,6	0.00	-	-		
86	OHX	6	2159	-	0,6,6	0.00	-	-		
86	OHX	5	4030	-	0,6,6	0.00	-	-		
86	OHX	5	3921	-	0,6,6	0.00	-	-		
86	OHX	5	4001	-	0,6,6	0.00	-	-		
86	OHX	6	2131	-	0,6,6	0.00	-	-		
86	OHX	2	2165	-	0,6,6	0.00	-	-		
86	OHX	5	4142	-	0,6,6	0.00	-	-		
86	OHX	5	4195	-	0,6,6	0.00	-	-		
86	OHX	2	2032	-	0,6,6	0.00	-	-		
86	OHX	6	2130	-	0,6,6	0.00	-	-		
86	OHX	1	3948	-	0,6,6	0.00	-	-		
86	OHX	5	4058	-	0,6,6	0.00	-	-		
86	OHX	2	2036	-	0,6,6	0.00	-	-		
86	OHX	1	4178	-	0,6,6	0.00	-	-		
86	OHX	O7	105	-	0,6,6	0.00	-	-		
86	OHX	5	4208	-	0,6,6	0.00	-	-		
86	OHX	5	4009	-	0,6,6	0.00	-	-		
86	OHX	6	2092	-	0,6,6	0.00	-	-		
86	OHX	1	3965	-	0,6,6	0.00	-	-		
86	OHX	5	4086	-	0,6,6	0.00	-	-		
86	OHX	5	4201	-	0,6,6	0.00	-	-		
86	OHX	2	2079	-	0,6,6	0.00	-	-		
86	OHX	1	3925	-	0,6,6	0.00	-	-		
86	OHX	5	4113	-	0,6,6	0.00	-	-		
86	OHX	2	2067	-	0,6,6	0.00	-	-		
86	OHX	2	2070	-	0,6,6	0.00	-	-		
86	OHX	2	2025	-	0,6,6	0.00	-	-		
86	OHX	M9	202	-	0,6,6	0.00	-	-		
86	OHX	5	4134	-	0,6,6	0.00	-	-		
86	OHX	1	3919	-	0,6,6	0.00	-	-		
86	OHX	1	3869	-	0,6,6	0.00	-	-		
86	OHX	1	3866	-	0,6,6	0.00	-	-		
86	OHX	6	2120	-	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	4228	-	0,6,6	0.00	-	-		
86	OHX	1	4171	-	0,6,6	0.00	-	-		
86	OHX	8	220	-	0,6,6	0.00	-	-		
86	OHX	1	4043	-	0,6,6	0.00	-	-		
86	OHX	5	3959	-	0,6,6	0.00	-	-		
86	OHX	5	3954	-	0,6,6	0.00	-	-		
86	OHX	5	3943	-	0,6,6	0.00	-	-		
86	OHX	1	3863	-	0,6,6	0.00	-	-		
86	OHX	5	4124	-	0,6,6	0.00	-	-		
86	OHX	1	3961	-	0,6,6	0.00	-	-		
86	OHX	1	4041	-	0,6,6	0.00	-	-		
86	OHX	5	4234	-	0,6,6	0.00	-	-		
86	OHX	5	3945	-	0,6,6	0.00	-	-		
86	OHX	6	2085	-	0,6,6	0.00	-	-		
86	OHX	6	2148	-	0,6,6	0.00	-	-		
86	OHX	1	3872	-	0,6,6	0.00	-	-		
86	OHX	6	2069	-	0,6,6	0.00	-	-		
86	OHX	5	4061	-	0,6,6	0.00	-	-		
86	OHX	2	2135	-	0,6,6	0.00	-	-		
86	OHX	1	3950	-	0,6,6	0.00	-	-		
86	OHX	5	4239	-	0,6,6	0.00	-	-		
86	OHX	1	3992	-	0,6,6	0.00	-	-		
86	OHX	1	4066	-	0,6,6	0.00	-	-		
86	OHX	6	2158	-	0,6,6	0.00	-	-		
86	OHX	1	3893	-	0,6,6	0.00	-	-		
86	OHX	1	3885	-	0,6,6	0.00	-	-		
86	OHX	M5	303	-	0,6,6	0.00	-	-		
86	OHX	5	3968	-	0,6,6	0.00	-	-		
86	OHX	5	3949	-	0,6,6	0.00	-	-		
86	OHX	1	4192	-	0,6,6	0.00	-	-		
86	OHX	1	4110	-	0,6,6	0.00	-	-		
86	OHX	5	4148	-	0,6,6	0.00	-	-		
86	OHX	1	3870	-	0,6,6	0.00	-	-		
86	OHX	1	4115	-	0,6,6	0.00	-	-		
86	OHX	1	3959	-	0,6,6	0.00	-	-		
86	OHX	5	4122	-	0,6,6	0.00	-	-		
86	OHX	1	3971	-	0,6,6	0.00	-	-		
86	OHX	1	3906	-	0,6,6	0.00	-	-		
86	OHX	6	2090	-	0,6,6	0.00	-	-		
86	OHX	4	227	-	0,6,6	0.00	-	-		
86	OHX	5	4170	-	0,6,6	0.00	-	-		
86	OHX	14	402	-	0,6,6	0.00	-	-		
86	OHX	5	4082	-	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	2145	-	0,6,6	0.00	-	-		
86	OHX	5	4008	-	0,6,6	0.00	-	-		
86	OHX	M7	207	-	0,6,6	0.00	-	-		
86	OHX	d4	201	-	0,6,6	0.00	-	-		
86	OHX	2	2137	-	0,6,6	0.00	-	-		
86	OHX	6	2062	-	0,6,6	0.00	-	-		
86	OHX	4	225	-	0,6,6	0.00	-	-		
86	OHX	1	3887	-	0,6,6	0.00	-	-		
86	OHX	6	2192	-	0,6,6	0.00	-	-		
86	OHX	5	4227	-	0,6,6	0.00	-	-		
86	OHX	1	4122	-	0,6,6	0.00	-	-		
86	OHX	5	4059	-	0,6,6	0.00	-	-		
86	OHX	1	4087	-	0,6,6	0.00	-	-		
86	OHX	5	4150	-	0,6,6	0.00	-	-		
86	OHX	6	2107	-	0,6,6	0.00	-	-		
