



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 07:42 PM BST

PDB ID : 4U4Z  
Title : Crystal structure of Phyllanthoside bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-24  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

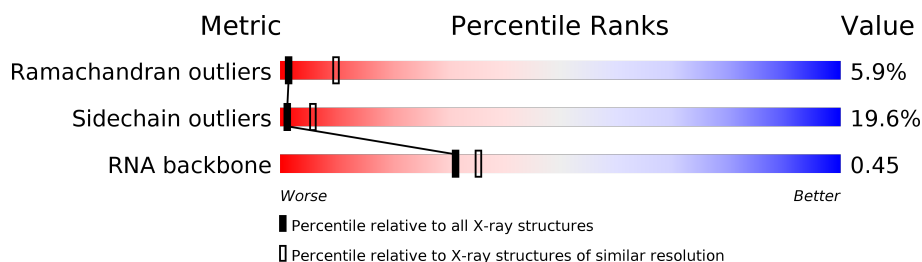
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)















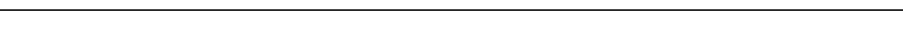




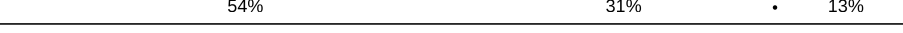





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	
1	6	1800	
2	S0	251	
2	s0	251	
3	S1	254	
3	s1	254	
4	S2	253	
4	s2	253	




















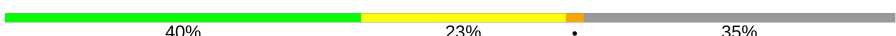





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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3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














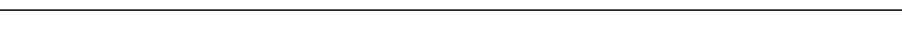











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Mol	Chain	Length	Quality of chain
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107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















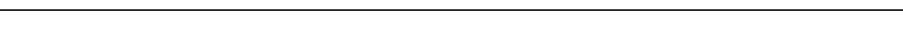




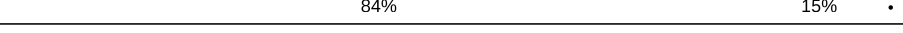





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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6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















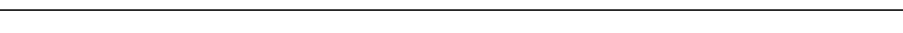




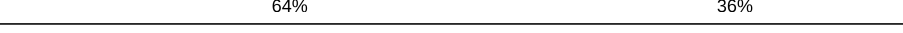





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Mol	Chain	Length	Quality of chain
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	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	 80% 19% .
68	o2	129	 78% 19% . .
69	O3	106	 90% 9% .
69	o3	106	 82% 16% .
70	O4	119	 77% 14% . 6%
70	o4	119	 76% 17% . 6%
71	O5	119	 75% 24% .
71	o5	119	 78% 21% .
72	O6	99	 76% 20% .
72	o6	99	 70% 28% .
73	O7	87	 76% 23% .
73	o7	87	 82% 16% .
74	O8	77	 73% 27%
74	o8	77	 77% 23%
75	O9	50	 80% 20%
75	o9	50	 80% 20%
76	Q0	52	 85% 15%
76	q0	52	 85% 15%
77	Q1	25	 64% 36%
77	q1	25	 72% 20% 8%
78	Q2	105	 80% 17% .
78	q2	105	 76% 22% . .
79	Q3	91	 81% 19%
79	q3	91	 82% 18%
80	e0	62	 74% 24% .

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

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411276 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1750	Total	C	N	O	P	0	0	0
			37283	16668	6591	12274	1750			
1	6	1795	Total	C	N	O	P	0	0	0
			38238	17095	6758	12590	1795			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	110	GLU	-	expression tag	UNP P87262
O4	111	ALA	-	expression tag	UNP P87262
O4	112	ALA	-	expression tag	UNP P87262

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Chain	Residue	Modelled	Actual	Comment	Reference
O4	113	LYS	-	expression tag	UNP P87262
O4	114	SER	-	expression tag	UNP P87262
O4	115	GLU	-	expression tag	UNP P87262
O4	116	LYS	-	expression tag	UNP P87262
O4	117	LYS	-	expression tag	UNP P87262
O4	118	ALA	-	expression tag	UNP P87262
O4	119	LYS	-	expression tag	UNP P87262
O4	120	LYS	-	expression tag	UNP P87262
o4	110	GLU	-	expression tag	UNP P87262
o4	111	ALA	-	expression tag	UNP P87262
o4	112	ALA	-	expression tag	UNP P87262
o4	113	LYS	-	expression tag	UNP P87262
o4	114	SER	-	expression tag	UNP P87262
o4	115	GLU	-	expression tag	UNP P87262
o4	116	LYS	-	expression tag	UNP P87262
o4	117	LYS	-	expression tag	UNP P87262
o4	118	ALA	-	expression tag	UNP P87262
o4	119	LYS	-	expression tag	UNP P87262
o4	120	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 Unknown protein m2.

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

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

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

- Molecule 83 is a protein called Unknown protein p1.

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

- Molecule 84 is a protein called Unknown protein p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	m6	2	Total 2	Mg 2	0	0
85	n8	5	Total 5	Mg 5	0	0
85	q3	2	Total 2	Mg 2	0	0
85	o1	1	Total 1	Mg 1	0	0
85	N5	1	Total 1	Mg 1	0	0
85	6	145	Total 145	Mg 145	0	0
85	sM	2	Total 2	Mg 2	0	0
85	O4	1	Total 1	Mg 1	0	0
85	m5	3	Total 3	Mg 3	0	0
85	l3	3	Total 3	Mg 3	0	0
85	M1	2	Total 2	Mg 2	0	0
85	n0	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0
85	2	121	Total 121	Mg 121	0	0
85	O3	1	Total 1	Mg 1	0	0
85	S6	1	Total 1	Mg 1	0	0
85	L4	2	Total 2	Mg 2	0	0
85	l7	3	Total 3	Mg 3	0	0
85	M5	1	Total 1	Mg 1	0	0
85	c9	1	Total 1	Mg 1	0	0
85	S2	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L8	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	o4	1	Total 1	Mg 1	0	0
85	M9	2	Total 2	Mg 2	0	0
85	q0	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	3	Total 3	Mg 3	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	497	Total 497	Mg 497	0	0
85	L5	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	1	471	Total 471	Mg 471	0	0
85	s2	1	Total 1	Mg 1	0	0
85	D0	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	2	Total 2	Mg 2	0	0
85	d3	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	M3	3	Total 3	Mg 3	0	0

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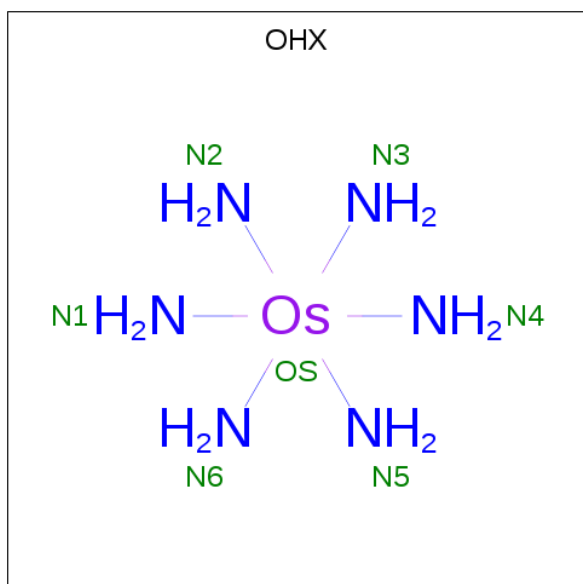
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N3	3	Total 3	Mg 3	0	0
85	4	23	Total 23	Mg 23	0	0
85	n6	1	Total 1	Mg 1	0	0
85	S4	1	Total 1	Mg 1	0	0
85	L2	2	Total 2	Mg 2	0	0
85	m1	1	Total 1	Mg 1	0	0
85	l5	2	Total 2	Mg 2	0	0
85	m7	5	Total 5	Mg 5	0	0
85	M7	4	Total 4	Mg 4	0	0
85	m4	1	Total 1	Mg 1	0	0
85	N8	3	Total 3	Mg 3	0	0
85	s1	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	l8	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	16	Total 16	Mg 16	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	3	Total 3	Mg 3	0	0
85	s4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N6	1	Total	Mg	0	0
			1	1		
85	8	15	Total	Mg	0	0
			15	15		
85	14	1	Total	Mg	0	0
			1	1		
85	M6	1	Total	Mg	0	0
			1	1		
85	N0	1	Total	Mg	0	0
			1	1		
85	3	13	Total	Mg	0	0
			13	13		

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



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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	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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86	1	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
			7	6	1		
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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86	1	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L4	1	Total	N	Os	0	0
			7	6	1		
86	M0	1	Total	N	Os	0	0
			7	6	1		
86	M5	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M9	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	N9	1	Total	N	Os	0	0
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86	O1	1	Total	N	Os	0	0
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86	O2	1	Total	N	Os	0	0
			7	6	1		
86	O3	1	Total	N	Os	0	0
			7	6	1		
86	O7	1	Total	N	Os	0	0
			7	6	1		
86	O7	1	Total	N	Os	0	0
			7	6	1		
86	Q2	1	Total	N	Os	0	0
			7	6	1		
86	6	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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86	6	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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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
86	6	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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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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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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			7	6	1		
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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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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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	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	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	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	m8	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q1	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).

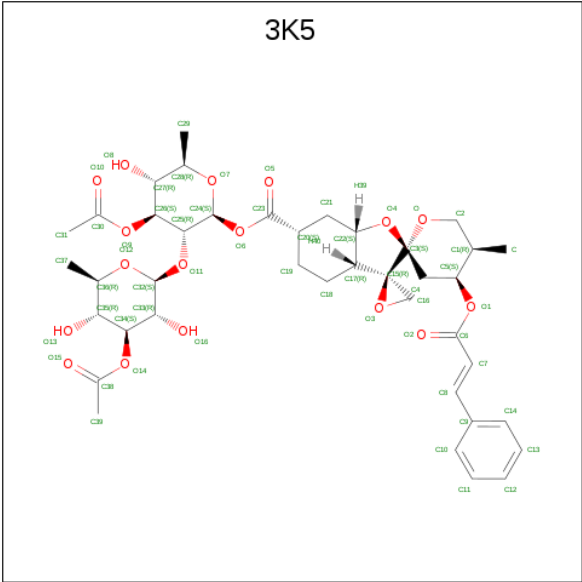
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		

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

- Molecule 88 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O-  
 {[ (2R,2'S,3a'R,4'S,5''R,6'S,7a'S)-5''-methyl-4''-{[(2E)-3-phenylprop-2-enoyl]oxy}decahy-  
 drodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl]carbonyl}-beta-D-glucopyranose  
 (three-letter code: 3K5) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>17</sub>).



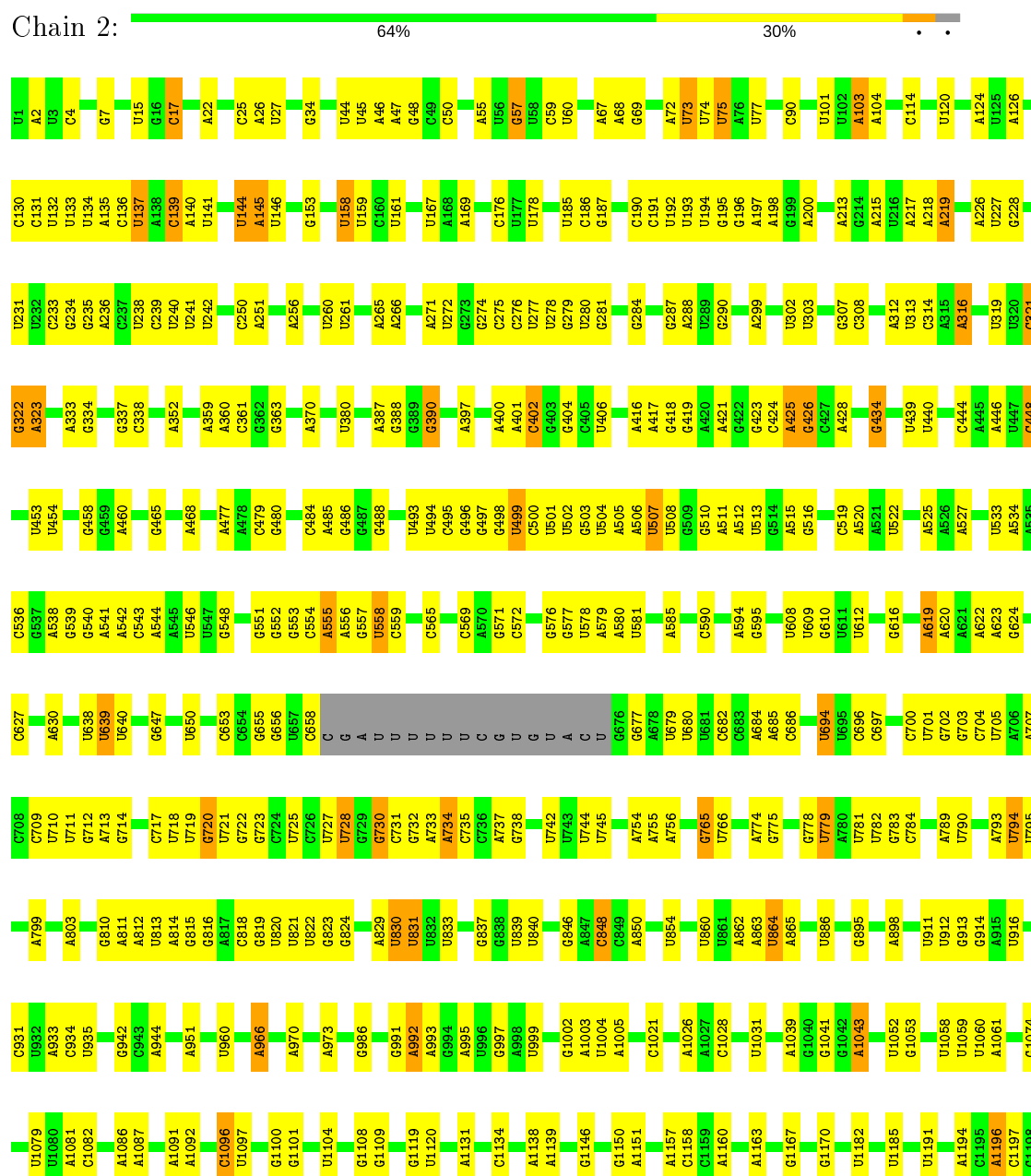
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	C	O	0	0
			57	40	17		
88	5	1	Total	C	O	0	0
			57	40	17		

### 3 Residue-property plots

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

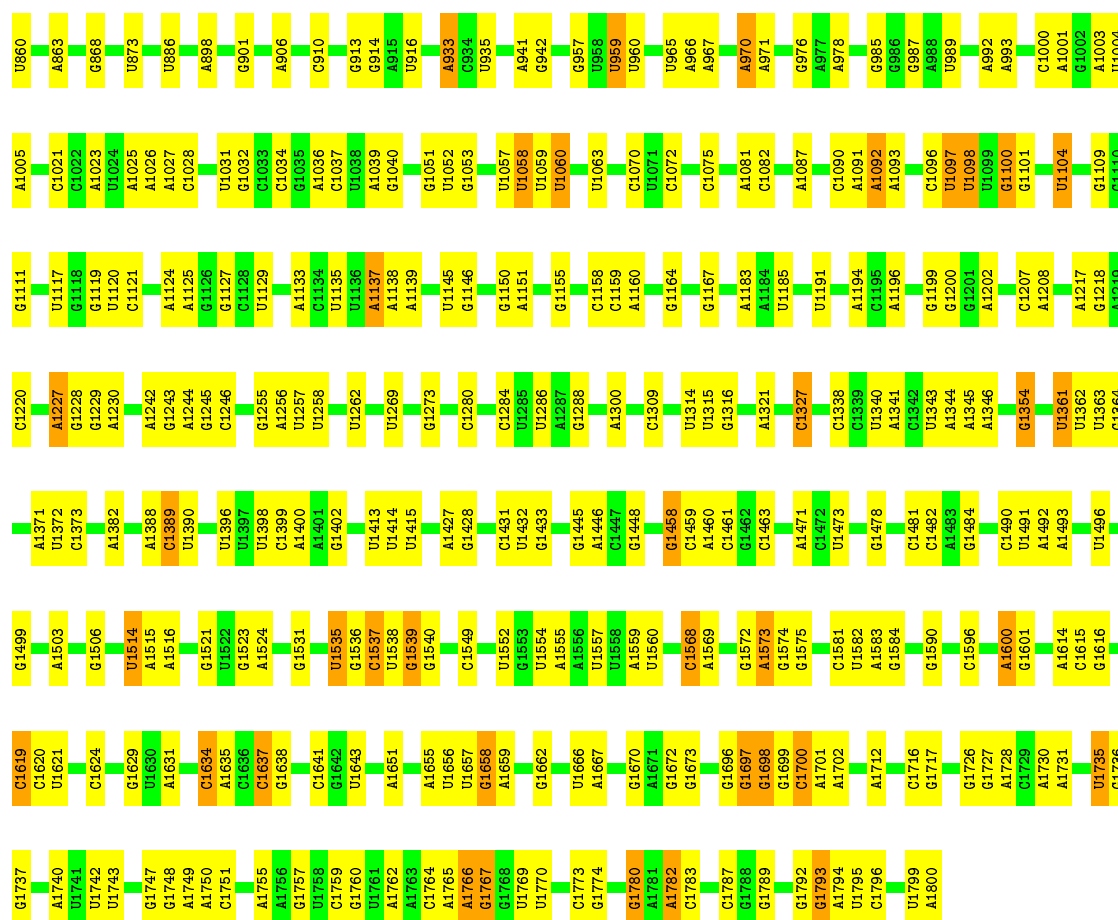
Note EDS failed to run properly.