86	OHX	1	3964	-	0,6,6	0.00	-	-		
86	OHX	2	2040	-	0,6,6	0.00	-	-		
86	OHX	5	4003	-	0,6,6	0.00	-	-		
86	OHX	5	4068	-	0,6,6	0.00	-	-		
86	OHX	2	2113	-	0,6,6	0.00	-	-		
86	OHX	5	3899	-	0,6,6	0.00	-	-		
86	OHX	6	2083	-	0,6,6	0.00	-	-		
86	OHX	5	4157	-	0,6,6	0.00	-	-		
86	OHX	6	2140	-	0,6,6	0.00	-	-		
86	OHX	2	2090	-	0,6,6	0.00	-	-		
86	OHX	4	235	-	0,6,6	0.00	-	-		
86	OHX	5	3987	-	0,6,6	0.00	-	-		
86	OHX	2	2121	-	0,6,6	0.00	-	-		
86	OHX	2	2173	-	0,6,6	0.00	-	-		
86	OHX	1	3989	-	0,6,6	0.00	-	-		
86	OHX	6	2135	-	0,6,6	0.00	-	-		
86	OHX	5	4247	-	0,6,6	0.00	-	-		
86	OHX	6	2126	-	0,6,6	0.00	-	-		
86	OHX	1	4042	-	0,6,6	0.00	-	-		
86	OHX	3	219	-	0,6,6	0.00	-	-		
86	OHX	2	2142	-	0,6,6	0.00	-	-		
86	OHX	1	4030	-	0,6,6	0.00	-	-		
86	OHX	5	4149	-	0,6,6	0.00	-	-		
86	OHX	5	4028	-	0,6,6	0.00	-	-		
86	OHX	1	3912	-	0,6,6	0.00	-	-		
86	OHX	2	2175	-	0,6,6	0.00	-	-		
86	OHX	1	4000	-	0,6,6	0.00	-	-		
86	OHX	1	3899	-	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	4165	-	0,6,6	0.00	-	-		
86	OHX	5	4199	-	0,6,6	0.00	-	-		
86	OHX	5	3966	-	0,6,6	0.00	-	-		
86	OHX	2	2156	-	0,6,6	0.00	-	-		
86	OHX	6	2067	-	0,6,6	0.00	-	-		
86	OHX	5	4241	-	0,6,6	0.00	-	-		
86	OHX	1	4104	-	0,6,6	0.00	-	-		
86	OHX	5	4109	-	0,6,6	0.00	-	-		
86	OHX	5	4128	-	0,6,6	0.00	-	-		
86	OHX	1	4095	-	0,6,6	0.00	-	-		
86	OHX	4	230	-	0,6,6	0.00	-	-		
86	OHX	1	4090	-	0,6,6	0.00	-	-		
86	OHX	1	3973	-	0,6,6	0.00	-	-		
86	OHX	2	2034	-	0,6,6	0.00	-	-		
86	OHX	6	2188	-	0,6,6	0.00	-	-		
86	OHX	5	4133	-	0,6,6	0.00	-	-		
86	OHX	2	2148	-	0,6,6	0.00	-	-		
86	OHX	S8	302	-	0,6,6	0.00	-	-		
86	OHX	2	2100	-	0,6,6	0.00	-	-		
86	OHX	s1	303	-	0,6,6	0.00	-	-		
86	OHX	1	4196	-	0,6,6	0.00	-	-		
86	OHX	5	4162	-	0,6,6	0.00	-	-		
86	OHX	1	4136	-	0,6,6	0.00	-	-		
86	OHX	1	3930	-	0,6,6	0.00	-	-		
86	OHX	6	2051	-	0,6,6	0.00	-	-		
86	OHX	6	2201	-	0,6,6	0.00	-	-		
86	OHX	1	3902	-	0,6,6	0.00	-	-		
86	OHX	5	4006	-	0,6,6	0.00	-	-		
86	OHX	D9	102	-	0,6,6	0.00	-	-		
86	OHX	1	4172	-	0,6,6	0.00	-	-		
86	OHX	5	4144	-	0,6,6	0.00	-	-		
86	OHX	1	4007	-	0,6,6	0.00	-	-		
86	OHX	5	4076	-	0,6,6	0.00	-	-		
86	OHX	8	225	-	0,6,6	0.00	-	-		
86	OHX	1	4134	-	0,6,6	0.00	-	-		
86	OHX	3	225	-	0,6,6	0.00	-	-		
86	OHX	1	4153	-	0,6,6	0.00	-	-		
86	OHX	2	2108	-	0,6,6	0.00	-	-		
86	OHX	8	219	-	0,6,6	0.00	-	-		
86	OHX	2	2102	-	0,6,6	0.00	-	-		
86	OHX	1	3868	-	0,6,6	0.00	-	-		
86	OHX	1	4035	-	0,6,6	0.00	-	-		
86	OHX	1	3983	-	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	4226	-	0,6,6	0.00	-	-		
86	OHX	5	3895	-	0,6,6	0.00	-	-		
86	OHX	1	4159	-	0,6,6	0.00	-	-		
86	OHX	5	4012	-	0,6,6	0.00	-	-		
86	OHX	5	4176	-	0,6,6	0.00	-	-		
86	OHX	5	4033	-	0,6,6	0.00	-	-		
86	OHX	5	3947	-	0,6,6	0.00	-	-		
86	OHX	1	3877	-	0,6,6	0.00	-	-		
86	OHX	1	4044	-	0,6,6	0.00	-	-		
86	OHX	7	229	-	0,6,6	0.00	-	-		
86	OHX	1	4077	-	0,6,6	0.00	-	-		
86	OHX	6	2118	-	0,6,6	0.00	-	-		
86	OHX	5	4013	-	0,6,6	0.00	-	-		
86	OHX	6	2059	-	0,6,6	0.00	-	-		
86	OHX	5	4078	-	0,6,6	0.00	-	-		
86	OHX	1	4089	-	0,6,6	0.00	-	-		
86	OHX	5	4051	-	0,6,6	0.00	-	-		
86	OHX	2	2178	-	0,6,6	0.00	-	-		
86	OHX	6	2047	-	0,6,6	0.00	-	-		
86	OHX	6	2152	-	0,6,6	0.00	-	-		
86	OHX	6	2186	-	0,6,6	0.00	-	-		