- Molecule 1: 18S ribosomal RNA



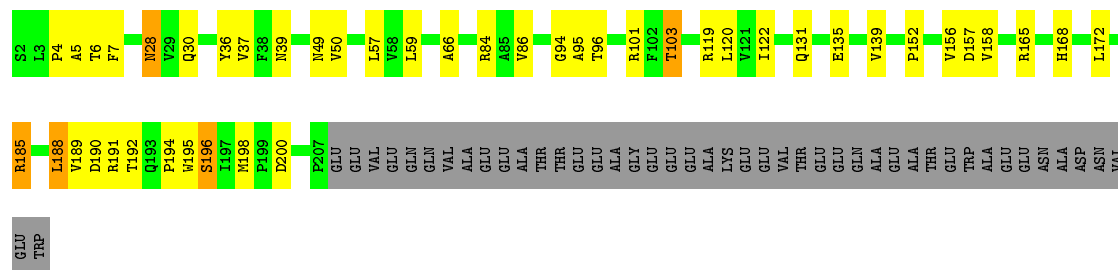




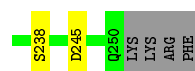


• Molecule 2: 40S ribosomal protein S0-A

Chain S0: 64% 16% 18%

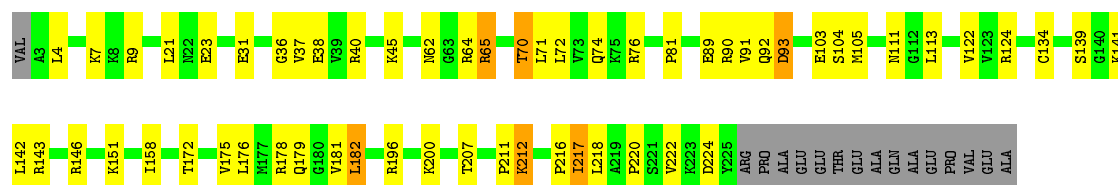


866	867	868	869	870	891	892	893	894	895	896		906	907		911	912	913	914	915	916	917	918	919	920	921		941	946		951	952	953		958	959	960	961		969		973	977	978	979	980	981	982	983	984	985								
ALA	PRO	GLU	ALA	GLN	GLN	GLN	LYS	ARG	GLY	GLY	PHE	GLY	GLY	GLY	ASN	ARG	ARG	GLY	ARG	PRO	ASN	ARG	GLY	PRO	ARG	ARG	ASN	THR	GLU	GLU	LYS	934		141		146		151	152	153		158	159	160	161		169		173	977	978	979	980	981	982	983	984	985



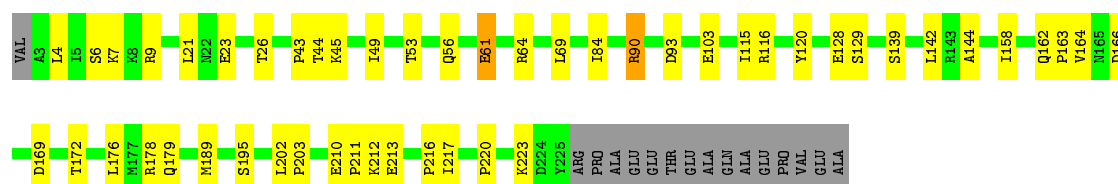
• Molecule 5: 40S ribosomal protein S3

Chain S3: 69% 22% 7%



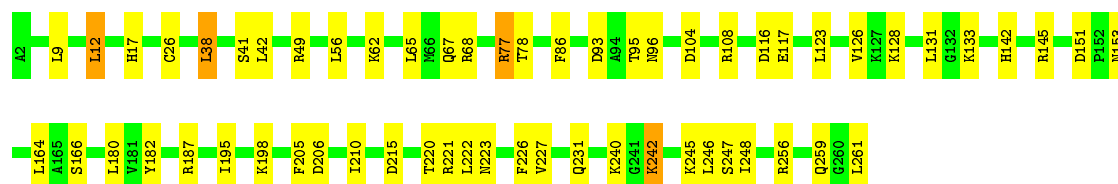
• Molecule 5: 40S ribosomal protein S3

Chain s3: 72% 20% 7%



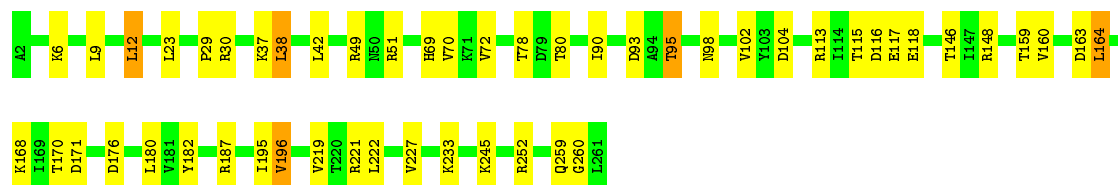
• Molecule 6: 40S ribosomal protein S4-A

Chain S4: 77% 21% 2%



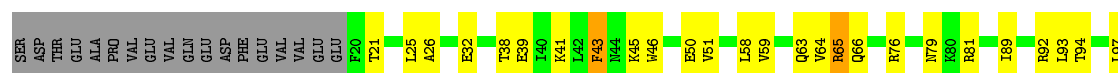
• Molecule 6: 40S ribosomal protein S4-A

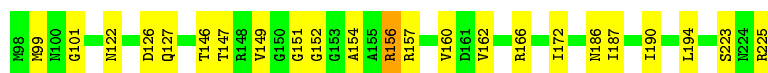
Chain s4: 80% 18% 2%



• Molecule 7: 40S ribosomal protein S5

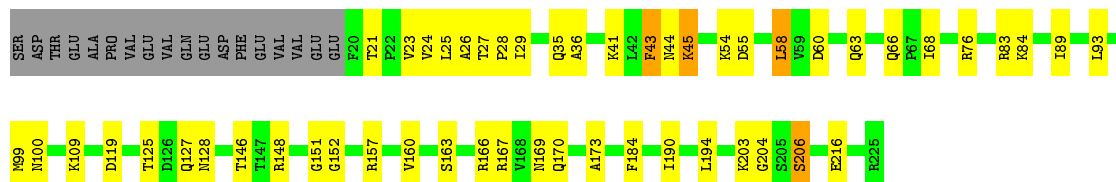
Chain S5: 70% 21% 8%





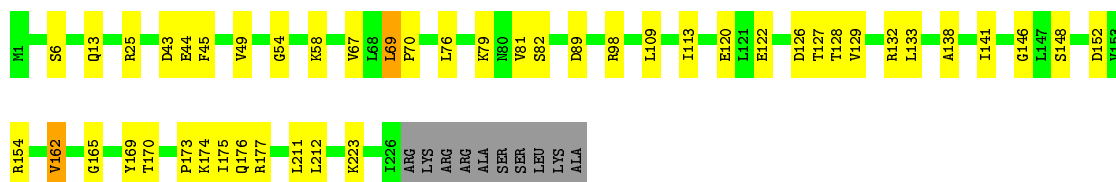
• Molecule 7: 40S ribosomal protein S5

Chain s5: 69% 21% 8%



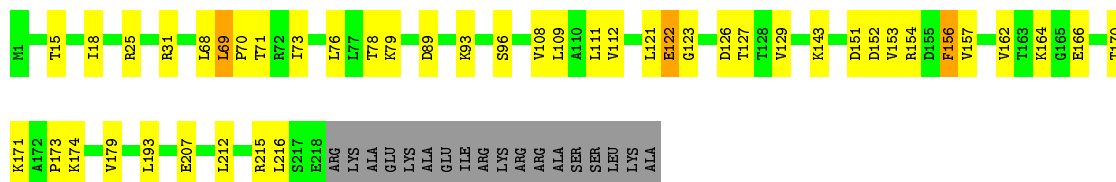
• Molecule 8: 40S ribosomal protein S6-A

Chain S6: 76% 19%



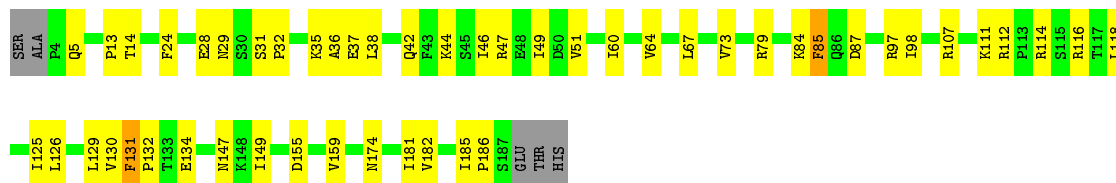
• Molecule 8: 40S ribosomal protein S6-A

Chain s6: 73% 18% 8%



• Molecule 9: 40S ribosomal protein S7-A

Chain S7: 71% 25%



• Molecule 9: 40S ribosomal protein S7-A

Chain s7: 78% 18%





- Molecule 10: 40S ribosomal protein S8-A

Chain S8: 78% 15% 6%



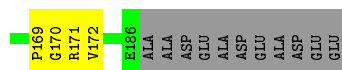
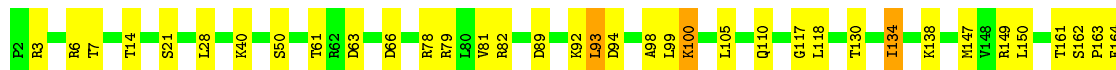
- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 74% 20% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain S9: 74% 19% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 73% 20% 6%

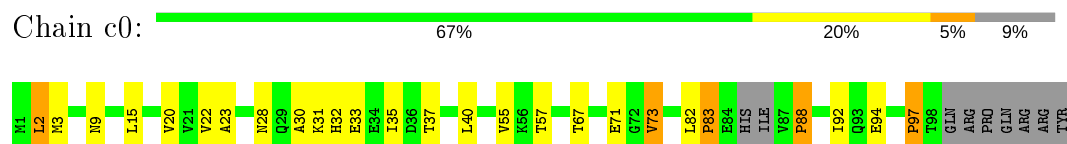


- Molecule 12: 40S ribosomal protein S10-A

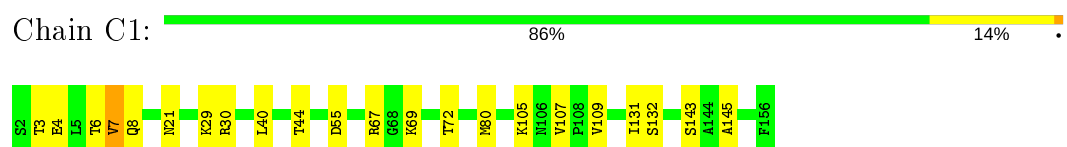
Chain C0: 74% 14% 9%



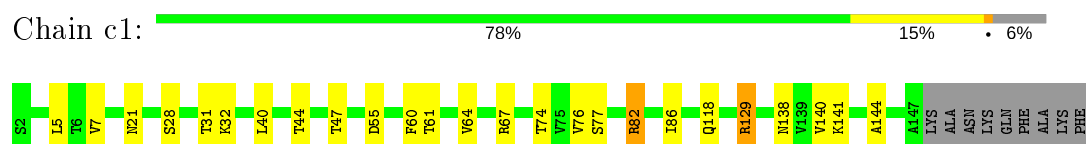
- Molecule 12: 40S ribosomal protein S10-A



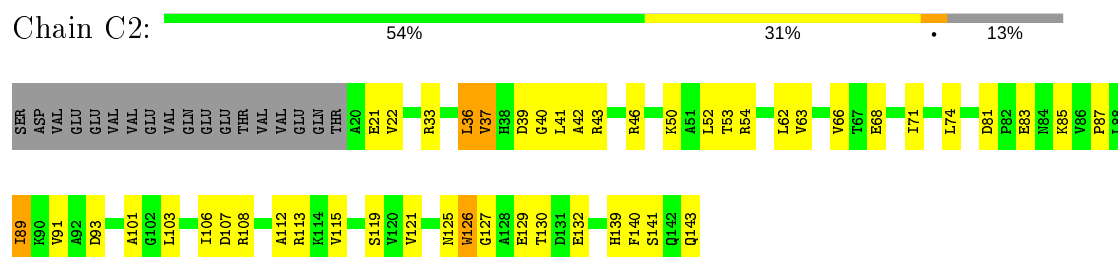
- Molecule 13: 40S ribosomal protein S11-A



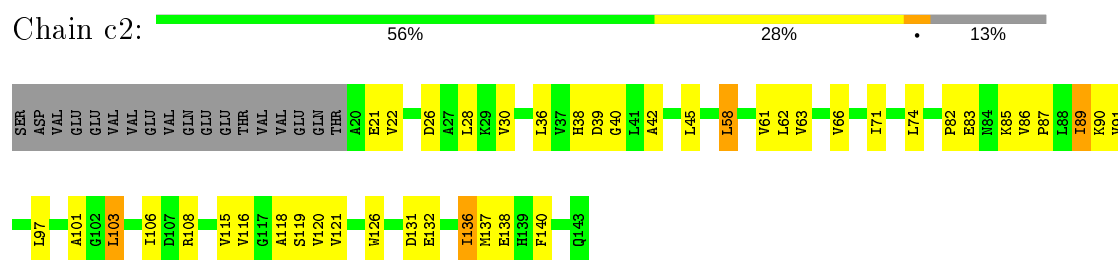
- Molecule 13: 40S ribosomal protein S11-A



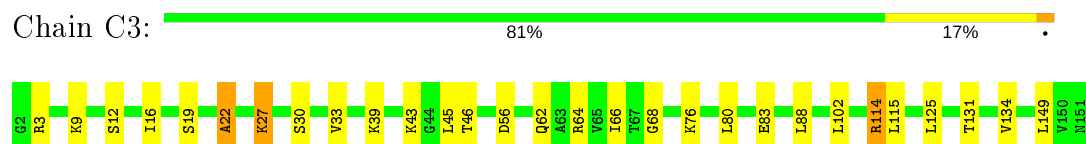
- Molecule 14: 40S ribosomal protein S12



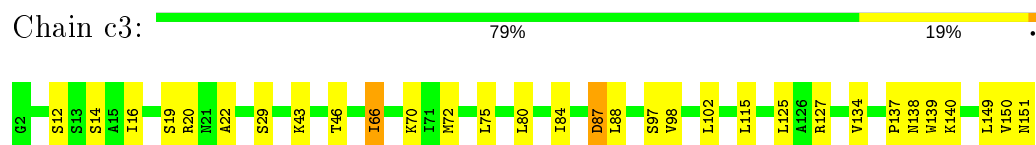
- Molecule 14: 40S ribosomal protein S12



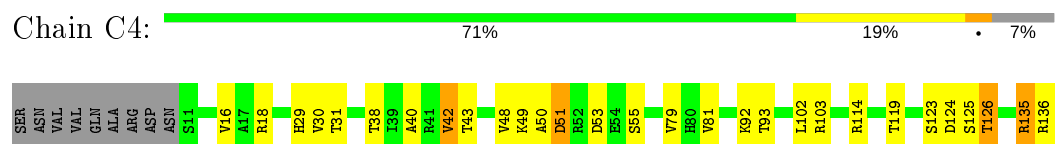
- Molecule 15: 40S ribosomal protein S13



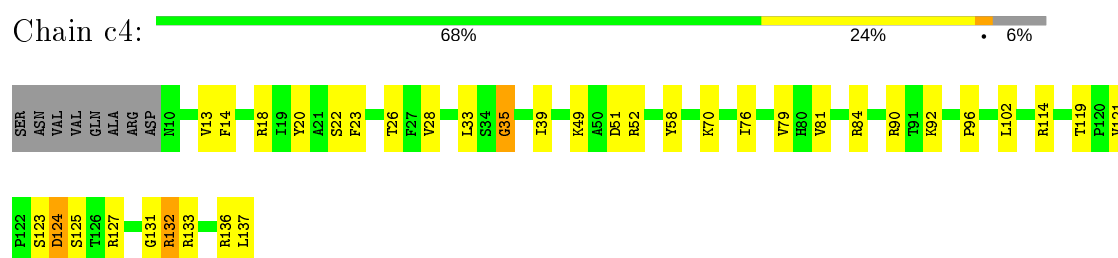
- Molecule 15: 40S ribosomal protein S13



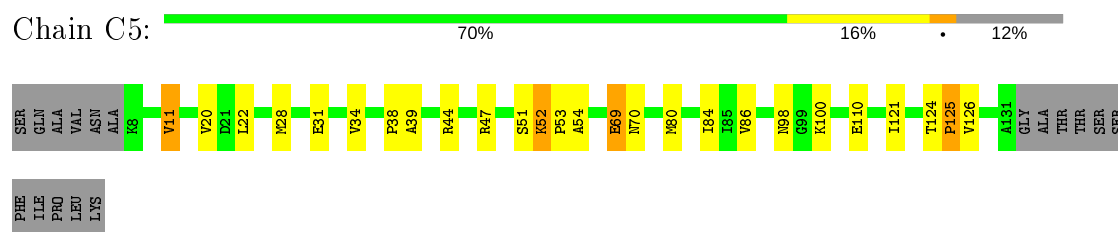
- Molecule 16: 40S ribosomal protein S14-A



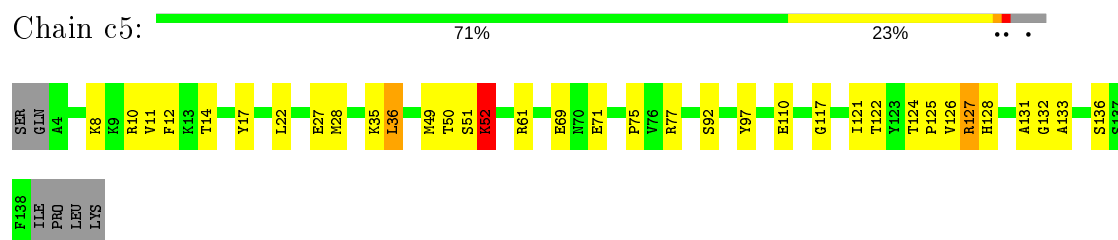
- Molecule 16: 40S ribosomal protein S14-A



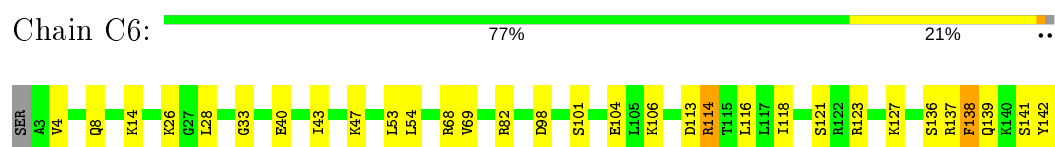
- Molecule 17: 40S ribosomal protein S15



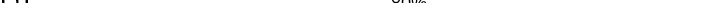
- Molecule 17: 40S ribosomal protein S15

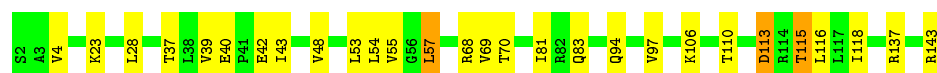


- Molecule 18: 40S ribosomal protein S16-A



- Molecule 18: 40S ribosomal protein S16-A

Chain c6:  80% 18% .