86	OHX	1	3963	-	0,6,6	0.00	-	-		
86	OHX	5	3914	-	0,6,6	0.00	-	-		
86	OHX	5	4091	-	0,6,6	0.00	-	-		
86	OHX	8	221	-	0,6,6	0.00	-	-		
86	OHX	m1	202	-	0,6,6	0.00	-	-		
86	OHX	6	2095	-	0,6,6	0.00	-	-		
86	OHX	1	4073	-	0,6,6	0.00	-	-		
86	OHX	1	4100	-	0,6,6	0.00	-	-		
86	OHX	1	4098	-	0,6,6	0.00	-	-		
86	OHX	6	2071	-	0,6,6	0.00	-	-		
86	OHX	5	4196	-	0,6,6	0.00	-	-		
86	OHX	2	2072	-	0,6,6	0.00	-	-		
86	OHX	5	4197	-	0,6,6	0.00	-	-		
86	OHX	5	4075	-	0,6,6	0.00	-	-		
86	OHX	1	4074	-	0,6,6	0.00	-	-		
86	OHX	5	3962	-	0,6,6	0.00	-	-		
86	OHX	5	4202	-	0,6,6	0.00	-	-		
86	OHX	1	4170	-	0,6,6	0.00	-	-		
86	OHX	5	3993	-	0,6,6	0.00	-	-		
86	OHX	5	4065	-	0,6,6	0.00	-	-		
86	OHX	1	4149	-	0,6,6	0.00	-	-		
86	OHX	1	3864	-	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	2105	-	0,6,6	0.00	-	-		
86	OHX	1	4168	-	0,6,6	0.00	-	-		
86	OHX	5	4000	-	0,6,6	0.00	-	-		
86	OHX	6	2129	-	0,6,6	0.00	-	-		
86	OHX	7	225	-	0,6,6	0.00	-	-		
86	OHX	1	4091	-	0,6,6	0.00	-	-		
86	OHX	6	2136	-	0,6,6	0.00	-	-		
86	OHX	5	4112	-	0,6,6	0.00	-	-		
86	OHX	2	2107	-	0,6,6	0.00	-	-		
86	OHX	1	4051	-	0,6,6	0.00	-	-		
86	OHX	5	3903	-	0,6,6	0.00	-	-		
86	OHX	5	4014	-	0,6,6	0.00	-	-		
86	OHX	5	4062	-	0,6,6	0.00	-	-		
86	OHX	6	2162	-	0,6,6	0.00	-	-		
86	OHX	6	2169	-	0,6,6	0.00	-	-		
86	OHX	2	2140	-	0,6,6	0.00	-	-		
86	OHX	4	237	-	0,6,6	0.00	-	-		
86	OHX	2	2167	-	0,6,6	0.00	-	-		
86	OHX	5	4089	-	0,6,6	0.00	-	-		
86	OHX	2	2042	-	0,6,6	0.00	-	-		
86	OHX	6	2204	-	0,6,6	0.00	-	-		
86	OHX	6	2142	-	0,6,6	0.00	-	-		
86	OHX	5	4054	-	0,6,6	0.00	-	-		
86	OHX	2	2089	-	0,6,6	0.00	-	-		
86	OHX	5	4155	-	0,6,6	0.00	-	-		
86	OHX	5	4020	-	0,6,6	0.00	-	-		
86	OHX	3	223	-	0,6,6	0.00	-	-		
86	OHX	5	3901	-	0,6,6	0.00	-	-		
86	OHX	1	4008	-	0,6,6	0.00	-	-		
88	BLS	1	4211	-	25,31,31	1.98	7 (28%)	23,43,43	2.77	8 (34%)
86	OHX	1	4067	-	0,6,6	0.00	-	-		
86	OHX	1	3949	-	0,6,6	0.00	-	-		
86	OHX	1	4009	-	0,6,6	0.00	-	-		
86	OHX	5	4021	-	0,6,6	0.00	-	-		
86	OHX	2	2085	-	0,6,6	0.00	-	-		
86	OHX	1	4204	-	0,6,6	0.00	-	-		
86	OHX	1	3871	-	0,6,6	0.00	-	-		
86	OHX	2	2077	-	0,6,6	0.00	-	-		
86	OHX	2	2076	-	0,6,6	0.00	-	-		
86	OHX	1	4135	-	0,6,6	0.00	-	-		
86	OHX	1	4120	-	0,6,6	0.00	-	-		
86	OHX	6	2087	-	0,6,6	0.00	-	-		
86	OHX	1	4084	-	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	4072	-	0,6,6	0.00	-	-		
86	OHX	6	2191	-	0,6,6	0.00	-	-		
86	OHX	1	4108	-	0,6,6	0.00	-	-		
86	OHX	1	3878	-	0,6,6	0.00	-	-		
86	OHX	8	229	-	0,6,6	0.00	-	-		
86	OHX	2	2030	-	0,6,6	0.00	-	-		
86	OHX	2	2105	-	0,6,6	0.00	-	-		
86	OHX	6	2184	-	0,6,6	0.00	-	-		
86	OHX	1	4129	-	0,6,6	0.00	-	-		
86	OHX	5	4123	-	0,6,6	0.00	-	-		
86	OHX	2	2133	-	0,6,6	0.00	-	-		
86	OHX	7	220	-	0,6,6	0.00	-	-		
86	OHX	6	2125	-	0,6,6	0.00	-	-		
86	OHX	1	4099	-	0,6,6	0.00	-	-		
86	OHX	5	3965	-	0,6,6	0.00	-	-		
86	OHX	5	4224	-	0,6,6	0.00	-	-		
86	OHX	6	2111	-	0,6,6	0.00	-	-		
86	OHX	6	2088	-	0,6,6	0.00	-	-		
86	OHX	1	4040	-	0,6,6	0.00	-	-		
86	OHX	6	2114	-	0,6,6	0.00	-	-		
86	OHX	5	4110	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	5	3900	-	0,6,6	0.00	-	-		
86	OHX	2	2027	-	0,6,6	0.00	-	-		
86	OHX	Q2	503	-	0,6,6	0.00	-	-		
86	OHX	5	3936	-	0,6,6	0.00	-	-		
86	OHX	5	4004	-	0,6,6	0.00	-	-		
86	OHX	1	4059	-	0,6,6	0.00	-	-		
86	OHX	4	226	-	0,6,6	0.00	-	-		
86	OHX	c5	201	-	0,6,6	0.00	-	-		
86	OHX	6	2141	-	0,6,6	0.00	-	-		
86	OHX	2	2138	-	0,6,6	0.00	-	-		
86	OHX	5	4066	-	0,6,6	0.00	-	-		
86	OHX	5	3920	-	0,6,6	0.00	-	-		
86	OHX	6	2084	-	0,6,6	0.00	-	-		
86	OHX	1	4039	-	0,6,6	0.00	-	-		
86	OHX	1	4033	-	0,6,6	0.00	-	-		
86	OHX	6	2134	-	0,6,6	0.00	-	-		
86	OHX	6	2113	-	0,6,6	0.00	-	-		
86	OHX	5	3950	-	0,6,6	0.00	-	-		
86	OHX	1	4038	-	0,6,6	0.00	-	-		
86	OHX	5	4053	-	0,6,6	0.00	-	-		
86	OHX	5	4118	-	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	3889	-	0,6,6	0.00	-	-		
86	OHX	1	4210	-	0,6,6	0.00	-	-		
86	OHX	5	4242	-	0,6,6	0.00	-	-		
86	OHX	5	4106	-	0,6,6	0.00	-	-		
86	OHX	5	3902	-	0,6,6	0.00	-	-		
86	OHX	1	3968	-	0,6,6	0.00	-	-		
86	OHX	1	4180	-	0,6,6	0.00	-	-		
86	OHX	8	217	-	0,6,6	0.00	-	-		
86	OHX	6	2132	-	0,6,6	0.00	-	-		
86	OHX	5	4073	-	0,6,6	0.00	-	-		
86	OHX	1	4034	-	0,6,6	0.00	-	-		
86	OHX	2	2083	-	0,6,6	0.00	-	-		
86	OHX	5	4173	-	0,6,6	0.00	-	-		
86	OHX	2	2066	-	0,6,6	0.00	-	-		
86	OHX	5	4049	-	0,6,6	0.00	-	-		
86	OHX	6	2178	-	0,6,6	0.00	-	-		
86	OHX	6	2155	-	0,6,6	0.00	-	-		
86	OHX	5	4207	-	0,6,6	0.00	-	-		
86	OHX	2	2069	-	0,6,6	0.00	-	-		
86	OHX	2	2116	-	0,6,6	0.00	-	-		
86	OHX	5	4192	-	0,6,6	0.00	-	-		
86	OHX	5	4060	-	0,6,6	0.00	-	-		
86	OHX	6	2119	-	0,6,6	0.00	-	-		
86	OHX	5	4154	-	0,6,6	0.00	-	-		
86	OHX	8	223	-	0,6,6	0.00	-	-		
86	OHX	1	3988	-	0,6,6	0.00	-	-		
86	OHX	6	2089	-	0,6,6	0.00	-	-		
86	OHX	1	4028	-	0,6,6	0.00	-	-		
86	OHX	1	3952	-	0,6,6	0.00	-	-		
86	OHX	5	4022	-	0,6,6	0.00	-	-		
86	OHX	1	4046	-	0,6,6	0.00	-	-		
86	OHX	5	3907	-	0,6,6	0.00	-	-		
86	OHX	6	2052	-	0,6,6	0.00	-	-		
86	OHX	5	3939	-	0,6,6	0.00	-	-		
86	OHX	2	2115	-	0,6,6	0.00	-	-		
86	OHX	1	4140	-	0,6,6	0.00	-	-		
86	OHX	5	4212	-	0,6,6	0.00	-	-		
86	OHX	5	4135	-	0,6,6	0.00	-	-		
86	OHX	2	2154	-	0,6,6	0.00	-	-		
86	OHX	6	2166	-	0,6,6	0.00	-	-		
86	OHX	o3	203	-	0,6,6	0.00	-	-		
86	OHX	5	4040	-	0,6,6	0.00	-	-		
86	OHX	1	4195	-	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	3904	-	0,6,6	0.00	-	-		
86	OHX	2	2153	-	0,6,6	0.00	-	-		
86	OHX	5	4102	-	0,6,6	0.00	-	-		
86	OHX	1	3999	-	0,6,6	0.00	-	-		
86	OHX	1	3991	-	0,6,6	0.00	-	-		
86	OHX	1	4005	-	0,6,6	0.00	-	-		
86	OHX	8	222	-	0,6,6	0.00	-	-		
86	OHX	2	2145	-	0,6,6	0.00	-	-		
86	OHX	1	4026	-	0,6,6	0.00	-	-		
86	OHX	SR	401	-	0,6,6	0.00	-	-		
86	OHX	1	3980	-	0,6,6	0.00	-	-		
86	OHX	2	2179	-	0,6,6	0.00	-	-		
86	OHX	5	4037	-	0,6,6	0.00	-	-		
86	OHX	2	2130	-	0,6,6	0.00	-	-		
86	OHX	5	3918	-	0,6,6	0.00	-	-		
86	OHX	5	4171	-	0,6,6	0.00	-	-		
86	OHX	2	2166	-	0,6,6	0.00	-	-		
86	OHX	2	2071	-	0,6,6	0.00	-	-		
86	OHX	2	2033	-	0,6,6	0.00	-	-		
86	OHX	15	306	-	0,6,6	0.00	-	-		
86	OHX	1	4137	-	0,6,6	0.00	-	-		
86	OHX	1	4169	-	0,6,6	0.00	-	-		
86	OHX	5	4042	-	0,6,6	0.00	-	-		
86	OHX	1	4193	-	0,6,6	0.00	-	-		
86	OHX	5	4179	-	0,6,6	0.00	-	-		
86	OHX	5	4079	-	0,6,6	0.00	-	-		
86	OHX	1	4158	-	0,6,6	0.00	-	-		
86	OHX	1	3974	-	0,6,6	0.00	-	-		
86	OHX	1	3922	-	0,6,6	0.00	-	-		
86	OHX	2	2065	-	0,6,6	0.00	-	-		
86	OHX	1	3929	-	0,6,6	0.00	-	-		