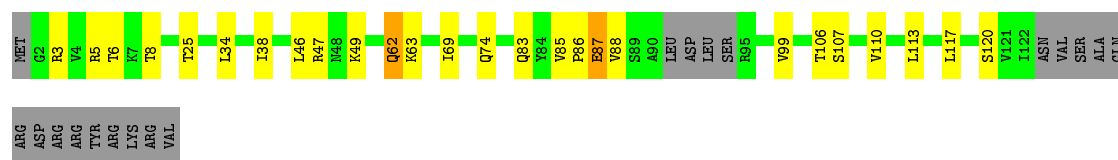
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:  66% 19% 0% 12%




- Molecule 19: 40S ribosomal protein S17-A

Chain c7:  67% 18% 14%



- Molecule 20: 40S ribosomal protein S18-A

Chain C8:  79% 19%



- Molecule 20: 40S ribosomal protein S18-A

Chain c8:  73% 25%




- Molecule 21: 40S ribosomal protein S19-A

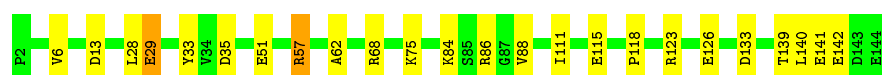
Chain C9:  80% 17% 3%



- Molecule 21: 40S ribosomal protein S19-A

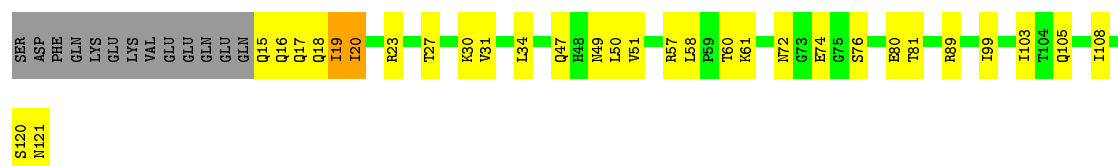


Chain c9:  83% 15% •



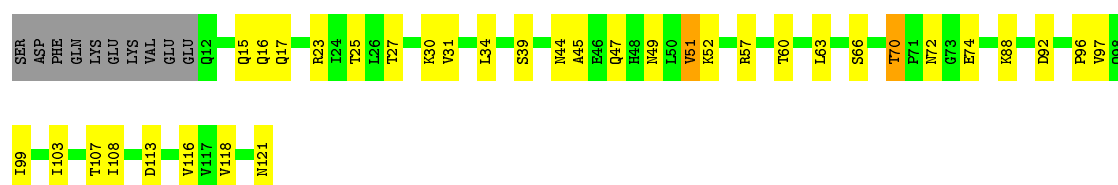
- Molecule 22: 40S ribosomal protein S20

Chain D0:  63% 24% • 11%




- Molecule 22: 40S ribosomal protein S20

Chain d0:  63% 28% • 8%



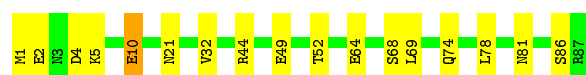
- Molecule 23: 40S ribosomal protein S21-A

Chain D1:  80% 17% •




- Molecule 23: 40S ribosomal protein S21-A

Chain d1:  80% 18% •



- Molecule 24: 40S ribosomal protein S22-A

Chain D2:  83% 14% •

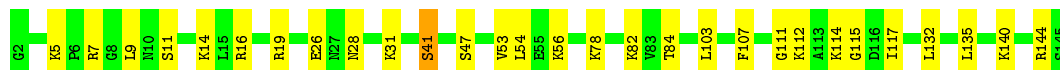
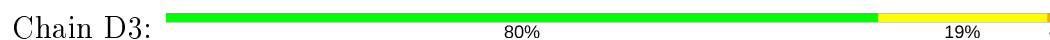


- Molecule 24: 40S ribosomal protein S22-A

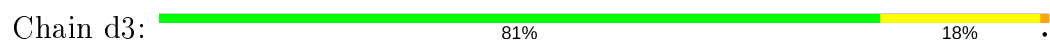
Chain d2:  87% 11% •



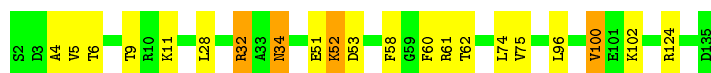
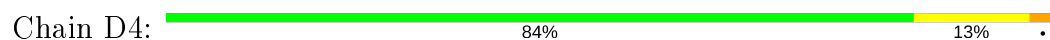
- Molecule 25: 40S ribosomal protein S23-A



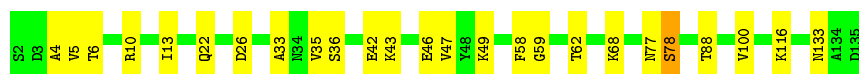
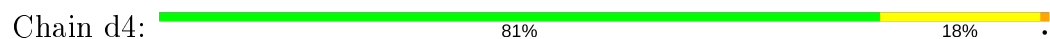
- Molecule 25: 40S ribosomal protein S23-A



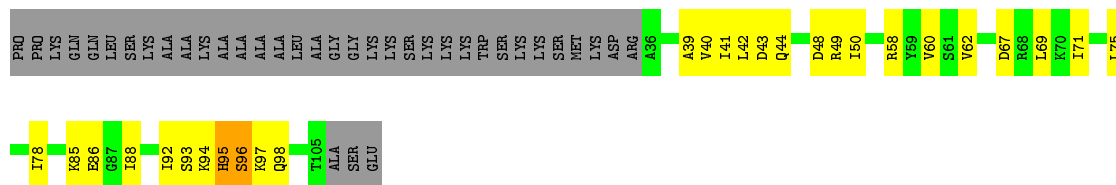
- Molecule 26: 40S ribosomal protein S24-A



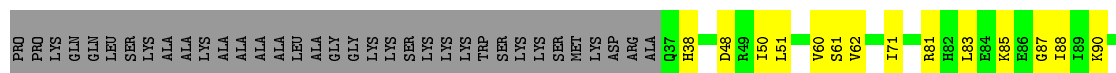
- Molecule 26: 40S ribosomal protein S24-A



- Molecule 27: 40S ribosomal protein S25-A



- Molecule 27: 40S ribosomal protein S25-A





- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 67% 27% 6%



- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 71% 29%



- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 81% 16% •



- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 83% 15% •



- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 70% 23% • 5%



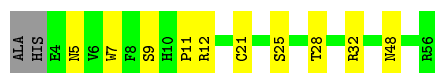
- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 76% 17% • 5%



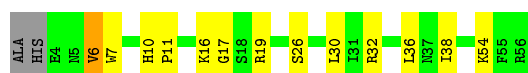
- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 78% 18% •



- Molecule 31: 40S ribosomal protein S29-A

Chain d9: 73% 22%



- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 77% 22%



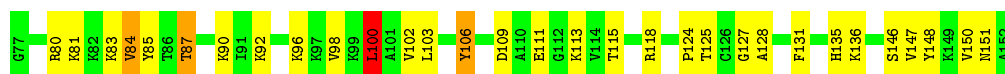
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 51% 36% 7% 7%



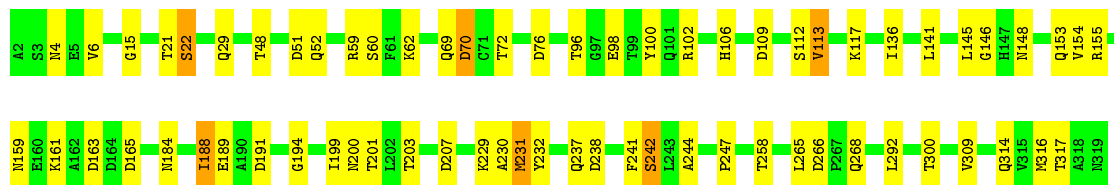
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 59% 36%



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

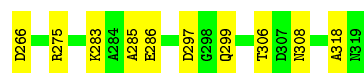
Chain SR: 79% 19%



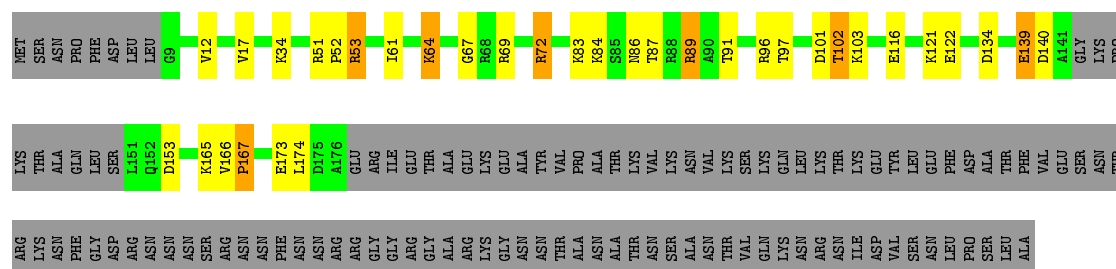
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR: 87% 13%

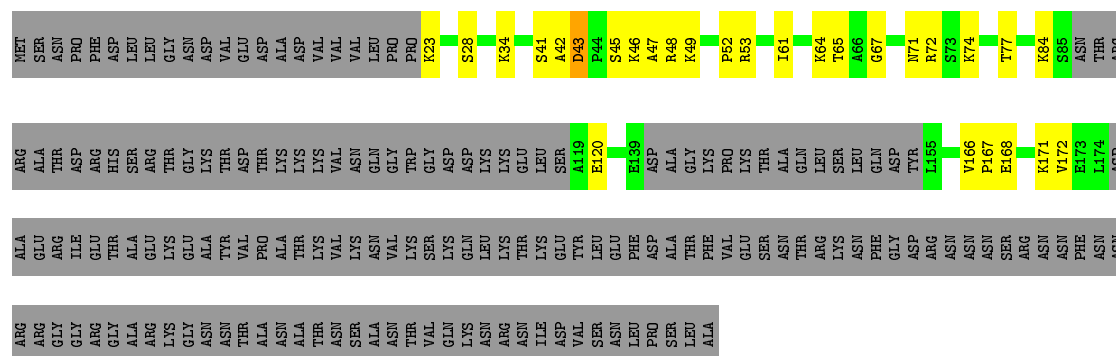




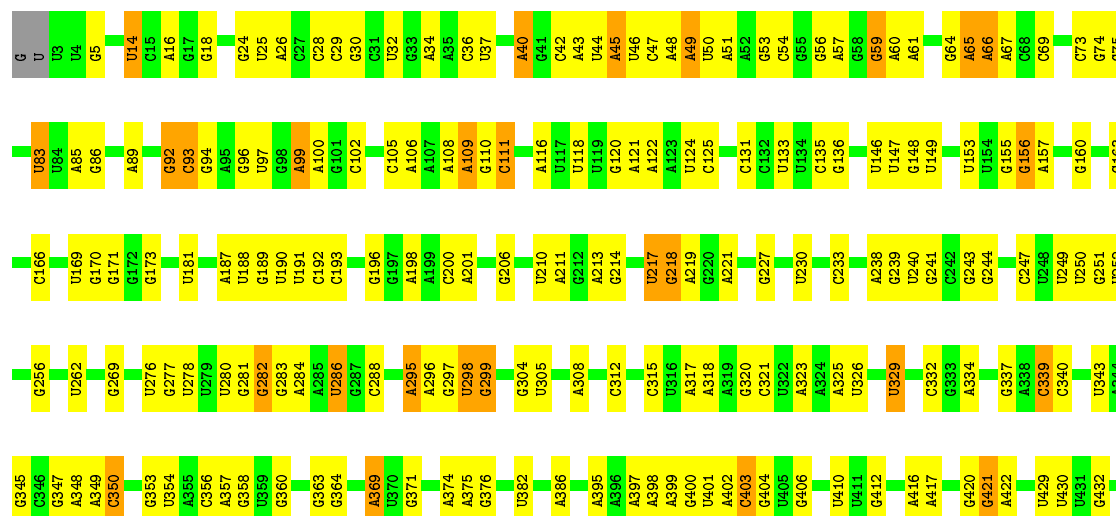
- Molecule 35: Suppressor protein STM1



- Molecule 35: Suppressor protein STM1



- Molecule 36: 25S ribosomal RNA



A1589	A1503	G1417	U1351	A1278	U1191	U1124	A1036	U954	A884	U797	G685	G610	C435
A1593	A1506	A1418	A1352	C1279	C1192	U1124	C1037	U955	U885	G798	A691	A611	A438
G1604	G1507	A1419	U1353	C1280	A1193	G1127	U1041	U956	C886	G799	A692	U612	C439
A1605	G1421	G1420	G1354	G1285	G1194	A1128	U1042	C957	C887	G800	A693	G613	A440
U1606	G1422	G1421	U1355	A1286	C1196	A1129	C1043	C958	C890	A801	C694	U614	U
	U1425	U1422	G1356	A1287	A1197	A1130	U1044	U960	C893	C802		G615	G
C1609		A1428	C1360	C1292	C1198	G1131	A1045	C961	C894	C803	A697	G616	G
C1615	G1513	A1429	C1364	U1293	C1199	C1132	A1046	C962	C894	C804	U698	G617	G
U1616	G1514	A1430	C1365	A1294	A1200	A1133	A1047	G963	C895	A806	U699	C618	U
G1617	A1515	U1430	G1365	C1295	C1201	G1134	A1048	G964	A895	A807	C700	A619	G
	C1516	G1431	A1366	G1296	A1202	A1135	C1049	A965	A896	A808	G701	U620	U
U1620		C1432	G1367	C1297	A1205	A1136	U1050	U966	U897	G809	C702	A621	U
U1629	U1526	A1433	U1368	C1298		C1137	U1051	A967	G900	A810		U622	U
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A1643	U1530	G1371	G1377	U1305	U1211	C1141	A1054	A970	A906	G813	U707	G633	G
	A1535			G1306	A1217	G1142	U1058	A971	G907		A708	C634	C
G1655	G1547	U1438	G1378	U1308	G1222	U1143	U1061	A972	G908	A816	A709	G635	C
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C1657	C1551	U1440	G1376	G1307	A1217		U1058	A973	U907	U819	A711	C637	U
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C1660	U1555	U1442	G1377	U1309					G909	A820		C639	U
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	A1557	G1444	U1378	U1309	G1226	G1148	A1064	U979	G912	G822	C717	U642	C
A1683	G1560	U1445	G1379	G1312	G1227	G1149	A1065	A980	A913		U718	U643	C
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U1695	C1562	U1447	A1381	U1314	C1232	U1151	C1068	C982	G915			U645	U
	U1564	U1448		U1315	C1233	A1152	C1069	A983	G916	G826		U646	G
G1712	G1565	U1449	U1384	U1316	G1234	A1153	U1069	U984	G917	A830	G725	A645	U
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G1727	G1571	U1453	G1389	G1323	U1241	A1159	G1083	A998	A925		G754	G651	U
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G1733	U1578	U1472	A1393	C1327	G1245	G1163	U1095	A1002	C931	C765	A578		G
G1736	C1579	G1473	G1395	U1328	U1246	A1164	U1096	A1003	U932	U766	G579		G
A1741	U1580	U1474	C1396	C1329	C1248	G1166	G1097	A933	A933	U767		G658	A
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	A1588	U1495	U1415	G1349	A1274	U1189	G1116	G1029	G950	C881	A608		G
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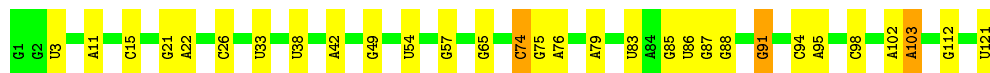


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U	A2133	C	A1841	A1704	G1576	U1495	C1328	C1219	G1147	U1060	U979	G909
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U	C2136	U	G1845	U1721	C1881	C1499	C1333	G1235	G1151	G1072	U985	A914
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G	A2138	G	A1847	U1725	C1883	G1504	G1413	G1236	A1153	A1076	U987	G916
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C	U2142	G	U1853	G1736	A1587	G1508	U1342	U1241	A1159	A1081	U991	A921
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C	A2149	C	G1863	U1765	A1515	G1429	U1353	G1262	G1174	U1094	A1002	U932
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U	G2198	G	G1864	U1822	U1565	C1478	A1398	C1316	C1049	G1140	C1049	C969
U	A2198	U	C1904	U1823	A1566	U1479	U1399	A1317	C1141	C1141	C1141	A970
U	G2199	A	G1905	U1824	U1567	G1480	G1399					
U	C2199	C	G1906	U1825	U1568	U1481	G1400					
U	C2204	A	A1909	U1833	U1570	A1482	U1399					
U	U2205	C	U1910	U1834	U1571	U1483	U1399					
U	G2206	G	A1911	U1837	U1572	U1484	U1400					
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A336	G3247	U3171	A3086	G2990	G2822	G2852	U2771	C2684	G2598	A	G2442	C2366	A2295	U2209
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A3342	U3249	A3173	G3174	G2996	C2928	U2854	C2773	A2686	U2505	U2504	C2444	A2372	U2297	U2211
G3343	G3175	A3174	A3091	U2997	C2929	G2857	U2775	A2689	U2506	U	A	A2374	A2302	A2214
A3344	G3176	C3093	C3092	A2996	A2930	U2858	C2776	G2690	C2507	A	A	G2375	A2303	A2222
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G3348	U3179	G3179	G3179	G2935	U2865	G2865	A2792	C2693	U2510	G	G	C2378	C2308	U2225
G3266	A3180	A3180	G3102	C3004	U2866	U2866	A2792	A2696	G2512	U	U	U2380	A2309	G2231
G3181	A3181	A3181	A3103	A3005	U2867	U2867	G2796	A2697	U2513	G	G	U2381	U2310	C2231
G3182	G3182	G3182	U3104	A3006	G2870	G2870	C2797	A2698	U2514	U	U	U2382	G2234	G2234
A3183	A3183	A3183	U3105	U3007	G2871	G2871	C2798	G2699	A2394	G	A	C2383	G2235	G2235
A3184	A3184	A3184	A3106	A3008	A2872	A2872	A2799	G2700	A2395	G	G	A2394	G2236	G2236
U3185	U3185	U3185	U3107	G3009	G2873	G2873	U2701	U2701	A2396	A	A	A2397	A2317	A2317
U3275	U3275	U3275	C3110	A3012	G2874	G2874	A2801	G2702	G2522	G	G	C2385	A2313	A2313
G3276	G3276	G3276	U3111	U3013	G2875	G2875	A2802	A2703	A2523	A	A	A2386	G2315	G2315
C3278	C3278	C3278	G3112	U3014	G2876	G2876	A2803	A2704	G2524	U	U	A2387	G2316	G2316
A3279	A3279	A3279	G3112	G3018	G2877	G2877	A2804	A2705	G2525	A	A	U2388	A2317	A2317
G3189	G3189	G3189	C3115	G3019	G2878	G2878	A2805	A2706	G2526	A	A	C2389	A2320	A2320
G3190	G3190	G3190	G3115	A3021	G2879	G2879	A2806	A2707	G2530	G	G	C2392	G2323	G2323
U3195	U3195	U3195	C3118	G3026	G2880	G2880	C2809	C2708	C2531	U	U	C2393	A2324	A2324
U3196	U3196	U3196	U3119	A3027	G2881	G2881	C2810	C2709	A2535	G	G	G2394	G2325	G2325
G3197	G3197	G3197	G3120	G3028	U2882	U2882	C2811	C2710	A2536	G	G	G2395	A2326	A2326
G3285	G3285	G3285	U3121	G3029	U2883	U2883	A2813	G2714	G2537	A	A	C2397	U2327	U2327
G3286	G3286	G3286	A3122	A3030	G2884	G2884	G2814	G2715	U2538	G	G	A2398	C2330	C2330
U3287	U3287	U3287	G3123	G3031	U2885	U2885	G2815	G2716	G2539	C	C	A2399	A2255	A2255
G3288	G3288	G3288	A3123	G3032	U2886	U2886	G2816	G2717	C2540	U	U	G2400	A2256	A2256
A3376	A3376	A3376	G3126	A3035	U2887	U2887	G2817	G2718	A2541	U	U	A2401	C2257	C2257
G3377	G3377	G3377	G3126	G3036	U2888	U2888	G2818	G2719	U2543	C	C	A2402	U2258	U2258
C3378	C3378	C3378	A3129	C3039	U2889	U2889	A2819	G2720	G2544	G	G	G2403	U2335	U2335
A3294	A3294	A3294	A3130	A3040	U2890	U2890	A2820	G2721	U2544	G	G	A2404	C2267	C2267
A3295	A3295	A3295	C3132	U3041	C2893	C2893	A2821	G2722	C2545	C	C	C2405	U2268	U2268
U3301	U3301	U3301	G3133	A3046	G2894	G2894	G2822	U2723	G2549	U	U	C2406	U2269	U2269
G3382	G3382	G3382	C3136	U3047	U2895	U2895	G2823	G2724	U2550	C	C	C2407	A2341	A2341
G3383	G3383	G3383	G3137	A3048	U2896	U2896	G2824	G2725	U2551	C	C	U2408	U2342	U2342
U3389	U3389	U3389	C3137	A3049	G2897	G2897	G2825	G2726	G2552	A	A	G2409	C2343	C2343
A3305	A3305	A3305	G3140	U3050	U2898	U2898	G2828	U2727	G2553	U	U	U2410	G2272	G2272
A3306	A3306	A3306	G3141	G3051	U2899	U2899	U2829	U2728	A2554	G	G	U2411	C2273	C2273
A3307	A3307	A3307	A3142	U3052	C2900	C2900	G2830	A2729	G2555	A	A	G2412	C2345	C2345
A3308	A3308	A3308	C3143	U3053	A2971	A2971	G2831	A2730	G2556	U	U	A2413	U2346	U2346
A3309	A3309	A3309	G3150	U3054	C2972	C2972	C2832	C2742	A2562	A	A	G2414	C2347	C2347
A3310	A3310	A3310	A3150	U3055	U2975	U2975	C2836	U2743	G2567	U	U	U2417	A2280	A2280
U3313	U3313	U3313	U3153	U3056	A2976	A2976	A2837	U2744	C2568	A	A	G2418	A2281	A2281
A3314	A3314	A3314	G3154	U3057	G2977	G2977	G2838	G2745	C2569	C	C	A2419	G2282	G2282
G3315	G3315	G3315	U3155	U3058	U2978	U2978	G2839	C2746	U2570	C	C	G2420	C2354	C2354
A3316	A3316	A3316	U3156	G3059	U2979	U2979	C2840	U2747	U2571	A	A	U2421	G2283	G2283
G3317	G3317	G3317	U3157	C3060	U2980	U2980	G2841	U2748	C2572	C	C	C2422	A2355	A2355
A3318	A3318	A3318	G3158	U3068	U2981	U2981	U2842	A2749	G2573	U	U	U2426	U2286	U2286
G3219	G3219	G3219	U3159	G3075	A2982	A2982	U2843	G2750	C2574	C	C	U2427	C2287	C2287
A3223	A3223	A3223	C3164	U3078	U2983	U2983	A2844	U2751	G2574	C	C	G2428	G2357	G2357
G3224	G3224	G3224	A3165	U3079	C2984	C2984	A2845	U2752	G2575	C	C	U2429	C2358	C2358
G3225	G3225	G3225	G3166	U3080	U2985	U2985	G2846	U2753	G2576	U	U	G2430	C2359	C2359
A3226	A3226	A3226	A3167	U3081	U2986	U2986	G2847	U2754	G2577	U	U	U2431	C2360	C2360
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G3229	G3229	G3229	A3245	U3084	U2989	U2989	G2850	U2757	G2580	A	A	U2434	C2361	C2361
G3327	G3327	G3327	G3246	U3085	U2990	U2990	G2851	U2758	G2581	U	U	U2435	A2290	A2290
G3239	G3239	G3239	A3169	U3086	U2991	U2991	G2852	U2759	G2582	U	U	U2436	C2362	C2362
A3330	A3330	A3330	G3169	U3087	U2992	U2992	G2853	U2760	G2583	U	U	U2437	A2291	A2291
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G3242	G3242	G3242	G3171	U3089	U2994	U2994	G2855	U2762	G2585	U	U	U2439	G2292	G2292
A3243	A3243	A3243	U3172	U3090	U2995	U2995	G2856	U2763	G2586	U	U	U2440	C2364	C2364
A3244	A3244	A3244	A3173	U3091	U2996	U2996	G2857	U2764	G2587	A	A	U2441	G2293	G2293
A3245	A3245	A3245	G3174	U3092	U2997	U2997	G2858	U2765	G2588	U	U	U2442	C2365	C2365
G3334	G3334	G3334	U3175	U3093	U2998	U2998	G2859	U2766	G2589	U	U	U2443	U2294	U2294
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G3346	G3346	G3346	G3177	U3095	U3000	U3000	G2861	U2768	G2591	U	U	U2445	U2296	U2296
G3347	G3347	G3347	U3178	U3096	U3001	U3001	G2862	U2769	G2592	U	U	U2446	U2297	U2297
G3348	G3348	G3348	U3179	U3097	U3002	U3002	G2863	U2770	G2593	U	U	U2447	U2298	U2298
G3349	G3349	G3349	U3180	U3098	U3003	U3003	G2864	U2771	G2594	U	U	U2448	U2299	U2299
G3350	G3350	G3350	U3181	U3099	U3004	U3004	G2865	U2772	G2595	U	U	U2449	U2300	U2300
G3351	G3351	G3351	U3182	U3100	U3005	U3005	G2866	U2773	G2596	U	U	U2450	U2301	U2301
G3352	G3352	G3352	U3183	U3101	U3006	U3006	G2867	U2774	G2597	U	U	U2451	U2302	U2302
G3353	G3353	G3353	U3184	U3102	U3007	U3007	G2868	U2775	G2598	U	U	U2452	U2303	U2303
G3354	G3354	G3354	U3185	U3103	U3008	U3008	G2869	U2776	G2599	U	U	U2453	U2304	U2304
G3355	G3355	G3355	U3186	U3104	U3009	U3009	G2870	U2777	G2600	U	U	U2454	U2305	U2305
G3356	G3356	G3356	U3187	U3105	U3010	U3010	G2871	U2778	G2601	U	U	U2455	U2306	U2306
A3357	A3357	A3357	U3188	U3106	U3011	U3011	G2872	U2779	G2602	U	U	U2456	U2307	U2307
U3358	U3358	U3358	U3189	U3107	U3012	U3012	G2873	U2780	G2603	U	U	U2457	U2308	U2308
G3359	G3359	G3359	U3190	U3108	U3013	U3013	G2874	U2781	G2604	U	U	U2458	U2309	U2309
A3362	A3362	A3362	U3191	U3109	U3014	U3014	G2875	U2782	G2605	U	U	U2459	U2310	U2310
U3363	U3363	U3363	U3192	U3110	U3015	U3015	G2876	U2783	G2606	U	U	U2460	U2311	U2311
U3364	U3364	U3364	U3193	U3111	U3016	U3016	G2877	U2784	G2607	U	U	U2461	U2312	U2312
U3365	U3365	U3365	U3194	U3112	U3017	U3017	G2878	U2785	G2608	U	U	U2462	U2313	U2313
U3366	U3366	U3366	U3195	U3113	U3018	U3018	G2879	U2786	G2609	U	U	U2463	U2314	U2314
U3367	U3367	U3367	U3196	U3114	U3019	U3019	G2880	U2787	G2610	U	U	U2464	U2315	U2315
U3368	U3368	U3368	U3197	U3115	U3020	U3020	G2881	U2788	G2611	U	U	U2465	U2316	U2316
G3369	G3369	G3369	U3198	U3116	U3021	U3021	G2882	U2789	G2612	U	U	U2466	U2317	U2317
G3370	G3370	G3370	U3199	U3117	U3022	U3022	G2883	U2790	G2613	U	U	U2467	U2318	U2318
A3372	A3372	A3												