86	OHX	1	4006	-	0,6,6	0.00	-	-		
86	OHX	1	4085	-	0,6,6	0.00	-	-		
86	OHX	5	3940	-	0,6,6	0.00	-	-		
86	OHX	1	3976	-	0,6,6	0.00	-	-		
86	OHX	5	3927	-	0,6,6	0.00	-	-		
86	OHX	5	4185	-	0,6,6	0.00	-	-		
86	OHX	2	2164	-	0,6,6	0.00	-	-		
86	OHX	2	2023	-	0,6,6	0.00	-	-		
86	OHX	5	4200	-	0,6,6	0.00	-	-		
86	OHX	1	4144	-	0,6,6	0.00	-	-		
86	OHX	6	2070	-	0,6,6	0.00	-	-		
86	OHX	5	4237	-	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	4018	-	0,6,6	0.00	-	-		
86	OHX	5	3937	-	0,6,6	0.00	-	-		
86	OHX	1	3857	-	0,6,6	0.00	-	-		
86	OHX	7	218	-	0,6,6	0.00	-	-		
86	OHX	1	3908	-	0,6,6	0.00	-	-		
86	OHX	1	4079	-	0,6,6	0.00	-	-		
86	OHX	2	2088	-	0,6,6	0.00	-	-		
86	OHX	5	4243	-	0,6,6	0.00	-	-		
86	OHX	1	4148	-	0,6,6	0.00	-	-		
86	OHX	1	4075	-	0,6,6	0.00	-	-		
86	OHX	15	305	-	0,6,6	0.00	-	-		
86	OHX	1	4088	-	0,6,6	0.00	-	-		
86	OHX	5	4172	-	0,6,6	0.00	-	-		
86	OHX	1	3962	-	0,6,6	0.00	-	-		
86	OHX	5	4182	-	0,6,6	0.00	-	-		
86	OHX	5	3986	-	0,6,6	0.00	-	-		
86	OHX	2	2158	-	0,6,6	0.00	-	-		
86	OHX	5	3997	-	0,6,6	0.00	-	-		
86	OHX	5	4084	-	0,6,6	0.00	-	-		
86	OHX	5	4186	-	0,6,6	0.00	-	-		
86	OHX	19	202	-	0,6,6	0.00	-	-		
86	OHX	1	4188	-	0,6,6	0.00	-	-		
86	OHX	6	2100	-	0,6,6	0.00	-	-		
86	OHX	6	2094	-	0,6,6	0.00	-	-		
86	OHX	6	2127	-	0,6,6	0.00	-	-		
86	OHX	2	2120	-	0,6,6	0.00	-	-		
86	OHX	1	4096	-	0,6,6	0.00	-	-		
86	OHX	5	4210	-	0,6,6	0.00	-	-		
86	OHX	5	4095	-	0,6,6	0.00	-	-		
86	OHX	2	2174	-	0,6,6	0.00	-	-		
86	OHX	5	4193	-	0,6,6	0.00	-	-		
86	OHX	5	3969	-	0,6,6	0.00	-	-		
86	OHX	1	4018	-	0,6,6	0.00	-	-		
86	OHX	5	3967	-	0,6,6	0.00	-	-		
86	OHX	2	2041	-	0,6,6	0.00	-	-		
86	OHX	1	4199	-	0,6,6	0.00	-	-		
86	OHX	5	4165	-	0,6,6	0.00	-	-		
86	OHX	1	3967	-	0,6,6	0.00	-	-		
86	OHX	5	4160	-	0,6,6	0.00	-	-		
86	OHX	5	4215	-	0,6,6	0.00	-	-		
86	OHX	6	2146	-	0,6,6	0.00	-	-		
86	OHX	5	3951	-	0,6,6	0.00	-	-		
86	OHX	1	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	4037	-	0,6,6	0.00	-	-		
86	OHX	M0	304	-	0,6,6	0.00	-	-		
86	OHX	1	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4183	-	0,6,6	0.00	-	-		
86	OHX	5	4189	-	0,6,6	0.00	-	-		
86	OHX	8	218	-	0,6,6	0.00	-	-		
86	OHX	s4	301	-	0,6,6	0.00	-	-		
86	OHX	1	3903	-	0,6,6	0.00	-	-		
86	OHX	5	3984	-	0,6,6	0.00	-	-		
86	OHX	1	4173	-	0,6,6	0.00	-	-		
86	OHX	1	3883	-	0,6,6	0.00	-	-		
86	OHX	5	3963	-	0,6,6	0.00	-	-		
86	OHX	5	3896	-	0,6,6	0.00	-	-		
86	OHX	2	2098	-	0,6,6	0.00	-	-		
86	OHX	1	3913	-	0,6,6	0.00	-	-		
86	OHX	5	4098	-	0,6,6	0.00	-	-		
86	OHX	5	4034	-	0,6,6	0.00	-	-		
86	OHX	1	3904	-	0,6,6	0.00	-	-		
86	OHX	2	2095	-	0,6,6	0.00	-	-		
86	OHX	4	228	-	0,6,6	0.00	-	-		
86	OHX	6	2167	-	0,6,6	0.00	-	-		
86	OHX	1	4167	-	0,6,6	0.00	-	-		
86	OHX	5	4085	-	0,6,6	0.00	-	-		
86	OHX	6	2197	-	0,6,6	0.00	-	-		
86	OHX	2	2129	-	0,6,6	0.00	-	-		
86	OHX	5	4120	-	0,6,6	0.00	-	-		
86	OHX	1	4048	-	0,6,6	0.00	-	-		
86	OHX	5	4213	-	0,6,6	0.00	-	-		
86	OHX	1	3859	-	0,6,6	0.00	-	-		
86	OHX	6	2165	-	0,6,6	0.00	-	-		
86	OHX	1	3970	-	0,6,6	0.00	-	-		
86	OHX	5	4206	-	0,6,6	0.00	-	-		
86	OHX	1	3921	-	0,6,6	0.00	-	-		
86	OHX	2	2051	-	0,6,6	0.00	-	-		
86	OHX	1	4053	-	0,6,6	0.00	-	-		
86	OHX	5	4069	-	0,6,6	0.00	-	-		