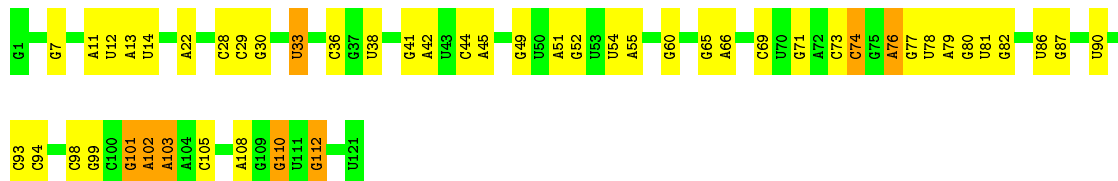
- Molecule 37: 5S ribosomal RNA

Chain 3:  75% 22%



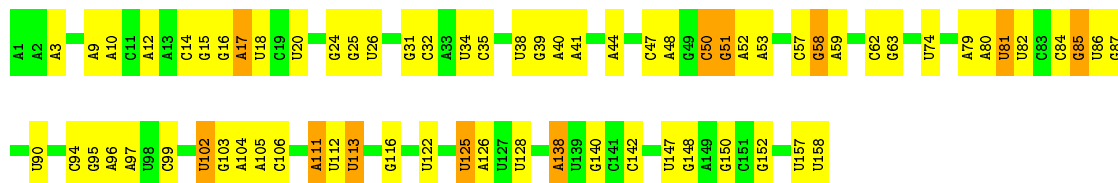
- Molecule 37: 5S ribosomal RNA

Chain 7:  60% 34% 7%



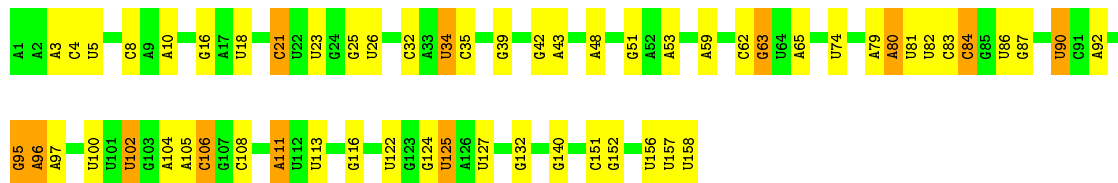
- Molecule 38: 5.8S ribosomal RNA

Chain 4:  56% 37% 7%




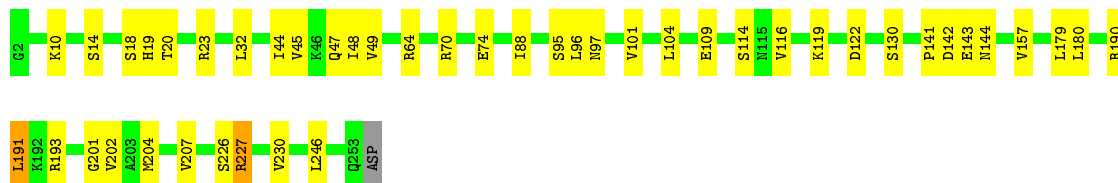
- Molecule 38: 5.8S ribosomal RNA

Chain 8:  63% 29% 8%




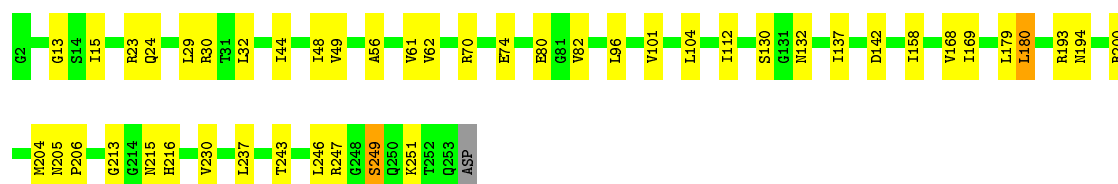
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:  82% 17%



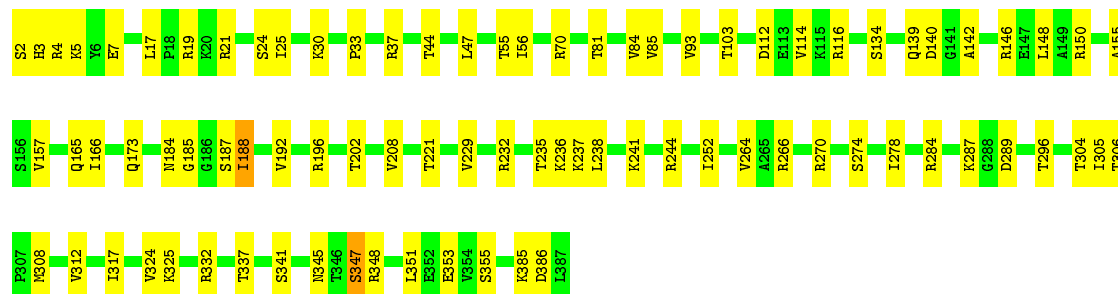
- Molecule 39: 60S ribosomal protein L2-A

Chain l2:  81% 17%



- Molecule 40: 60S ribosomal protein L3

Chain L3: 78% 21% .



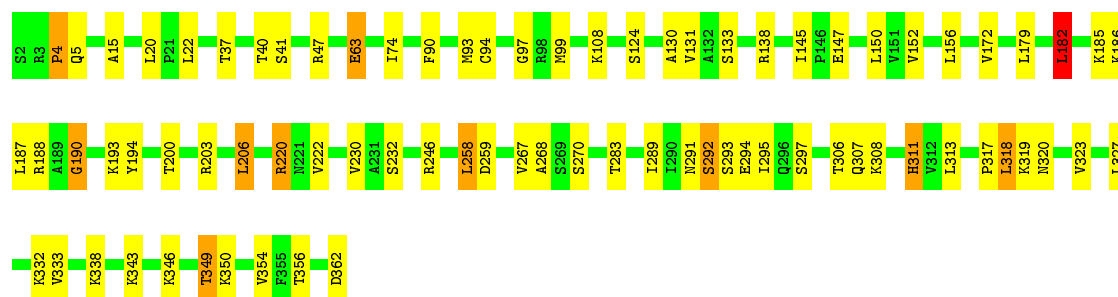
- Molecule 40: 60S ribosomal protein L3

Chain l3: 79% 20% .



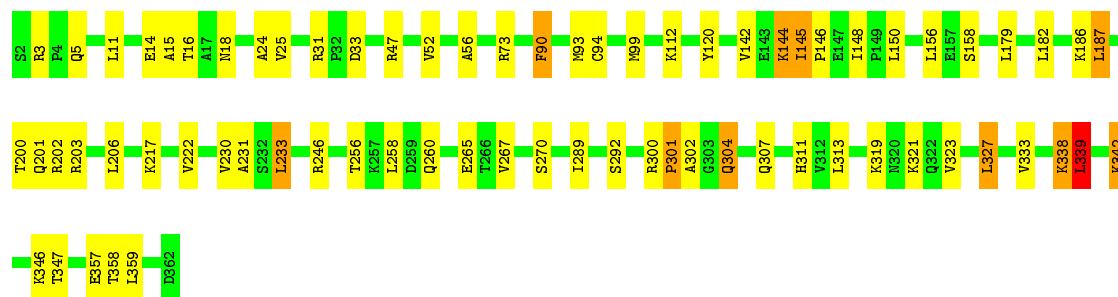
- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 78% 19% .



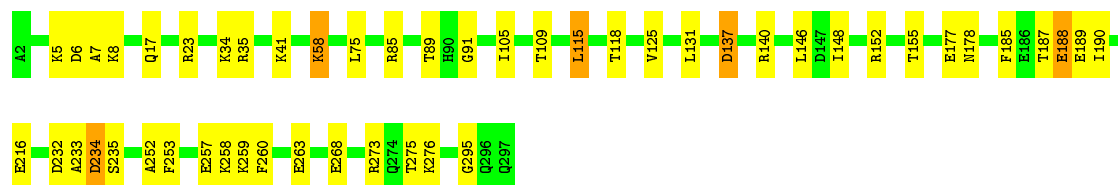
- Molecule 41: 60S ribosomal protein L4-A

Chain l4: 80% 17% .



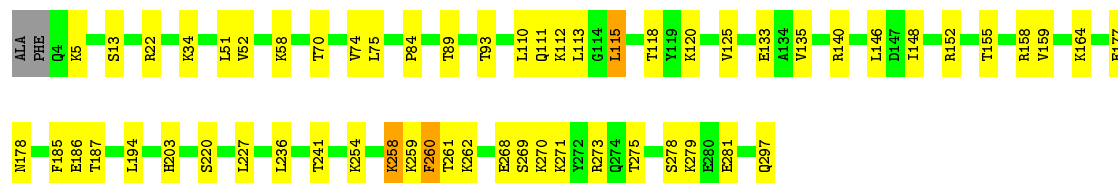
- Molecule 42: 60S ribosomal protein L5

Chain L5: 83% 15% .



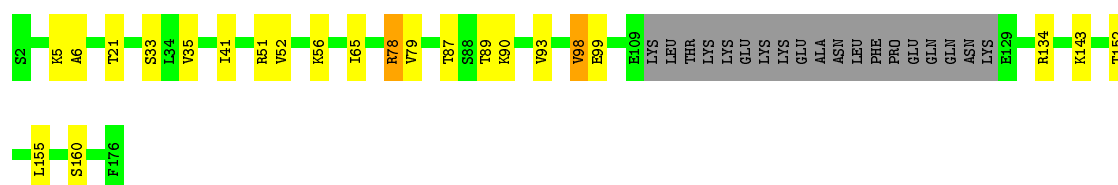
- Molecule 42: 60S ribosomal protein L5

Chain L5: 80% 19% ..



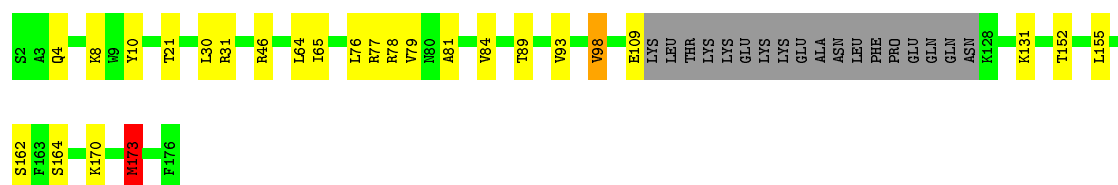
- Molecule 43: 60S ribosomal protein L6-A

Chain L6: 76% 12% . 11%




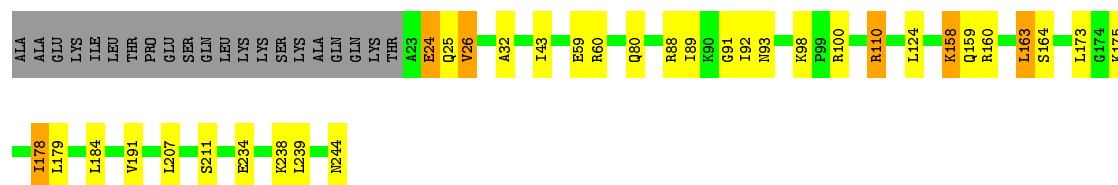
- Molecule 43: 60S ribosomal protein L6-A

Chain L6: 75% 14% .. 10%




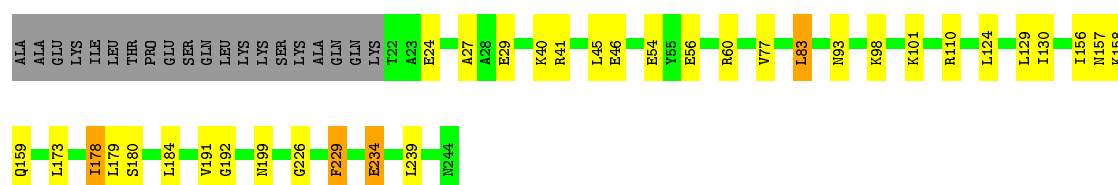
- Molecule 44: 60S ribosomal protein L7-A

Chain L7:  77% 12% 9%




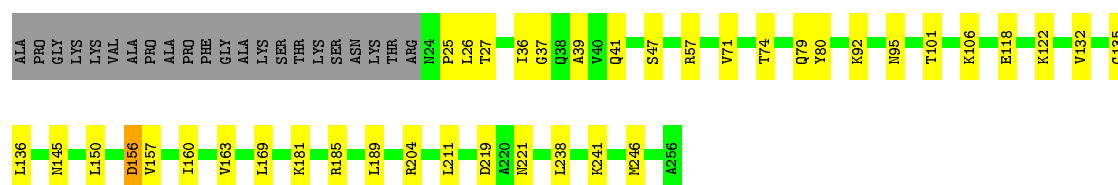
- Molecule 44: 60S ribosomal protein L7-A

Chain l7:  77% 13% 8%



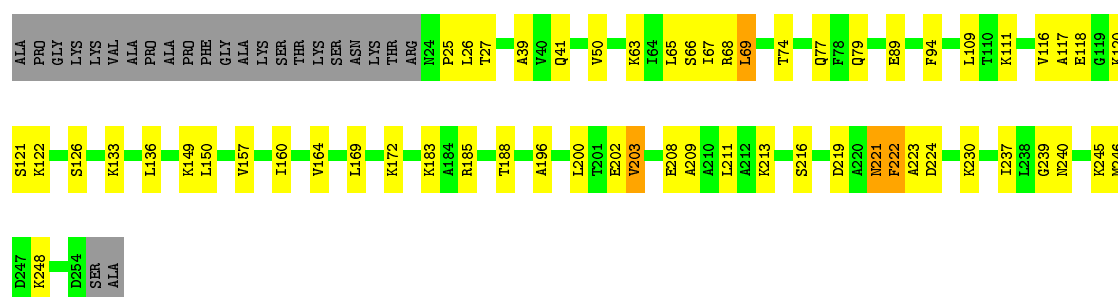
- Molecule 45: 60S ribosomal protein L8-A