86	OHX	5	4121	-	0,6,6	0.00	-	-		
86	OHX	5	3938	-	0,6,6	0.00	-	-		
86	OHX	1	4162	-	0,6,6	0.00	-	-		
86	OHX	2	2092	-	0,6,6	0.00	-	-		
86	OHX	1	4111	-	0,6,6	0.00	-	-		
86	OHX	5	4071	-	0,6,6	0.00	-	-		
86	OHX	l3	405	-	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	2123	-	0,6,6	0.00	-	-		
86	OHX	4	231	-	0,6,6	0.00	-	-		
86	OHX	1	3987	-	0,6,6	0.00	-	-		
86	OHX	1	4121	-	0,6,6	0.00	-	-		
86	OHX	5	4100	-	0,6,6	0.00	-	-		
86	OHX	1	4011	-	0,6,6	0.00	-	-		
86	OHX	2	2159	-	0,6,6	0.00	-	-		
86	OHX	1	4049	-	0,6,6	0.00	-	-		
86	OHX	5	3908	-	0,6,6	0.00	-	-		
86	OHX	1	4164	-	0,6,6	0.00	-	-		
86	OHX	1	4208	-	0,6,6	0.00	-	-		
86	OHX	1	3951	-	0,6,6	0.00	-	-		
86	OHX	5	4245	-	0,6,6	0.00	-	-		
86	OHX	5	3981	-	0,6,6	0.00	-	-		
86	OHX	1	3917	-	0,6,6	0.00	-	-		
86	OHX	5	4007	-	0,6,6	0.00	-	-		
86	OHX	1	3986	-	0,6,6	0.00	-	-		
86	OHX	1	4127	-	0,6,6	0.00	-	-		
86	OHX	2	2039	-	0,6,6	0.00	-	-		
86	OHX	2	2035	-	0,6,6	0.00	-	-		
86	OHX	5	4111	-	0,6,6	0.00	-	-		
86	OHX	s9	201	-	0,6,6	0.00	-	-		
86	OHX	1	4126	-	0,6,6	0.00	-	-		
86	OHX	1	4131	-	0,6,6	0.00	-	-		
86	OHX	8	228	-	0,6,6	0.00	-	-		
86	OHX	m4	202	-	0,6,6	0.00	-	-		
86	OHX	2	2155	-	0,6,6	0.00	-	-		
86	OHX	1	3892	-	0,6,6	0.00	-	-		
86	OHX	1	4020	-	0,6,6	0.00	-	-		
86	OHX	1	3898	-	0,6,6	0.00	-	-		
86	OHX	5	4159	-	0,6,6	0.00	-	-		
86	OHX	1	4187	-	0,6,6	0.00	-	-		
86	OHX	1	3996	-	0,6,6	0.00	-	-		
86	OHX	2	2147	-	0,6,6	0.00	-	-		
86	OHX	1	4024	-	0,6,6	0.00	-	-		
86	OHX	1	4157	-	0,6,6	0.00	-	-		
86	OHX	l5	304	-	0,6,6	0.00	-	-		
86	OHX	6	2075	-	0,6,6	0.00	-	-		
86	OHX	5	4141	-	0,6,6	0.00	-	-		
86	OHX	1	4143	-	0,6,6	0.00	-	-		
86	OHX	5	4161	-	0,6,6	0.00	-	-		
86	OHX	5	3961	-	0,6,6	0.00	-	-		
86	OHX	5	3994	-	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	2137	-	0,6,6	0.00	-	-		
86	OHX	m6	203	-	0,6,6	0.00	-	-		
86	OHX	1	3891	-	0,6,6	0.00	-	-		
86	OHX	2	2068	-	0,6,6	0.00	-	-		
86	OHX	5	4117	-	0,6,6	0.00	-	-		
86	OHX	6	2198	-	0,6,6	0.00	-	-		
86	OHX	2	2029	-	0,6,6	0.00	-	-		
86	OHX	1	4047	-	0,6,6	0.00	-	-		
86	OHX	6	2099	-	0,6,6	0.00	-	-		
86	OHX	8	215	-	0,6,6	0.00	-	-		
86	OHX	6	2182	-	0,6,6	0.00	-	-		
86	OHX	C3	201	-	0,6,6	0.00	-	-		
86	OHX	6	2101	-	0,6,6	0.00	-	-		
86	OHX	6	2096	-	0,6,6	0.00	-	-		
86	OHX	1	3960	-	0,6,6	0.00	-	-		
86	OHX	1	3927	-	0,6,6	0.00	-	-		
86	OHX	1	4130	-	0,6,6	0.00	-	-		
86	OHX	5	3912	-	0,6,6	0.00	-	-		
86	OHX	5	3924	-	0,6,6	0.00	-	-		
86	OHX	2	2141	-	0,6,6	0.00	-	-		
86	OHX	5	4181	-	0,6,6	0.00	-	-		
86	OHX	1	4001	-	0,6,6	0.00	-	-		
86	OHX	6	2055	-	0,6,6	0.00	-	-		
86	OHX	1	3861	-	0,6,6	0.00	-	-		
86	OHX	1	4113	-	0,6,6	0.00	-	-		
86	OHX	6	2102	-	0,6,6	0.00	-	-		
86	OHX	5	4107	-	0,6,6	0.00	-	-		
86	OHX	2	2128	-	0,6,6	0.00	-	-		
86	OHX	2	2127	-	0,6,6	0.00	-	-		
86	OHX	5	3922	-	0,6,6	0.00	-	-		
86	OHX	2	2038	-	0,6,6	0.00	-	-		
86	OHX	2	2044	-	0,6,6	0.00	-	-		
86	OHX	5	4097	-	0,6,6	0.00	-	-		
86	OHX	1	4069	-	0,6,6	0.00	-	-		
86	OHX	1	4185	-	0,6,6	0.00	-	-		
86	OHX	1	4036	-	0,6,6	0.00	-	-		
86	OHX	1	4107	-	0,6,6	0.00	-	-		
86	OHX	5	4052	-	0,6,6	0.00	-	-		
86	OHX	5	4145	-	0,6,6	0.00	-	-		
86	OHX	1	4205	-	0,6,6	0.00	-	-		
86	OHX	5	4232	-	0,6,6	0.00	-	-		
86	OHX	5	3892	-	0,6,6	0.00	-	-		