Chain L8:  76% 15% 9%




- Molecule 45: 60S ribosomal protein L8-A

Chain l8:  67% 22% 9%



- Molecule 46: 60S ribosomal protein L9-A

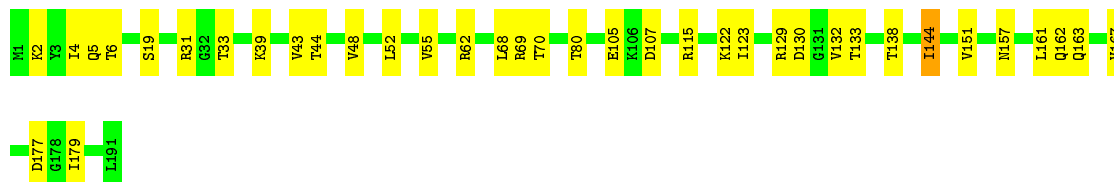
Chain L9:  75% 24%





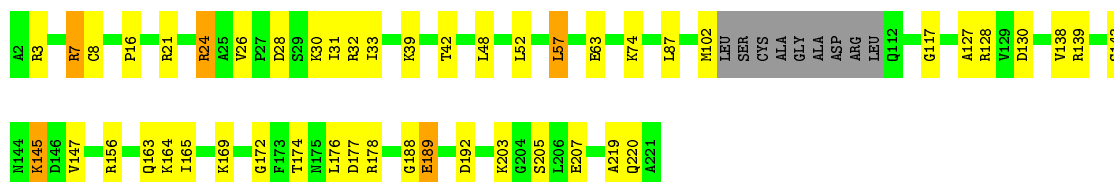
- Molecule 46: 60S ribosomal protein L9-A

Chain l9: 81% 19%



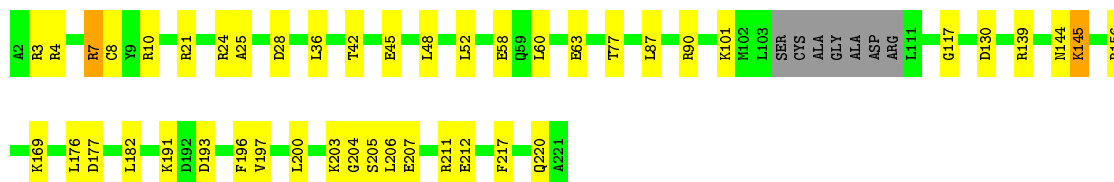
- Molecule 47: 60S ribosomal protein L10

Chain M0: 74% 20%



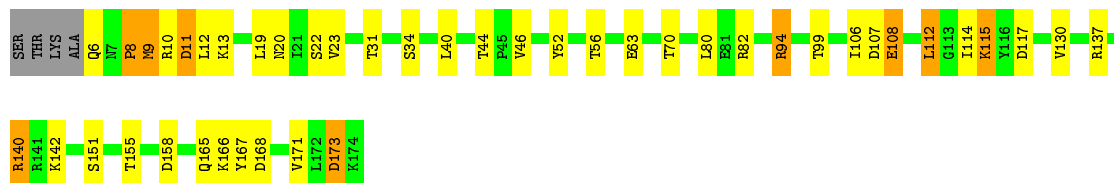
- Molecule 47: 60S ribosomal protein L10

Chain m0: 76% 20%



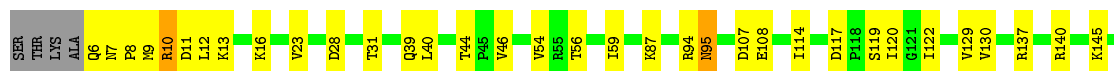
- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 72% 20% 5%



- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 73% 23%





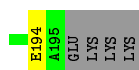
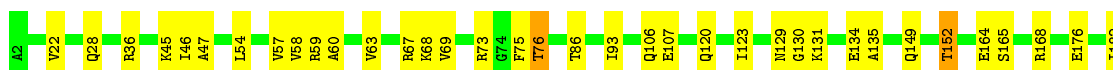
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 78% 18%



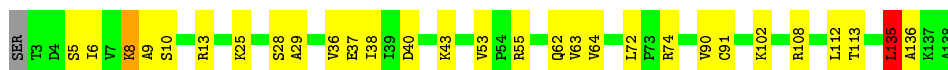
- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 79% 18%



- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 78% 20%



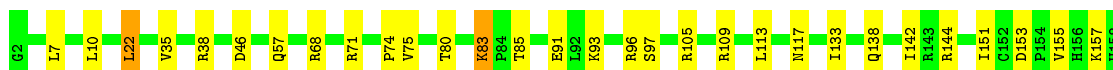
- Molecule 50: 60S ribosomal protein L14-A

Chain m4: 85% 13%



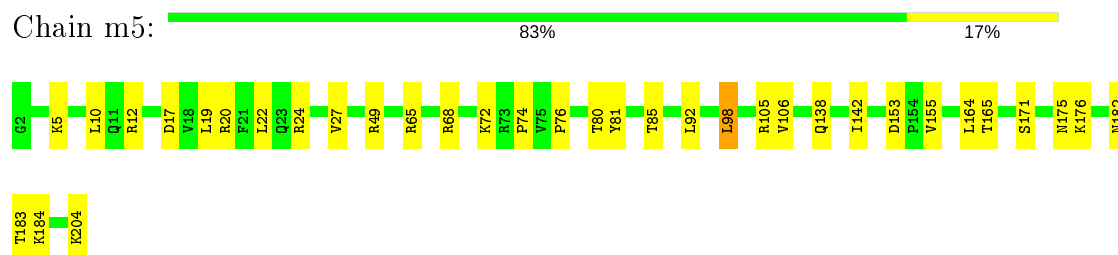
- Molecule 51: 60S ribosomal protein L15-A

Chain M5: 80% 19%

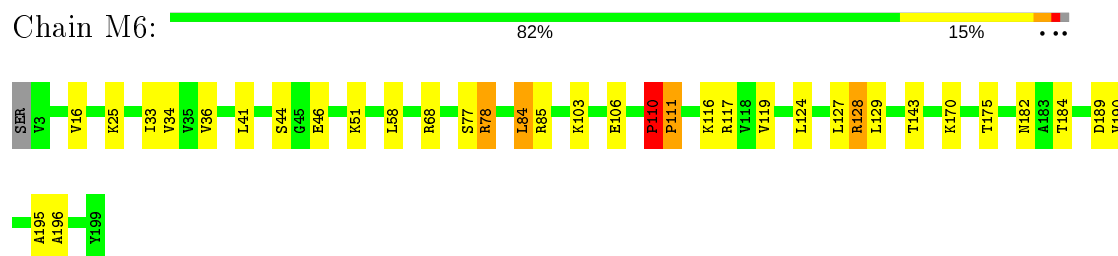


- Molecule 51: 60S ribosomal protein L15-A

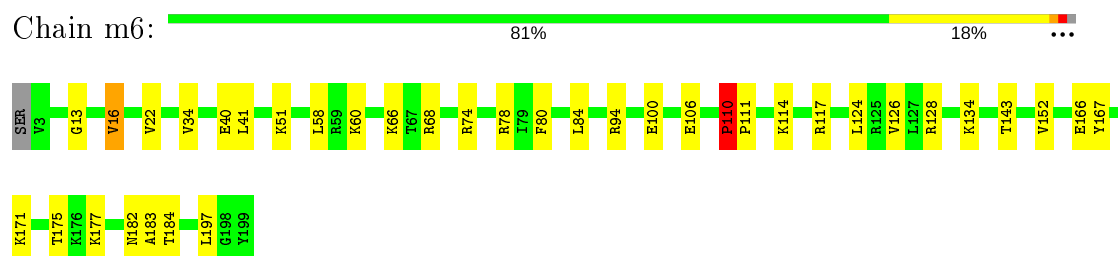




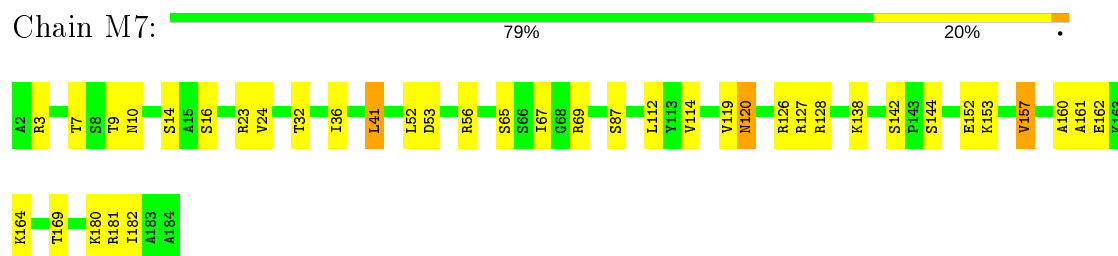
- Molecule 52: 60S ribosomal protein L16-A



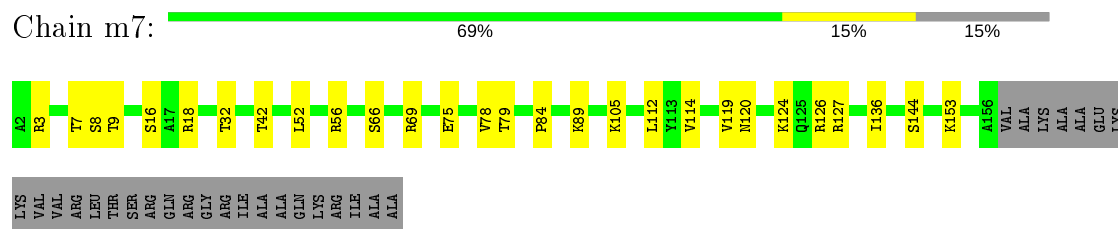
- Molecule 52: 60S ribosomal protein L16-A



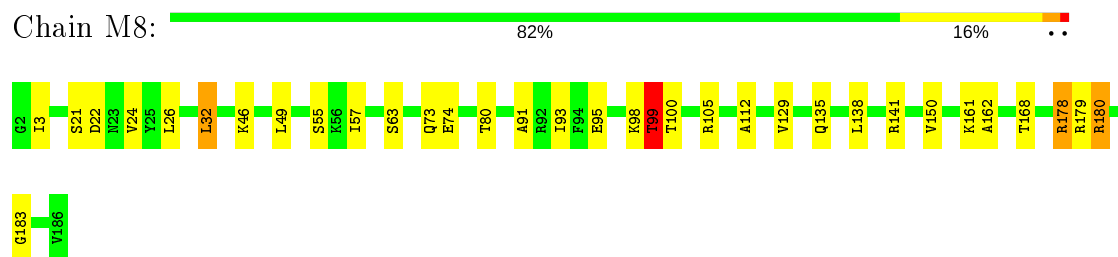
- Molecule 53: 60S ribosomal protein L17-A



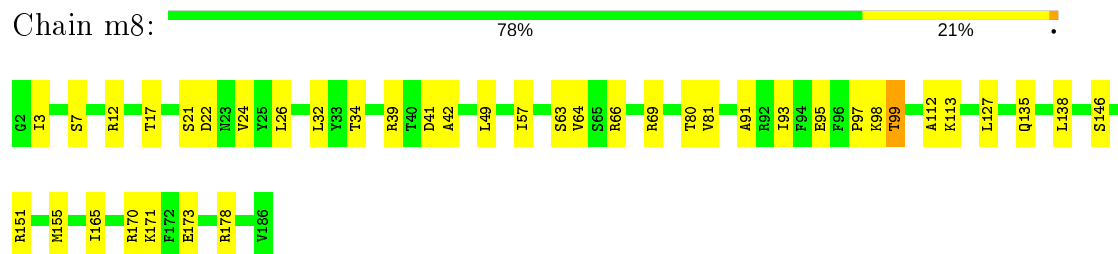
- Molecule 53: 60S ribosomal protein L17-A



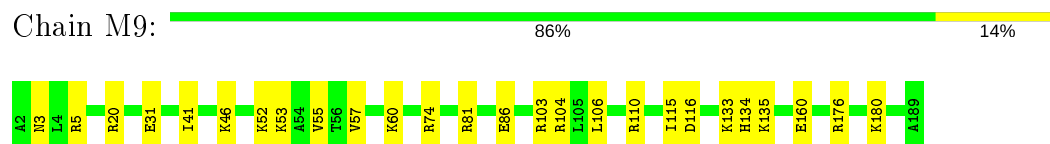
- Molecule 54: 60S ribosomal protein L18-A



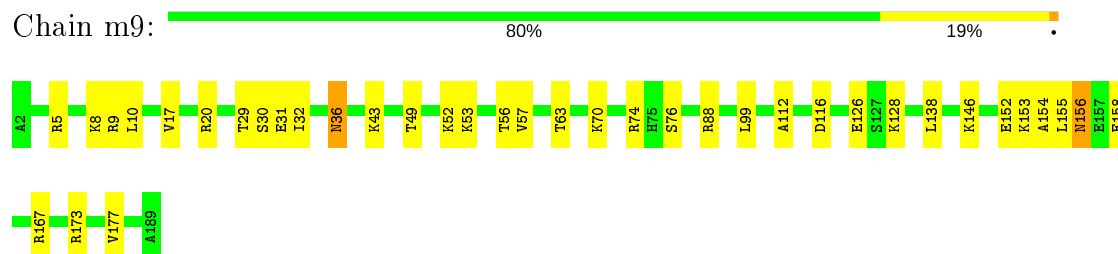
- Molecule 54: 60S ribosomal protein L18-A



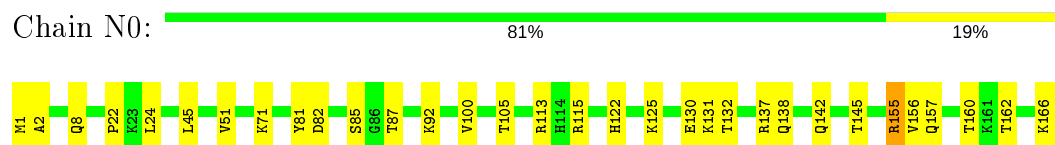
- Molecule 55: 60S ribosomal protein L19-A



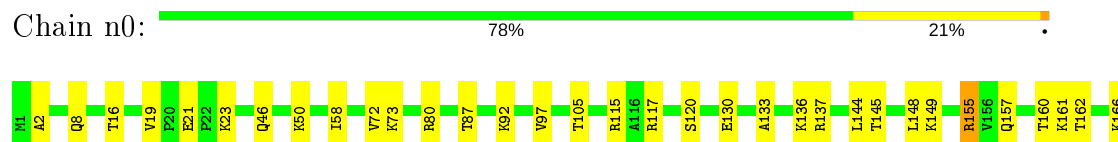
- Molecule 55: 60S ribosomal protein L19-A

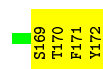


- Molecule 56: 60S ribosomal protein L20-A



- Molecule 56: 60S ribosomal protein L20-A





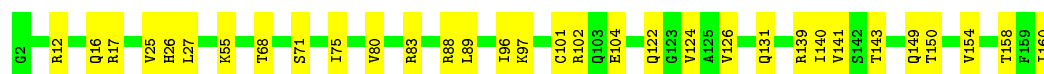
- Molecule 57: 60S ribosomal protein L21-A

Chain N1: 81% 16%



- Molecule 57: 60S ribosomal protein L21-A

Chain n1: 80% 20%



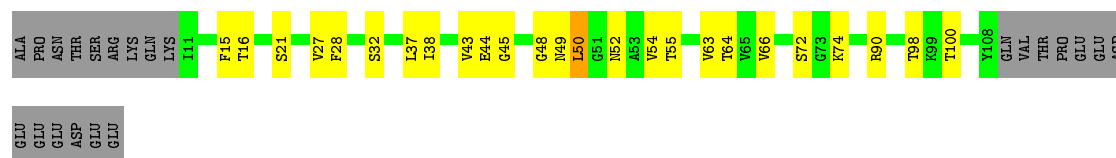
- Molecule 58: 60S ribosomal protein L22-A

Chain N2: 68% 14% 17%



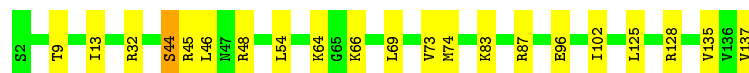
- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 61% 20% 18%



- Molecule 59: 60S ribosomal protein L23-A

Chain N3: 85% 15%



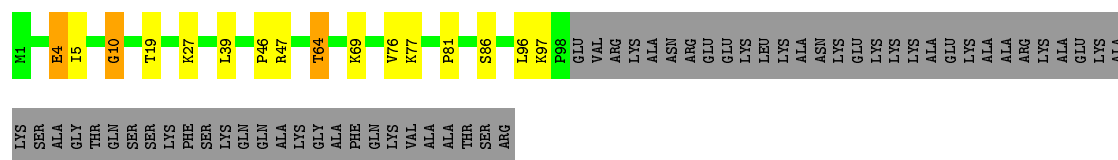
- Molecule 59: 60S ribosomal protein L23-A

Chain n3: 88% 11%



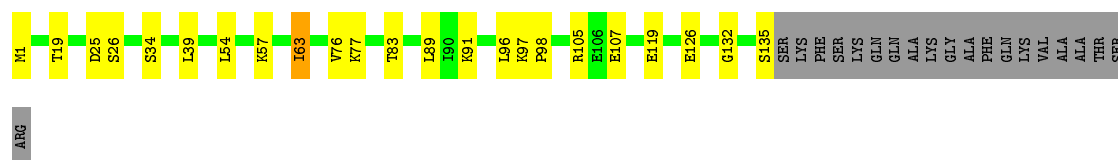
- Molecule 60: 60S ribosomal protein L24-A

Chain N4:  53% 8% 37%



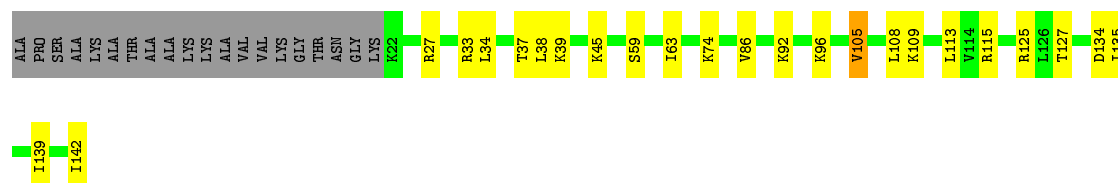
- Molecule 60: 60S ribosomal protein L24-A

Chain n4:  72% 14% • 13%



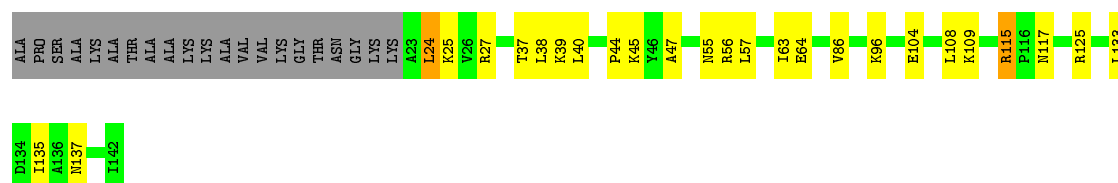
- Molecule 61: 60S ribosomal protein L25

Chain N5:  69% 16% • 14%




- Molecule 61: 60S ribosomal protein L25

Chain n5:  67% 17% • 15%




- Molecule 62: 60S ribosomal protein L26-A

Chain N6:  79% 21%



- Molecule 62: 60S ribosomal protein L26-A

Chain n6:  80% 19% .



- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 79% 20%



- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 78% 17%



- Molecule 64: 60S ribosomal protein L28

Chain N8: 82% 16%



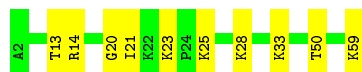
- Molecule 64: 60S ribosomal protein L28

Chain n8: 84% 15%



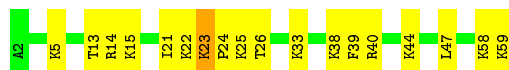
- Molecule 65: 60S ribosomal protein L29

Chain N9: 83% 17%



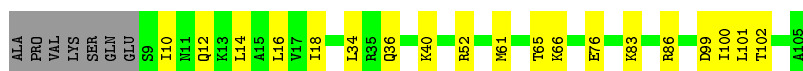
- Molecule 65: 60S ribosomal protein L29

Chain n9: 69% 29%

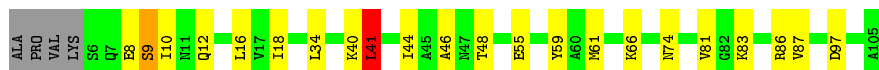


- Molecule 66: 60S ribosomal protein L30

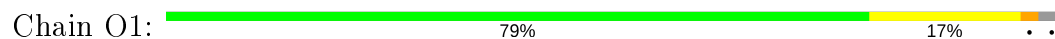
Chain O0: 75% 18% 7%



- Molecule 66: 60S ribosomal protein L30



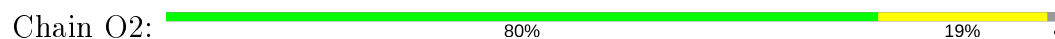
- Molecule 67: 60S ribosomal protein L31-A



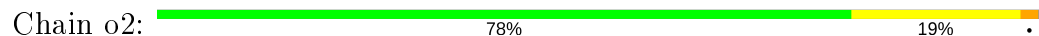
- Molecule 67: 60S ribosomal protein L31-A



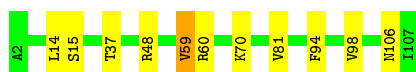
- Molecule 68: 60S ribosomal protein L32



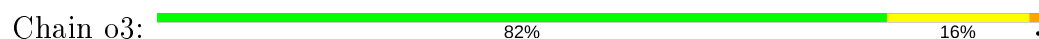
- Molecule 68: 60S ribosomal protein L32

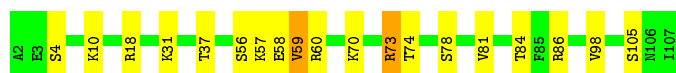


- Molecule 69: 60S ribosomal protein L33-A



- Molecule 69: 60S ribosomal protein L33-A





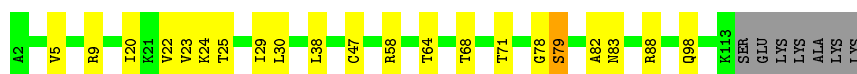
- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 77% 14% 6%



- Molecule 70: 60S ribosomal protein L34-A

Chain o4: 76% 17% 6%



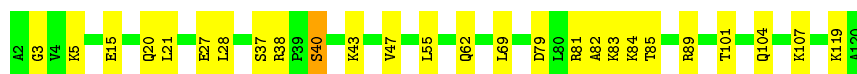
- Molecule 71: 60S ribosomal protein L35-A

Chain O5: 75% 24% 1%



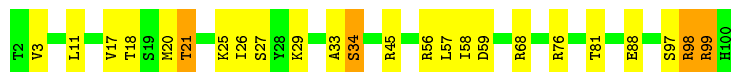
- Molecule 71: 60S ribosomal protein L35-A

Chain o5: 78% 21% 1%



- Molecule 72: 60S ribosomal protein L36-A

Chain O6: 76% 20% 4%



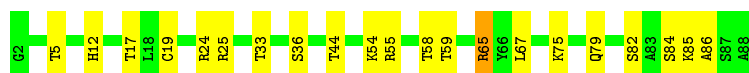
- Molecule 72: 60S ribosomal protein L36-A

Chain o6: 70% 28% 2%



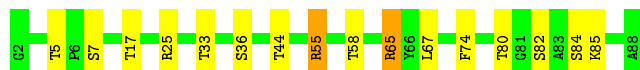
- Molecule 73: 60S ribosomal protein L37-A

Chain O7: 76% 23% 1%



- Molecule 73: 60S ribosomal protein L37-A

Chain o7: 82% 16%



- Molecule 74: 60S ribosomal protein L38

Chain O8: 73% 27%



- Molecule 74: 60S ribosomal protein L38

Chain o8: 77% 23%



- Molecule 75: 60S ribosomal protein L39

Chain O9: 80% 20%



- Molecule 75: 60S ribosomal protein L39

Chain o9: 80% 20%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0: 85% 15%



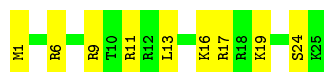
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0: 85% 15%





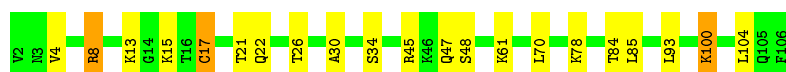
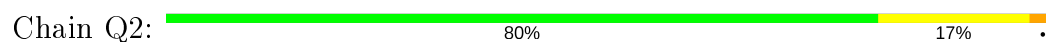
- Molecule 77: 60S ribosomal protein L41-A



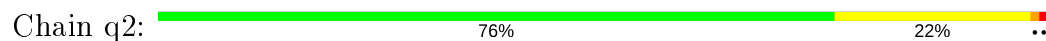
- Molecule 77: 60S ribosomal protein L41-A



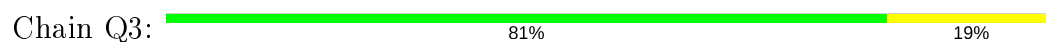
- Molecule 78: 60S ribosomal protein L42-A



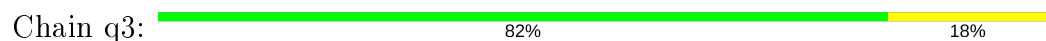
- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A



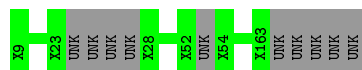
- Molecule 80: 40S ribosomal protein S30-A





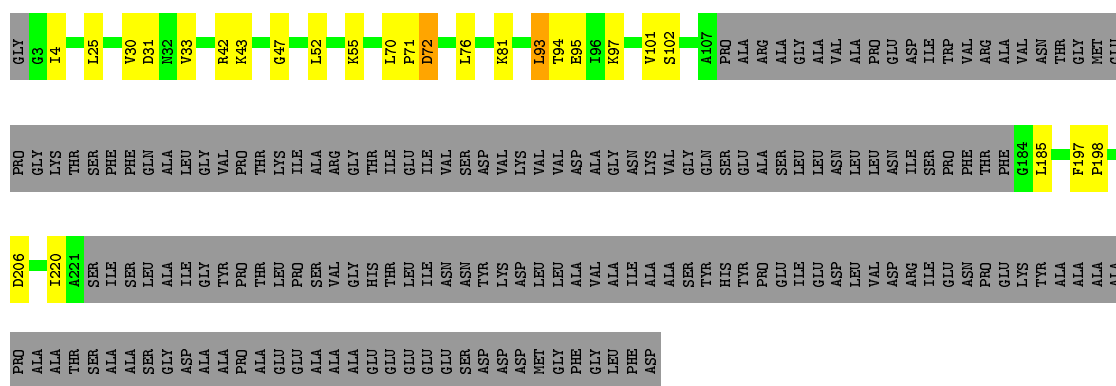
- Molecule 81: Unknown protein m2

Chain m2:  94% 6%



- Molecule 82: 60S acidic ribosomal protein P0

Chain p0:  38% 8% 54%



- Molecule 83: Unknown protein p1

Chain p1:  100%

There are no outlier residues recorded for this chain.

- Molecule 84: Unknown protein p2

Chain p2:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	434.98Å 287.50Å 303.22Å 90.00° 98.85° 90.00°	Depositor
Resolution (Å)	299.60 – 3.10	Depositor
% Data completeness (in resolution range)	100.0 (299.60-3.10)	Depositor
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.202 , 0.252	Depositor
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtriage
Anisotropy	0.178	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411276	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 3K5, ZN, OHX, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	2	0.73	5/41698 (0.0%)	1.28	279/64972 (0.4%)
1	6	0.89	29/42765 (0.1%)	1.39	455/66634 (0.7%)
2	S0	0.48	0/1617	0.67	0/2215
2	s0	0.50	0/1623	0.68	0/2222
3	S1	0.37	0/1735	0.68	1/2335 (0.0%)
3	s1	0.53	0/1748	0.70	0/2352
4	S2	0.51	0/1665	0.66	0/2263
4	s2	0.59	0/1665	0.77	0/2263
5	S3	0.51	0/1759	0.70	1/2368 (0.0%)
5	s3	0.47	0/1759	0.61	0/2368
6	S4	0.50	0/2109	0.72	0/2839
6	s4	0.56	0/2109	0.76	1/2839 (0.0%)
7	S5	0.41	0/1629	0.61	0/2202
7	s5	0.47	0/1629	0.66	0/2202
8	S6	0.49	0/1823	0.67	0/2439
8	s6	0.57	0/1779	0.71	0/2379
9	S7	0.44	0/1506	0.67	0/2028
9	s7	0.49	0/1516	0.72	1/2043 (0.0%)
10	S8	0.56	0/1514	0.74	2/2021 (0.1%)
10	s8	0.65	0/1514	0.78	0/2021
11	S9	0.49	0/1519	0.68	1/2035 (0.0%)
11	s9	0.59	0/1519	0.74	0/2035
12	C0	0.42	0/790	0.64	1/1069 (0.1%)
12	c0	0.40	0/777	0.64	3/1049 (0.3%)
13	C1	0.61	0/1240	0.75	0/1675
13	c1	0.65	0/1194	0.77	0/1610
14	C2	0.38	0/900	0.64	0/1224
14	c2	0.30	0/900	0.59	1/1224 (0.1%)
15	C3	0.51	0/1215	0.72	3/1638 (0.2%)
15	c3	0.60	0/1215	0.73	0/1638
16	C4	0.38	0/901	0.63	0/1217
16	c4	0.54	0/960	0.78	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	C5	0.46	0/998	0.71	0/1341
17	c5	0.52	0/1060	0.69	1/1426 (0.1%)
18	C6	0.46	0/1125	0.67	0/1510
18	c6	0.50	0/1131	0.72	1/1518 (0.1%)
19	C7	0.44	0/935	0.63	0/1254
19	c7	0.50	0/914	0.71	0/1224
20	C8	0.45	0/1211	0.65	1/1628 (0.1%)
20	c8	0.50	0/1211	0.70	1/1628 (0.1%)
21	C9	0.46	0/1130	0.68	1/1517 (0.1%)
21	c9	0.50	0/1130	0.67	1/1517 (0.1%)
22	D0	0.48	0/865	0.66	0/1169
22	d0	0.50	0/892	0.66	0/1205
23	D1	0.45	0/693	0.62	1/935 (0.1%)
23	d1	0.57	0/693	0.73	0/935
24	D2	0.52	0/1038	0.73	1/1395 (0.1%)
24	d2	0.63	0/1038	0.75	1/1395 (0.1%)
25	D3	0.62	0/1139	0.76	1/1518 (0.1%)
25	d3	0.74	0/1139	0.87	3/1518 (0.2%)
26	D4	0.46	0/1087	0.62	0/1449
26	d4	0.57	0/1087	0.74	0/1449
27	D5	0.40	0/571	0.73	1/768 (0.1%)
27	d5	0.41	0/566	0.64	0/761
28	D6	0.47	0/782	0.68	0/1047
28	d6	0.57	0/782	0.70	0/1047
29	D7	0.43	0/620	0.67	0/838
29	d7	0.49	0/620	0.71	0/838
30	D8	0.36	0/499	0.59	0/670
30	d8	0.45	0/499	0.66	0/670
31	D9	0.55	0/452	0.74	0/600
31	d9	0.57	0/452	0.69	0/600
32	E0	0.48	0/483	0.62	0/643
33	E1	0.46	0/577	0.78	0/770
33	e1	0.42	0/619	0.73	1/822 (0.1%)
34	SR	0.41	0/2494	0.64	0/3393
34	sR	0.40	0/2495	0.60	0/3395
35	SM	0.52	0/1113	0.73	2/1502 (0.1%)
35	sM	0.48	0/682	0.68	1/921 (0.1%)
36	1	1.17	163/75394 (0.2%)	1.66	1841/117545 (1.6%)
36	5	1.20	181/75414 (0.2%)	1.67	1895/117575 (1.6%)
37	3	0.96	1/2883 (0.0%)	1.41	24/4491 (0.5%)
37	7	1.17	3/2883 (0.1%)	1.66	57/4491 (1.3%)
38	4	1.15	2/3746 (0.1%)	1.64	82/5832 (1.4%)
38	8	1.04	3/3746 (0.1%)	1.50	53/5832 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	L2	0.74	0/1948	0.86	3/2617 (0.1%)
39	l2	0.74	0/1946	0.89	3/2614 (0.1%)
40	L3	0.72	0/3146	0.81	0/4228
40	l3	0.86	0/3146	0.90	5/4228 (0.1%)
41	L4	0.84	2/2800 (0.1%)	0.95	6/3790 (0.2%)
41	l4	0.75	1/2800 (0.0%)	0.92	6/3790 (0.2%)
42	L5	0.60	0/2425	0.71	1/3271 (0.0%)
42	l5	0.70	0/2408	0.79	1/3248 (0.0%)
43	L6	0.76	0/1260	0.84	1/1694 (0.1%)
43	l6	0.78	0/1269	0.85	3/1705 (0.2%)
44	L7	0.82	0/1821	0.94	3/2451 (0.1%)
44	l7	0.85	1/1828 (0.1%)	0.89	2/2461 (0.1%)
45	L8	0.60	0/1836	0.69	1/2481 (0.0%)
45	l8	0.57	0/1795	0.70	1/2429 (0.0%)
46	L9	0.67	0/1539	0.78	1/2073 (0.0%)
46	l9	0.79	0/1539	0.81	0/2073
47	M0	0.77	2/1741 (0.1%)	0.87	2/2335 (0.1%)
47	m0	0.78	1/1758 (0.1%)	0.87	3/2358 (0.1%)
48	M1	0.55	0/1374	0.74	1/1842 (0.1%)
48	m1	0.65	0/1374	0.78	1/1842 (0.1%)
49	M3	0.77	0/1568	0.88	2/2106 (0.1%)
49	m3	0.67	0/1573	0.79	1/2113 (0.0%)
50	M4	0.72	0/1068	0.80	1/1438 (0.1%)
50	m4	0.85	0/1074	0.87	2/1446 (0.1%)
51	M5	0.80	0/1757	0.87	3/2354 (0.1%)
51	m5	0.69	0/1757	0.82	2/2354 (0.1%)
52	M6	0.85	0/1585	0.91	5/2128 (0.2%)
52	m6	1.03	4/1585 (0.3%)	0.98	3/2128 (0.1%)
53	M7	0.77	0/1443	0.86	2/1944 (0.1%)
53	m7	0.90	0/1250	0.84	0/1683
54	M8	0.79	0/1465	0.90	4/1965 (0.2%)
54	m8	0.76	0/1465	0.91	2/1965 (0.1%)
55	M9	0.55	0/1538	0.69	0/2050
55	m9	0.63	0/1538	0.71	0/2050
56	N0	0.82	0/1481	0.87	0/1990
56	n0	0.88	0/1481	0.88	2/1990 (0.1%)
57	N1	0.77	0/1300	0.84	2/1743 (0.1%)
57	n1	0.83	1/1300 (0.1%)	0.81	0/1743
58	N2	0.48	0/812	0.64	0/1099
58	n2	0.51	0/794	0.69	0/1076
59	N3	0.73	0/1018	0.81	0/1369
59	n3	0.88	0/1018	0.90	3/1369 (0.2%)
60	N4	0.57	0/712	0.71	1/958 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	n4	0.71	0/1052	0.76	0/1398
61	N5	0.64	0/979	0.81	1/1321 (0.1%)
61	n5	0.68	0/974	0.85	1/1314 (0.1%)
62	N6	0.73	0/1004	0.91	0/1341
62	n6	0.68	0/1004	0.84	0/1341
63	N7	0.52	0/1118	0.66	0/1497
63	n7	0.49	0/1118	0.72	3/1497 (0.2%)
64	N8	0.80	0/1204	0.90	2/1612 (0.1%)
64	n8	0.78	0/1204	0.87	0/1612
65	N9	0.72	0/473	0.79	0/629
65	n9	0.80	0/473	0.87	0/629
66	O0	0.50	0/751	0.72	0/1008
66	o0	0.52	0/775	0.68	1/1040 (0.1%)
67	O1	0.63	0/890	0.78	0/1196
67	o1	0.79	0/897	0.89	0/1205
68	O2	0.86	0/1041	0.90	1/1394 (0.1%)
68	o2	0.85	0/1041	0.92	2/1394 (0.1%)
69	O3	0.90	0/868	0.89	0/1168
69	o3	0.92	0/868	0.90	3/1168 (0.3%)
70	O4	0.63	0/890	0.83	2/1189 (0.2%)
70	o4	0.65	0/890	0.83	0/1189
71	O5	0.73	0/978	0.76	1/1301 (0.1%)
71	o5	0.62	0/974	0.74	1/1297 (0.1%)
72	O6	0.67	0/778	0.78	0/1034
72	o6	0.63	0/777	0.71	0/1033
73	O7	0.80	0/696	0.93	2/923 (0.2%)
73	o7	0.77	0/696	0.88	1/923 (0.1%)
74	O8	0.53	0/618	0.64	0/826
74	o8	0.50	0/614	0.66	0/822
75	O9	0.76	0/443	0.98	1/588 (0.2%)
75	o9	0.71	0/443	0.79	0/588
76	Q0	0.71	0/423	0.80	0/562
76	q0	0.94	0/423	0.94	0/562
77	Q1	0.74	0/234	0.89	0/300
77	q1	0.76	0/234	0.94	1/300 (0.3%)
78	Q2	0.89	1/860 (0.1%)	0.88	1/1136 (0.1%)
78	q2	0.80	1/860 (0.1%)	0.82	0/1136
79	Q3	0.76	0/701	0.83	0/934
79	q3	0.75	0/701	0.80	1/934 (0.1%)
80	e0	0.56	0/499	0.81	0/665
82	p0	0.47	0/1091	0.63	0/1472
All	All	0.92	401/430072 (0.1%)	1.31	4824/631360 (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
2	s0	0	1
7	s5	0	2
9	S7	0	1
9	s7	0	1
12	c0	0	1
16	c4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	1
22	d0	0	1
25	D3	0	1
26	d4	0	1
27	D5	0	2
33	E1	0	1
39	L2	0	2
41	L4	0	1
43	L6	0	1
44	l7	0	2
45	l8	0	1
48	M1	0	1
49	M3	0	1
50	M4	0	1
52	M6	0	2
52	m6	0	1
53	M7	0	1
56	n0	0	2
57	N1	0	1
63	N7	0	1
64	N8	0	1
64	n8	0	3
65	N9	0	1
67	O1	0	1
All	All	0	43

All (401) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-12.58	1.27	1.38
78	Q2	17	CYS	CB-SG	11.86	2.02	1.82
36	5	960	U	N1-C2	10.74	1.48	1.38
36	5	2971	A	N9-C4	9.52	1.43	1.37
78	q2	17	CYS	CB-SG	8.98	1.97	1.82
36	5	2358	A	N9-C4	-8.86	1.32	1.37
36	5	1143	A	N3-C4	-8.43	1.29	1.34
36	1	907	G	N7-C5	-8.12	1.34	1.39
36	1	3181	C	N3-C4	-7.89	1.28	1.33
36	5	1152	G	N3-C4	-7.82	1.29	1.35
36	1	1428	A	C5-C6	-7.61	1.34	1.41
1	6	163	G	N9-C4	-7.57	1.31	1.38
1	6	337	G	C2-N3	7.55	1.38	1.32
36	5	63	A	N7-C5	-7.48	1.34	1.39
36	5	1143	A	N9-C4	-7.41	1.33	1.37
36	1	2138	A	N7-C5	-7.37	1.34	1.39
36	1	654	C	N1-C6	-7.33	1.32	1.37
36	5	2943	G	N7-C5	-7.32	1.34	1.39
36	1	34	A	N9-C4	-7.30	1.33	1.37
36	5	2280	A	N9-C4	-7.26	1.33	1.37
36	1	804	C	N1-C6	-7.15	1.32	1.37
36	5	2147	A	C5-C6	-7.10	1.34	1.41
47	M0	8	CYS	CB-SG	-7.03	1.70	1.82
36	1	2714	G	N9-C4	-6.95	1.32	1.38
36	1	1326	A	N9-C4	-6.91	1.33	1.37
36	1	296	A	N9-C4	6.87	1.42	1.37
36	5	2885	C	N1-C6	-6.87	1.33	1.37
36	5	2941	A	N3-C4	-6.84	1.30	1.34
38	8	80	A	N9-C4	6.84	1.42	1.37
1	6	1537	C	N1-C6	6.83	1.41	1.37
36	1	1132	C	N3-C4	-6.82	1.29	1.33
36	5	1332	A	N3-C4	-6.81	1.30	1.34
36	1	2971	A	N9-C4	6.79	1.42	1.37
1	6	119	A	N9-C4	-6.77	1.33	1.37
36	5	875	G	N7-C5	6.75	1.43	1.39
36	1	907	G	N3-C4	6.70	1.40	1.35
36	1	1392	G	C5-C4	-6.70	1.33	1.38
36	5	2726	C	N3-C4	-6.70	1.29	1.33
36	5	3209	A	C5-C4	6.67	1.43	1.38
38	4	15	G	N7-C5	-6.67	1.35	1.39
36	5	40	A	N7-C5	-6.65	1.35	1.39
36	1	716	A	C5-C6	-6.61	1.35	1.41
36	5	3008	A	N9-C4	-6.61	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	642	U	N1-C2	-6.58	1.32	1.38
36	5	1159	A	N7-C5	-6.58	1.35	1.39
36	5	2639	G	N7-C5	-6.58	1.35	1.39
36	5	1152	G	C5-C6	-6.53	1.35	1.42
36	1	49	A	N9-C4	-6.52	1.33	1.37
36	5	3084	C	N1-C6	-6.50	1.33	1.37
36	1	1153	A	N7-C5	-6.50	1.35	1.39
36	1	1103	A	N9-C4	6.46	1.41	1.37
36	1	1371	G	N9-C8	-6.45	1.33	1.37
36	5	2401	A	N7-C5	6.45	1.43	1.39
36	1	1114	U	C2-N3	-6.43	1.33	1.37
36	5	971	G	N7-C5	-6.43	1.35	1.39
41	L4	63	GLU	CG-CD	6.42	1.61	1.51
36	5	1152	G	C8-N7	6.41	1.34	1.30
36	1	1103	A	N3-C4	6.40	1.38	1.34
1	6	1765	A	N9-C4	-6.39	1.34	1.37
36	5	1116	G	C8-N7	6.38	1.34	1.30
36	5	2954	U	N1-C2	6.38	1.44	1.38
36	5	2335	G	C5-C4	-6.38	1.33	1.38
36	5	423	A	N7-C5	-6.37	1.35	1.39
36	5	924	G	N3-C4	-6.37	1.30	1.35
36	5	981	U	N1-C2	6.35	1.44	1.38
36	1	2397	A	C6-N1	6.35	1.40	1.35
36	5	706	A	N9-C4	-6.31	1.34	1.37
1	2	558	U	N1-C2	6.31	1.44	1.38
36	5	2139	A	N3-C4	-6.28	1.31	1.34
36	5	2980	U	C2-O2	-6.27	1.16	1.22
36	5	366	A	C5-C6	-6.26	1.35	1.41
1	6	1655	A	N3-C4	-6.26	1.31	1.34
36	1	3273	A	N3-C4	-6.24	1.31	1.34
36	1	2404	A	N7-C5	6.23	1.43	1.39
52	m6	80	PHE	CB-CG	-6.23	1.40	1.51
36	1	1308	A	N7-C5	-6.21	1.35	1.39
36	1	2404	A	N3-C4	6.20	1.38	1.34
36	5	2386	A	N7-C5	-6.19	1.35	1.39
36	1	2187	G	N7-C5	-6.18	1.35	1.39
36	5	3106	A	N7-C5	-6.18	1.35	1.39
36	1	2983	C	N3-C4	-6.17	1.29	1.33
36	5	1912	U	N1-C2	-6.15	1.33	1.38
36	5	2640	A	N9-C4	-6.15	1.34	1.37
36	5	2996	U	N1-C2	6.13	1.44	1.38
36	1	25	U	C4-O4	6.13	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	1115	G	N3-C4	-6.13	1.31	1.35
36	1	1138	U	C2-N3	-6.12	1.33	1.37
36	5	1159	A	N9-C4	-6.09	1.34	1.37
36	1	2361	A	N9-C4	6.08	1.41	1.37
36	5	2138	A	N7-C5	-6.08	1.35	1.39
36	5	2385	G	N9-C4	-6.07	1.33	1.38
36	1	2355	G	N7-C5	-6.07	1.35	1.39
36	1	1192	C	N1-C2	6.07	1.46	1.40
36	5	883	A	N3-C4	-6.07	1.31	1.34
36	1	1103	A	N7-C5	6.07	1.42	1.39
36	1	1002	A	N9-C4	-6.06	1.34	1.37
36	1	404	G	N7-C5	-6.06	1.35	1.39
36	1	2165	G	N7-C5	-6.05	1.35	1.39
36	5	1149	G	N9-C8	-6.05	1.33	1.37
1	6	65	A	N9-C4	-6.04	1.34	1.37
36	1	317	A	C5-C6	-6.04	1.35	1.41
36	1	1835	A	N9-C4	-6.03	1.34	1.37
1	6	623	A	N9-C4	-6.03	1.34	1.37
36	5	2399	A	N9-C4	-6.01	1.34	1.37
36	1	1143	A	N3-C4	-6.00	1.31	1.34
36	5	2335	G	N1-C2	-5.97	1.32	1.37
36	1	1158	A	N7-C5	-5.97	1.35	1.39
36	5	1847	A	N9-C4	-5.96	1.34	1.37
36	1	1556	C	N1-C2	5.95	1.46	1.40
36	1	1394	A	N9-C4	-5.95	1.34	1.37
36	1	1416	C	N3-C4	-5.94	1.29	1.33
36	1	354	U	C2-N3	-5.93	1.33	1.37
47	m0	8	CYS	CB-SG	-5.92	1.72	1.81
1	6	630	A	C5-C6	-5.92	1.35	1.41
36	1	699	A	N9-C4	-5.91	1.34	1.37
1	6	1748	G	N9-C8	-5.91	1.33	1.37
36	1	884	A	N9-C4	-5.91	1.34	1.37
36	1	1103	A	C6-N1	5.90	1.39	1.35
36	5	647	A	C6-N1	-5.89	1.31	1.35
36	1	716	A	N9-C4	-5.89	1.34	1.37
1	6	1750	A	N9-C4	-5.86	1.34	1.37
36	5	3245	A	C5-C6	-5.86	1.35	1.41
36	5	922	U	C4-O4	-5.85	1.19	1.23
36	5	3172	A	N9-C4	-5.85	1.34	1.37
37	7	76	A	N9-C4	-5.85	1.34	1.37
36	5	3103	A	N3-C4	-5.84	1.31	1.34
1	6	538	A	N9-C4	5.84	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2320	A	N9-C4	-5.83	1.34	1.37
36	1	1328	C	N1-C6	-5.82	1.33	1.37
36	5	3006	A	N3-C4	-5.82	1.31	1.34
36	5	1524	A	N9-C4	-5.82	1.34	1.37
36	5	646	A	C6-N1	-5.81	1.31	1.35
36	5	884	A	N9-C4	-5.81	1.34	1.37
36	5	2944	U	C2-N3	-5.80	1.33	1.37
41	L4	94	CYS	CB-SG	-5.80	1.72	1.81
36	1	925	A	N3-C4	-5.78	1.31	1.34
36	5	875	G	C6-N1	-5.78	1.35	1.39
36	5	657	A	C5-C4	-5.77	1.34	1.38
36	5	2985	C	N1-C6	-5.77	1.33	1.37
36	5	1849	C	N1-C6	-5.76	1.33	1.37
36	1	2144	A	N9-C8	-5.75	1.33	1.37
1	6	163	G	N3-C4	-5.75	1.31	1.35
36	5	1177	G	N3-C4	-5.74	1.31	1.35
36	1	653	A	N7-C5	-5.73	1.35	1.39
36	1	1135	A	N3-C4	-5.73	1.31	1.34
36	5	807	A	N9-C4	-5.73	1.34	1.37
36	1	1116	G	N7-C5	-5.72	1.35	1.39
36	5	924	G	C2-N3	-5.72	1.28	1.32
36	1	3008	A	N9-C4	-5.72	1.34	1.37
1	6	1659	A	N9-C4	-5.71	1.34	1.37
36	1	304	G	C2-N3	-5.71	1.28	1.32
36	1	363	G	C5-C6	-5.71	1.36	1.42
36	1	106	A	N9-C4	-5.70	1.34	1.37
36	5	2335	G	C6-N1	-5.70	1.35	1.39
36	5	953	G	C5-C4	-5.70	1.34	1.38
36	1	2910	A	N9-C4	-5.70	1.34	1.37
36	1	2401	A	N9-C8	5.70	1.42	1.37
36	5	2761	G	N7-C5	-5.70	1.35	1.39
36	1	826	G	C5-C4	-5.69	1.34	1.38
36	5	2755	C	N1-C6	-5.68	1.33	1.37
36	1	916	G	C6-N1	-5.68	1.35	1.39
36	1	937	G	N9-C8	-5.67	1.33	1.37
1	2	555	A	N9-C4	5.66	1.41	1.37
36	5	1303	A	N9-C4	-5.66	1.34	1.37
36	5	2360	C	C4-C5	-5.65	1.38	1.43
36	1	659	G	C5-C4	-5.65	1.34	1.38
36	5	861	C	N1-C6	-5.65	1.33	1.37
36	1	2144	A	C5-C4	-5.65	1.34	1.38
36	1	85	A	C6-N1	-5.64	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	40	A	C5-C6	-5.64	1.35	1.41
36	1	627	U	N1-C2	-5.63	1.33	1.38
1	6	1728	A	N9-C4	-5.63	1.34	1.37
36	5	921	A	N7-C5	-5.63	1.35	1.39
36	5	1180	A	C6-N1	-5.63	1.31	1.35
36	1	1326	A	N3-C4	-5.62	1.31	1.34
36	1	2982	A	N9-C8	-5.62	1.33	1.37
36	5	2379	U	C2-N3	-5.60	1.33	1.37
36	1	282	G	N1-C2	-5.60	1.33	1.37
36	1	3375	A	N3-C4	-5.60	1.31	1.34
36	1	2276	G	N7-C5	-5.59	1.35	1.39
1	6	1119	G	N7-C5	-5.59	1.35	1.39
36	5	1159	A	C5-C6	-5.59	1.36	1.41
36	1	895	A	C5-C6	-5.59	1.36	1.41
36	1	1154	A	N3-C4	-5.58	1.31	1.34
36	5	1199	C	N1-C6	-5.57	1.33	1.37
36	5	421	G	N1-C2	-5.57	1.33	1.37
36	5	3245	A	N9-C4	-5.57	1.34	1.37
36	5	3132	C	N1-C6	-5.56	1.33	1.37
36	5	420	G	C5-C4	-5.56	1.34	1.38
36	5	3047	U	C2-N3	-5.56	1.33	1.37
36	5	1047	A	N7-C5	-5.55	1.35	1.39
37	7	102	A	N9-C4	-5.54	1.34	1.37
36	1	1335	C	N3-C4	-5.53	1.30	1.33
36	1	3142	A	N3-C4	-5.53	1.31	1.34
36	5	2814	G	N7-C5	-5.53	1.35	1.39
36	5	2920	U	C4-O4	-5.53	1.19	1.23
36	1	1367	G	N7-C5	-5.52	1.35	1.39
37	3	91	G	N7-C5	-5.52	1.35	1.39
36	5	1315	U	N1-C2	-5.52	1.33	1.38
36	5	2903	A	N9-C4	-5.52	1.34	1.37
36	1	2326	A	N9-C4	-5.52	1.34	1.37
36	5	649	A	C5-C6	-5.51	1.36	1.41
36	5	2937	G	C5-C4	-5.51	1.34	1.38
36	5	2334	U	C4-O4	-5.50	1.19	1.23
36	1	2811	A	N7-C5	-5.50	1.35	1.39
36	5	3314	A	N9-C4	-5.50	1.34	1.37
36	5	1841	A	N7-C5	-5.49	1.35	1.39
36	1	36	C	N1-C6	-5.48	1.33	1.37
1	6	1537	C	C2-N3	5.48	1.40	1.35
36	5	2400	G	N9-C4	-5.48	1.33	1.38
36	1	1369	A	N7-C5	-5.47	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2879	C	N1-C6	-5.47	1.33	1.37
36	1	710	A	C5-C6	-5.47	1.36	1.41
36	1	2356	A	N9-C4	-5.46	1.34	1.37
1	6	397	A	N9-C4	-5.46	1.34	1.37
36	5	3137	C	N3-C4	-5.46	1.30	1.33
36	5	2937	G	N7-C5	-5.46	1.35	1.39
37	7	14	U	C2-N3	-5.46	1.33	1.37
36	5	941	G	C6-N1	-5.45	1.35	1.39
36	5	1372	C	N1-C6	-5.45	1.33	1.37
36	1	189	G	C6-N1	-5.45	1.35	1.39
36	5	421	G	C2-N3	-5.45	1.28	1.32
36	5	971	G	N9-C8	-5.44	1.34	1.37
36	5	2967	A	C6-N1	-5.44	1.31	1.35
36	5	934	G	C5-C6	-5.44	1.36	1.42
52	m6	167	TYR	CE1-CZ	-5.42	1.31	1.38
36	1	921	A	N7-C5	-5.42	1.36	1.39
1	6	1748	G	C5-C4	-5.42	1.34	1.38
36	1	40	A	C8-N7	-5.42	1.27	1.31
36	1	2147	A	N9-C4	-5.41	1.34	1.37
36	1	1402	C	N3-C4	-5.40	1.30	1.33
1	6	542	A	N7-C5	-5.40	1.36	1.39
52	m6	16	VAL	CB-CG2	-5.40	1.41	1.52
36	1	1149	G	N3-C4	-5.40	1.31	1.35
36	1	2616	C	N1-C6	-5.39	1.33	1.37
36	1	2384	A	C5-C6	-5.39	1.36	1.41
36	5	1048	A	C6-N1	-5.39	1.31	1.35
36	5	3197	G	N9-C8	5.38	1.41	1.37
36	1	2188	A	N3-C4	-5.38	1.31	1.34
1	6	630	A	N7-C5	-5.37	1.36	1.39
36	5	2117	A	C5-C4	-5.37	1.34	1.38
36	5	3052	G	C2-N3	-5.37	1.28	1.32
36	1	2404	A	C5-C6	5.37	1.45	1.41
36	5	3209	A	C6-N1	5.36	1.39	1.35
36	1	799	G	N3-C4	-5.36	1.31	1.35
36	1	2821	C	N3-C4	5.36	1.37	1.33
44	17	234	GLU	CD-OE2	5.36	1.31	1.25
36	1	638	C	N1-C6	-5.36	1.33	1.37
1	2	1119	G	N7-C5	-5.35	1.36	1.39
36	1	2401	A	C5-C4	5.35	1.42	1.38
36	1	364	G	N9-C4	-5.34	1.33	1.38
36	1	1164	G	N7-C5	-5.34	1.36	1.39
1	6	426	G	C6-N1	-5.34	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	1537	C	C5-C6	5.33	1.38	1.34
36	1	710	A	N7-C5	-5.33	1.36	1.39
36	5	2872	A	N9-C4	-5.32	1.34	1.37
36	5	1192	C	N1-C2	5.32	1.45	1.40
36	5	2825	C	N1-C6	-5.32	1.33	1.37
36	1	2617	U	N3-C4	-5.32	1.33	1.38
36	5	2976	A	N3-C4	-5.31	1.31	1.34
36	5	3091	A	N3-C4	-5.31	1.31	1.34
36	1	942	U	C5-C6	-5.31	1.29	1.34
36	5	874	U	N1-C2	-5.31	1.33	1.38
36	5	2851	A	N9-C4	-5.31	1.34	1.37
36	5	2690	G	N3-C4	-5.30	1.31	1.35
36	5	981	U	C2-N3	5.30	1.41	1.37
36	1	1133	A	N9-C4	-5.30	1.34	1.37
36	1	2853	A	N7-C5	-5.29	1.36	1.39
36	1	1318	A	N9-C4	-5.29	1.34	1.37
36	1	699	A	N3-C4	-5.29	1.31	1.34
36	1	1606	U	N1-C2	-5.29	1.33	1.38
36	5	2911	A	N7-C5	-5.29	1.36	1.39
36	5	3107	U	C2-N3	-5.29	1.34	1.37
36	1	579	G	C5-C4	-5.28	1.34	1.38
38	8	106	C	N1-C6	-5.28	1.33	1.37
36	1	2407	C	N1-C6	-5.28	1.33	1.37
36	5	2804	A	N9-C4	-5.27	1.34	1.37
36	1	2726	C	N3-C4	-5.27	1.30	1.33
36	1	2418	G	O3'-P	5.27	1.67	1.61
36	5	95	A	C5-C6	-5.27	1.36	1.41
36	5	609	G	N3-C4	-5.27	1.31	1.35
36	1	48	A	N7-C5	-5.26	1.36	1.39
36	5	1113	G	N3-C4	-5.26	1.31	1.35
36	1	2382	G	N1-C2	-5.26	1.33	1.37
36	1	2762	A	N3-C4	-5.26	1.31	1.34
36	1	3273	A	C6-N1	-5.26	1.31	1.35
36	5	2848	G	N7-C5	-5.26	1.36	1.39
36	5	2993	G	C5-C4	-5.26	1.34	1.38
36	1	29	C	N1-C6	-5.25	1.33	1.37
36	5	644	G	N7-C5	-5.25	1.36	1.39
36	1	92	G	N1-C2	-5.25	1.33	1.37
36	1	887	G	N9-C8	-5.24	1.34	1.37
36	1	1140	G	C6-N1	-5.24	1.35	1.39
36	1	1452	A	N9-C4	-5.24	1.34	1.37
36	1	1140	G	N1-C2	-5.24	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	12	A	N9-C4	-5.24	1.34	1.37
36	5	1371	G	C5-C4	-5.24	1.34	1.38
36	5	345	G	N7-C5	-5.23	1.36	1.39
36	1	830	A	N7-C5	-5.23	1.36	1.39
36	5	2819	A	N9-C4	-5.23	1.34	1.37
1	6	985	G	C6-N1	-5.23	1.35	1.39
36	1	420	G	N9-C8	-5.23	1.34	1.37
36	1	2305	G	N7-C5	-5.23	1.36	1.39
36	5	1152	G	N9-C8	5.22	1.41	1.37
36	1	66	A	N9-C4	-5.22	1.34	1.37
36	5	1332	A	C5-C4	-5.22	1.35	1.38
36	1	2875	U	C2-N3	5.21	1.41	1.37
36	1	3141	A	N9-C4	-5.21	1.34	1.37
36	1	2177	G	N7-C5	-5.21	1.36	1.39
36	1	1159	A	N3-C4	-5.21	1.31	1.34
36	5	2286	U	C2-N3	-5.21	1.34	1.37
36	5	2704	A	N9-C4	-5.21	1.34	1.37
36	5	2607	G	N7-C5	-5.21	1.36	1.39
36	5	642	U	C2-N3	-5.20	1.34	1.37
36	1	1901	A	N9-C4	-5.20	1.34	1.37
36	5	420	G	N9-C8	-5.18	1.34	1.37
36	5	2815	G	N9-C8	-5.18	1.34	1.37
1	6	46	A	N3-C4	-5.18	1.31	1.34
36	5	1195	A	N9-C4	-5.18	1.34	1.37
36	1	1313	G	C5-C6	-5.18	1.37	1.42
36	1	659	G	N1-C2	-5.17	1.33	1.37
1	6	337	G	C2-N2	5.17	1.39	1.34
36	5	1048	A	C5-C6	-5.17	1.36	1.41
36	5	2819	A	N3-C4	-5.17	1.31	1.34
36	5	1915	A	C5-C4	-5.17	1.35	1.38
36	5	1195	A	N3-C4	-5.17	1.31	1.34
41	14	94	CYS	CB-SG	-5.17	1.73	1.81
36	5	924	G	N9-C4	-5.17	1.33	1.38
36	5	800	G	N9-C8	-5.16	1.34	1.37
36	5	1117	G	C5-C4	-5.16	1.34	1.38
36	1	1430	U	N1-C6	-5.16	1.33	1.38
36	5	2281	A	N9-C4	-5.16	1.34	1.37
36	5	2145	A	C6-N1	-5.15	1.31	1.35
36	1	890	C	N3-C4	-5.15	1.30	1.33
36	1	2714	G	N9-C8	5.15	1.41	1.37
36	5	2591	A	N9-C4	-5.15	1.34	1.37
36	5	3050	U	N3-C4	-5.15	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	1773	C	N3-C4	5.14	1.37	1.33
36	1	286	U	C2-N3	-5.14	1.34	1.37
36	5	43	A	C5-C6	-5.13	1.36	1.41
36	1	213	A	N9-C4	-5.13	1.34	1.37
36	1	2409	G	N3-C4	-5.13	1.31	1.35
36	5	2400	G	C5-C4	-5.13	1.34	1.38
36	5	2830	G	N3-C4	-5.13	1.31	1.35
36	1	1154	A	N7-C5	-5.13	1.36	1.39
1	2	1746	A	N9-C4	-5.12	1.34	1.37
36	1	649	A	N3-C4	-5.12	1.31	1.34
36	1	1153	A	C5-C6	-5.12	1.36	1.41
36	1	2381	G	N3-C4	-5.12	1.31	1.35
36	5	865	U	N1-C2	-5.12	1.33	1.38
36	5	1897	G	N3-C4	-5.12	1.31	1.35
36	1	816	A	N9-C4	5.12	1.41	1.37
57	n1	101	CYS	CB-SG	5.12	1.91	1.82
36	5	95	A	N9-C4	-5.11	1.34	1.37
36	5	1203	A	C5-C6	-5.11	1.36	1.41
36	5	1383	G	N3-C4	-5.11	1.31	1.35
36	5	2342	U	C2-N3	-5.10	1.34	1.37
36	5	1833	G	C5-C4	-5.10	1.34	1.38
38	8	39	G	N7-C5	-5.10	1.36	1.39
36	1	706	A	N9-C4	-5.10	1.34	1.37
36	5	1504	A	N3-C4	-5.10	1.31	1.34
1	2	1754	A	N9-C4	-5.09	1.34	1.37
36	1	2404	A	N9-C4	5.08	1.40	1.37
36	1	1447	G	N3-C4	-5.08	1.31	1.35
36	1	658	G	C8-N7	-5.07	1.27	1.30
1	6	1773	C	C2-N3	5.07	1.39	1.35
36	5	647	A	N3-C4	-5.07	1.31	1.34
36	5	1148	G	N3-C4	5.07	1.39	1.35
36	1	2157	G	N7-C5	-5.07	1.36	1.39
36	1	2406	C	N1-C6	-5.07	1.34	1.37
36	5	2411	U	C2-N3	-5.07	1.34	1.37
36	5	1927	G	N3-C4	-5.07	1.31	1.35
36	5	1462	A	N9-C4	-5.06	1.34	1.37
36	5	3185	U	N1-C6	-5.06	1.33	1.38
36	1	1401	A	N7-C5	-5.06	1.36	1.39
36	1	2142	A	N3-C4	-5.05	1.31	1.34
36	5	958	C	N1-C6	-5.05	1.34	1.37
36	5	1844	C	N3-C4	-5.05	1.30	1.33
52	m6	40	GLU	CG-CD	5.05	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	1129	U	C2-N3	-5.05	1.34	1.37
36	1	972	A	N9-C4	-5.05	1.34	1.37
36	1	2867	C	C2-N3	-5.05	1.31	1.35
36	1	34	A	N3-C4	-5.05	1.31	1.34
36	1	2419	A	N9-C4	-5.05	1.34	1.37
47	M0	127	ALA	CA-CB	-5.04	1.41	1.52
36	5	804	C	N1-C6	-5.04	1.34	1.37
36	5	1849	C	N3-C4	-5.04	1.30	1.33
36	5	1451	C	N1-C6	-5.04	1.34	1.37
36	5	652	G	C5-C4	-5.03	1.34	1.38
36	1	1308	A	P-OP2	-5.03	1.40	1.49
36	5	1874	A	N9-C4	-5.03	1.34	1.37
36	5	2117	A	N9-C8	-5.03	1.33	1.37
36	5	1348	U	N1-C2	5.02	1.43	1.38
36	5	2138	A	N9-C4	-5.02	1.34	1.37
36	5	943	U	C2-N3	-5.02	1.34	1.37
36	5	2364	G	N7-C5	-5.02	1.36	1.39
36	5	1131	G	N9-C8	-5.02	1.34	1.37
36	1	2867	C	N3-C4	-5.01	1.30	1.33
36	1	1133	A	C5-C4	-5.01	1.35	1.38
36	1	1100	U	N1-C2	-5.00	1.34	1.38
36	1	1328	C	C4-C5	-5.00	1.39	1.43