86	OHX	5	4180	-	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	4061	-	0,6,6	0.00	-	-		
86	OHX	5	4010	-	0,6,6	0.00	-	-		
86	OHX	5	4152	-	0,6,6	0.00	-	-		
86	OHX	1	4141	-	0,6,6	0.00	-	-		
86	OHX	5	3979	-	0,6,6	0.00	-	-		
86	OHX	5	4015	-	0,6,6	0.00	-	-		
86	OHX	6	2112	-	0,6,6	0.00	-	-		
86	OHX	5	4114	-	0,6,6	0.00	-	-		
86	OHX	1	4166	-	0,6,6	0.00	-	-		
86	OHX	5	4219	-	0,6,6	0.00	-	-		
86	OHX	2	2111	-	0,6,6	0.00	-	-		
86	OHX	5	3934	-	0,6,6	0.00	-	-		
86	OHX	6	2081	-	0,6,6	0.00	-	-		
86	OHX	5	4070	-	0,6,6	0.00	-	-		
86	OHX	2	2170	-	0,6,6	0.00	-	-		
86	OHX	5	3960	-	0,6,6	0.00	-	-		
86	OHX	5	4169	-	0,6,6	0.00	-	-		
86	OHX	2	2078	-	0,6,6	0.00	-	-		
86	OHX	7	227	-	0,6,6	0.00	-	-		
86	OHX	1	3910	-	0,6,6	0.00	-	-		
86	OHX	5	4129	-	0,6,6	0.00	-	-		
86	OHX	1	4123	-	0,6,6	0.00	-	-		
86	OHX	2	2052	-	0,6,6	0.00	-	-		
86	OHX	1	3958	-	0,6,6	0.00	-	-		
86	OHX	2	2058	-	0,6,6	0.00	-	-		
86	OHX	2	2057	-	0,6,6	0.00	-	-		
86	OHX	1	4163	-	0,6,6	0.00	-	-		
86	OHX	1	4186	-	0,6,6	0.00	-	-		
86	OHX	1	3946	-	0,6,6	0.00	-	-		
86	OHX	L4	404	-	0,6,6	0.00	-	-		
86	OHX	5	3906	-	0,6,6	0.00	-	-		
86	OHX	1	4076	-	0,6,6	0.00	-	-		
86	OHX	5	4188	-	0,6,6	0.00	-	-		
86	OHX	5	4041	-	0,6,6	0.00	-	-		
86	OHX	5	4064	-	0,6,6	0.00	-	-		
86	OHX	6	2079	-	0,6,6	0.00	-	-		
86	OHX	1	3975	-	0,6,6	0.00	-	-		
86	OHX	1	3862	-	0,6,6	0.00	-	-		
86	OHX	1	4124	-	0,6,6	0.00	-	-		
86	OHX	1	4027	-	0,6,6	0.00	-	-		
86	OHX	1	4021	-	0,6,6	0.00	-	-		
86	OHX	1	4177	-	0,6,6	0.00	-	-		
86	OHX	1	3937	-	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	3996	-	0,6,6	0.00	-	-		
86	OHX	6	2196	-	0,6,6	0.00	-	-		
86	OHX	2	2050	-	0,6,6	0.00	-	-		
86	OHX	5	4139	-	0,6,6	0.00	-	-		
86	OHX	1	4012	-	0,6,6	0.00	-	-		
86	OHX	6	2098	-	0,6,6	0.00	-	-		
86	OHX	1	4070	-	0,6,6	0.00	-	-		
86	OHX	m7	207	-	0,6,6	0.00	-	-		
86	OHX	5	3990	-	0,6,6	0.00	-	-		
86	OHX	2	2056	-	0,6,6	0.00	-	-		
86	OHX	1	3981	-	0,6,6	0.00	-	-		
86	OHX	1	3984	-	0,6,6	0.00	-	-		
86	OHX	5	4044	-	0,6,6	0.00	-	-		
86	OHX	5	3931	-	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
88	BLS	5	4248	-	-	7/17/38/38	0/2/2/2
88	BLS	1	4211	-	-	3/17/38/38	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	5	4248	BLS	C11-N12	-5.35	1.36	1.47
88	1	4211	BLS	C6-N1	4.43	1.41	1.35
88	1	4211	BLS	C2-N3	-4.20	1.29	1.38
88	1	4211	BLS	C5-C4	3.59	1.49	1.41
88	1	4211	BLS	C11-N12	3.19	1.53	1.47
88	1	4211	BLS	C1'-N1	-2.87	1.40	1.49
88	1	4211	BLS	C6-C5	-2.53	1.32	1.38
88	5	4248	BLS	C14-N12	2.33	1.40	1.35
88	1	4211	BLS	C4-N3	-2.21	1.32	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4211	BLS	C2-N3-C4	10.01	126.48	116.34
88	5	4248	BLS	O5'-C1'-C2'	-5.93	109.92	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	5	4248	BLS	C2-N3-C4	4.27	120.66	116.34
88	1	4211	BLS	N4-C4-N3	3.65	122.25	116.49
88	1	4211	BLS	C4'-N6-C7	3.44	126.81	123.13
88	1	4211	BLS	C6-N1-C2	-2.78	116.78	121.20
88	1	4211	BLS	O5'-C1'-C2'	2.74	114.61	113.13
88	5	4248	BLS	N15-C14-N12	-2.69	115.32	118.53
88	1	4211	BLS	C5-C4-N3	-2.68	118.62	121.72
88	1	4211	BLS	C11-C10-C9	-2.48	109.86	114.52
88	1	4211	BLS	N15-C14-N12	-2.43	115.63	118.53

There are no chirality outliers.

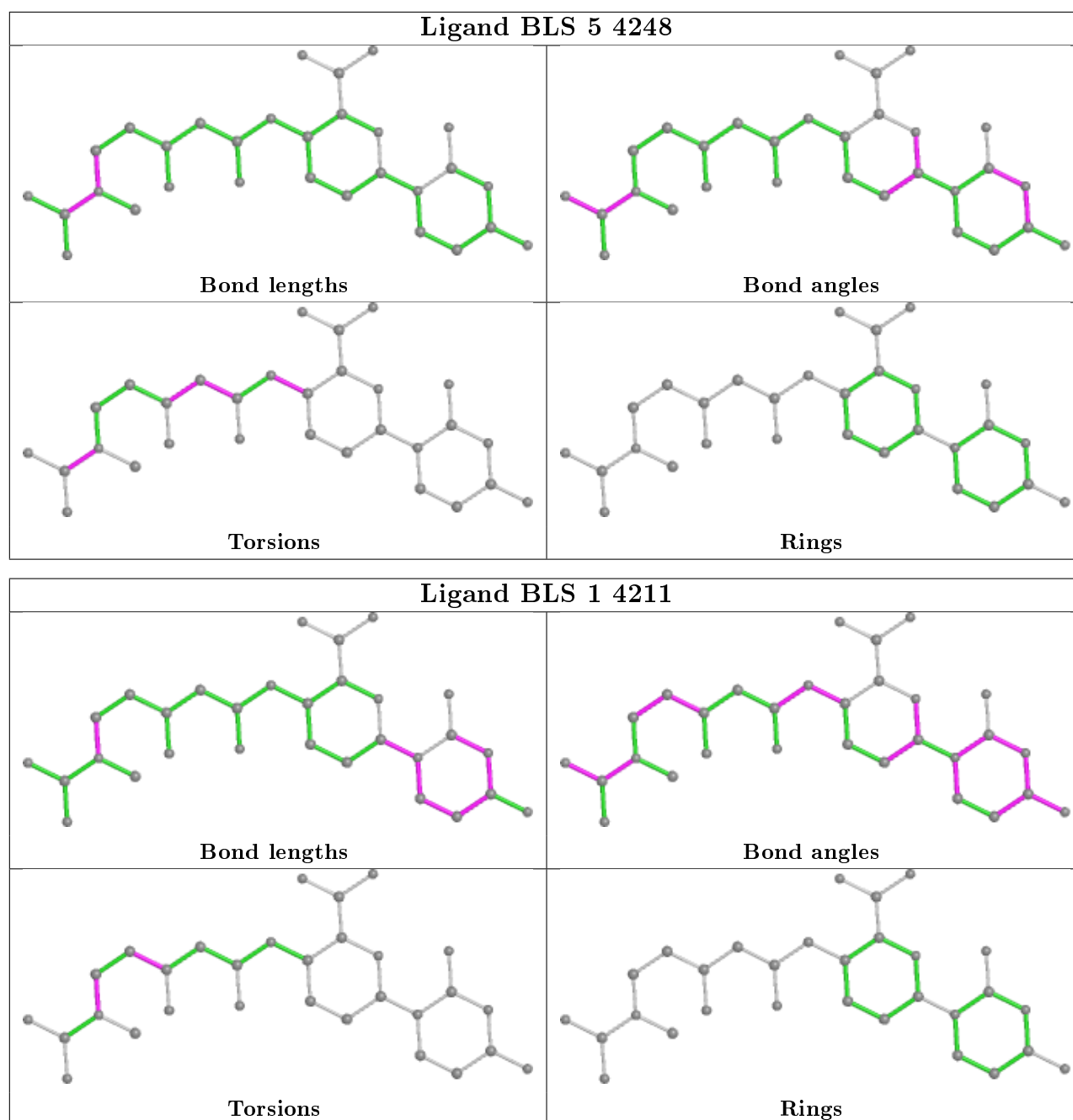
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	5	4248	BLS	C3'-C4'-N6-C7
88	5	4248	BLS	C7-C8-C9-N9
88	5	4248	BLS	N14-C14-N12-C11
88	5	4248	BLS	N15-C14-N12-C11
88	1	4211	BLS	C11-C10-C9-C8
88	1	4211	BLS	C11-C10-C9-N9
88	5	4248	BLS	O7-C7-C8-C9
88	5	4248	BLS	N6-C7-C8-C9
88	1	4211	BLS	C10-C11-N12-C13
88	5	4248	BLS	C5'-C4'-N6-C7

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.