All (4824) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	C2-N3-C4	-23.10	100.35	111.90
36	5	1152	G	N3-C4-C5	23.05	140.12	128.60
36	5	1152	G	N3-C4-N9	-22.76	112.34	126.00
36	1	2714	G	N3-C4-C5	15.18	136.19	128.60
36	1	1308	A	O5'-P-OP2	-14.90	92.29	105.70
36	5	2385	G	O5'-P-OP1	-14.30	92.83	105.70
36	1	716	A	N1-C6-N6	13.71	126.83	118.60
36	1	86	G	O5'-P-OP2	-13.29	93.74	105.70
36	1	1308	A	C8-N9-C4	-13.10	100.56	105.80
36	1	2808	A	N1-C6-N6	12.98	126.39	118.60
36	5	2726	C	C5-C4-N4	12.69	129.08	120.20
36	1	2714	G	N3-C4-N9	-12.58	118.45	126.00
36	1	639	G	N1-C6-O6	12.47	127.39	119.90
1	6	1773	C	N3-C4-C5	-12.41	116.94	121.90
36	1	406	G	O4'-C1'-N9	12.40	118.12	108.20
36	1	2846	U	N3-C2-O2	-12.33	113.57	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2818	U	O5'-P-OP1	-12.23	94.69	105.70
1	2	553	G	N1-C6-O6	12.22	127.23	119.90
36	5	642	U	O5'-P-OP2	-12.14	94.78	105.70
36	1	2996	U	C2-N1-C1'	12.07	132.18	117.70
1	6	163	G	N3-C4-N9	-12.06	118.76	126.00
36	5	1152	G	C5-N7-C8	-11.96	98.32	104.30
36	5	2726	C	C6-N1-C2	-11.93	115.53	120.30
36	5	2726	C	N3-C2-O2	-11.92	113.56	121.90
36	5	3245	A	C5-N7-C8	-11.84	97.98	103.90
36	1	1428	A	N1-C6-N6	11.79	125.67	118.60
36	5	922	U	C5-C6-N1	-11.76	116.82	122.70
36	5	1006	A	O5'-P-OP2	-11.75	95.12	105.70
36	5	2400	G	C5-C6-O6	-11.72	121.57	128.60
36	1	939	U	C5-C4-O4	-11.65	118.91	125.90
1	6	1537	C	C6-N1-C2	-11.61	115.66	120.30
36	1	2764	C	C2-N3-C4	11.49	125.65	119.90
36	1	716	A	N9-C4-C5	-11.49	101.20	105.80
36	1	1902	G	N1-C6-O6	11.43	126.76	119.90
36	5	881	C	N1-C2-O2	11.40	125.74	118.90
36	1	54	C	N3-C4-C5	11.36	126.44	121.90
36	5	1152	G	C8-N9-C1'	11.36	141.76	127.00
36	5	63	A	N1-C6-N6	11.35	125.41	118.60
36	1	2868	U	N1-C2-O2	11.34	130.74	122.80
36	1	939	U	N1-C2-O2	-11.31	114.88	122.80
36	5	2400	G	N1-C6-O6	11.29	126.67	119.90
36	1	2617	U	C5-C4-O4	11.25	132.65	125.90
36	1	1150	A	O5'-P-OP2	-11.21	95.61	105.70
36	5	1513	G	C8-N9-C4	-11.16	101.94	106.40
36	1	1365	G	N3-C4-C5	-11.16	123.02	128.60
36	1	1132	C	O5'-P-OP1	-11.09	95.72	105.70
36	1	2884	C	N3-C4-C5	11.05	126.32	121.90
36	5	2372	A	C8-N9-C4	-11.05	101.38	105.80
36	1	794	U	O5'-P-OP2	-11.00	95.80	105.70
36	1	645	A	N1-C6-N6	-10.95	112.03	118.60
36	1	363	G	C5-C6-O6	-10.94	122.03	128.60
36	5	2334	U	O5'-P-OP2	-10.94	95.86	105.70
1	6	144	U	N3-C2-O2	-10.89	114.58	122.20
36	1	2726	C	N3-C2-O2	-10.86	114.30	121.90
36	5	2935	U	O5'-P-OP2	-10.82	95.96	105.70
36	1	1428	A	C5-C6-N6	-10.82	115.04	123.70
36	1	1902	G	C5-C6-O6	-10.80	122.12	128.60
38	8	80	A	C8-N9-C4	-10.80	101.48	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	610	G	O5'-P-OP2	-10.77	96.01	105.70
1	6	402	C	O5'-P-OP2	-10.73	96.04	105.70
36	5	2617	U	O5'-P-OP2	-10.72	96.06	105.70
36	1	1489	A	N1-C6-N6	10.71	125.03	118.60
36	1	2617	U	N1-C2-N3	10.71	121.32	114.90
36	5	421	G	O5'-P-OP2	-10.70	96.07	105.70
36	5	1452	A	N1-C6-N6	10.64	124.98	118.60
36	1	859	G	N9-C4-C5	-10.63	101.15	105.40
36	5	222	A	O5'-P-OP2	-10.62	96.14	105.70
36	1	339	C	OP1-P-OP2	-10.62	103.67	119.60
36	1	1495	U	C5-C6-N1	-10.61	117.39	122.70
36	5	2290	C	C6-N1-C2	10.57	124.53	120.30
36	5	966	U	N1-C2-O2	10.51	130.16	122.80
36	1	1495	U	C4-C5-C6	10.44	125.96	119.70
36	5	2392	C	N3-C4-C5	10.44	126.08	121.90
36	5	1481	A	C8-N9-C4	-10.42	101.63	105.80
36	5	1902	G	C5-C6-O6	-10.42	122.35	128.60
36	1	2996	U	C6-N1-C1'	-10.42	106.62	121.20
36	5	3245	A	C2-N3-C4	-10.41	105.39	110.60
36	1	1192	C	N1-C2-O2	10.41	125.14	118.90
36	1	1385	C	N1-C2-O2	-10.37	112.68	118.90
36	1	1902	G	C6-C5-N7	-10.33	124.20	130.40
36	5	2821	C	N1-C2-O2	-10.32	112.71	118.90
36	1	1838	G	N1-C6-O6	10.27	126.06	119.90
36	5	1152	G	N3-C2-N2	-10.26	112.72	119.90
36	5	1902	G	N1-C6-O6	10.25	126.05	119.90
36	5	1152	G	C4-N9-C1'	-10.23	113.20	126.50
36	1	1133	A	N1-C6-N6	10.22	124.73	118.60
36	5	585	A	O5'-P-OP2	-10.21	96.51	105.70
36	1	942	U	C5-C4-O4	-10.21	119.78	125.90
36	1	969	C	N1-C2-O2	-10.20	112.78	118.90
36	5	2354	C	N3-C2-O2	10.19	129.03	121.90
36	1	2827	U	C5-C4-O4	10.18	132.01	125.90
36	5	2383	C	N1-C2-O2	-10.18	112.79	118.90
36	5	966	U	N3-C2-O2	-10.16	115.08	122.20
36	1	1381	A	O5'-P-OP2	10.16	122.89	110.70
1	6	1100	G	N3-C4-C5	-10.14	123.53	128.60
36	1	1133	A	C5-C6-N6	-10.14	115.59	123.70
36	5	2392	C	C6-N1-C2	10.12	124.35	120.30
36	5	2945	G	O5'-P-OP1	10.12	122.84	110.70
36	1	1495	U	N1-C2-N3	10.10	120.96	114.90
36	1	2617	U	C5-C6-N1	-10.09	117.66	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	20	U	O5'-P-OP2	-10.09	96.62	105.70
1	2	558	U	N1-C2-O2	10.08	129.86	122.80
36	1	2764	C	N3-C4-C5	-10.07	117.87	121.90
36	5	860	G	O5'-P-OP2	-10.06	96.64	105.70
36	5	2403	G	O5'-P-OP2	-10.04	96.66	105.70
36	1	2197	C	C6-N1-C2	10.04	124.31	120.30
37	7	49	G	N1-C6-O6	10.04	125.92	119.90
36	1	1307	G	N9-C4-C5	10.03	109.41	105.40
1	2	639	U	N3-C2-O2	-10.03	115.18	122.20
36	1	2818	U	O5'-P-OP1	-10.03	96.67	105.70
36	1	2165	G	N1-C6-O6	10.01	125.90	119.90
36	1	2661	G	O5'-P-OP1	-10.00	96.70	105.70
37	7	93	C	O5'-P-OP2	-9.97	96.73	105.70
36	5	3218	A	N1-C6-N6	9.96	124.58	118.60
36	1	1556	C	N3-C2-O2	-9.95	114.94	121.90
36	1	1433	A	O5'-P-OP1	-9.93	96.77	105.70
36	5	2333	C	C6-N1-C2	9.92	124.27	120.30
36	1	2617	U	C4-C5-C6	9.91	125.65	119.70
36	5	2389	C	N3-C4-C5	9.85	125.84	121.90
36	5	960	U	N1-C2-O2	9.84	129.69	122.80
36	1	1428	A	C4-C5-N7	9.84	115.62	110.70
36	5	960	U	N3-C2-O2	-9.83	115.32	122.20
38	8	80	A	N7-C8-N9	9.81	118.71	113.80
36	1	2870	C	C2-N1-C1'	-9.80	108.02	118.80
36	1	830	A	N1-C6-N6	9.79	124.47	118.60
36	1	1308	A	N7-C8-N9	9.78	118.69	113.80
36	1	2714	G	C2-N3-C4	-9.77	107.02	111.90
36	5	2699	G	C5-C6-O6	-9.76	122.74	128.60
36	1	282	G	O5'-P-OP1	-9.76	96.92	105.70
36	1	895	A	O5'-P-OP1	-9.75	96.93	105.70
36	1	397	A	N1-C6-N6	-9.74	112.75	118.60
36	5	3197	G	N3-C2-N2	-9.74	113.08	119.90
36	5	2699	G	N1-C6-O6	9.72	125.73	119.90
36	1	2936	A	O5'-P-OP1	-9.72	96.95	105.70
36	1	2384	A	N1-C6-N6	9.71	124.43	118.60
36	5	2978	U	C5-C6-N1	-9.70	117.85	122.70
1	6	163	G	N3-C4-C5	9.68	133.44	128.60
36	5	640	U	N1-C2-O2	-9.67	116.03	122.80
36	5	1200	A	N1-C6-N6	9.63	124.38	118.60
36	1	2397	A	N1-C6-N6	9.62	124.38	118.60
36	1	339	C	N3-C4-N4	-9.61	111.27	118.00
36	5	2400	G	N3-C4-C5	9.60	133.40	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1773	C	N3-C4-N4	9.58	124.71	118.00
36	5	1520	G	C5-C6-O6	-9.56	122.86	128.60
36	5	2147	A	N1-C6-N6	9.55	124.33	118.60
36	5	2426	U	C5-C4-O4	9.52	131.61	125.90
36	1	640	U	N3-C4-O4	9.52	126.06	119.40
36	5	3245	A	C4-C5-N7	9.50	115.45	110.70
38	4	44	A	N1-C6-N6	9.49	124.30	118.60
36	1	3278	C	N1-C2-O2	9.48	124.59	118.90
36	1	66	A	O5'-P-OP1	-9.47	97.18	105.70
36	1	1902	G	C4-C5-N7	9.46	114.58	110.80
36	5	41	G	C4-C5-N7	9.46	114.58	110.80
36	1	2812	C	O5'-P-OP2	9.44	122.03	110.70
36	1	770	G	O4'-C1'-N9	9.43	115.74	108.20
36	1	662	U	O5'-P-OP2	-9.42	97.22	105.70
36	5	1481	A	N7-C8-N9	9.42	118.51	113.80
36	1	1389	G	C4-C5-N7	9.41	114.56	110.80
36	1	67	A	O5'-P-OP1	-9.38	97.26	105.70
36	5	40	A	O5'-P-OP1	-9.37	97.27	105.70
36	1	1389	G	N1-C6-O6	9.36	125.52	119.90
36	1	1556	C	C6-N1-C2	-9.36	116.55	120.30
36	5	911	C	C5-C6-N1	-9.33	116.33	121.00
36	5	3005	A	O5'-P-OP2	-9.33	97.30	105.70
1	6	941	A	N1-C6-N6	-9.32	113.01	118.60
36	1	3098	G	O5'-P-OP2	-9.31	97.32	105.70
36	1	3181	C	N3-C2-O2	-9.31	115.38	121.90
36	1	1103	A	O5'-P-OP1	-9.31	97.32	105.70
36	1	1846	C	O5'-P-OP1	-9.28	97.34	105.70
36	1	2237	C	C6-N1-C2	9.28	124.01	120.30
36	1	1153	A	O5'-P-OP1	-9.27	97.35	105.70
36	1	2846	U	C5-C4-O4	9.27	131.46	125.90
36	5	806	A	O5'-P-OP1	-9.24	97.38	105.70
36	1	716	A	C8-N9-C4	9.23	109.49	105.80
36	1	2700	G	C5-C6-O6	-9.23	123.06	128.60
36	1	2165	G	C5-C6-O6	-9.23	123.06	128.60
3	S1	218	LEU	CA-CB-CG	9.23	136.52	115.30
36	1	2355	G	N1-C6-O6	9.23	125.44	119.90
36	5	1390	A	N1-C6-N6	-9.23	113.06	118.60
36	1	2572	C	N1-C2-O2	9.22	124.44	118.90
36	5	776	U	C5-C6-N1	-9.22	118.09	122.70
36	5	3245	A	N7-C8-N9	9.22	118.41	113.80
36	1	672	A	N1-C6-N6	9.20	124.12	118.60
36	5	398	A	O5'-P-OP2	-9.19	97.43	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1537	C	N3-C4-C5	-9.18	118.23	121.90
36	5	2400	G	C8-N9-C4	9.18	110.07	106.40
36	1	1001	G	N1-C6-O6	9.18	125.41	119.90
1	2	558	U	N3-C2-O2	-9.17	115.78	122.20
36	5	2644	C	O5'-P-OP1	-9.15	97.47	105.70
36	1	640	U	N1-C2-O2	-9.13	116.41	122.80
36	1	1904	C	C6-N1-C2	-9.13	116.65	120.30
36	1	3183	A	N1-C6-N6	9.11	124.07	118.60
36	1	2808	A	C6-C5-N7	-9.10	125.93	132.30
36	5	981	U	C5-C6-N1	9.10	127.25	122.70
36	5	922	U	N3-C2-O2	-9.09	115.83	122.20
36	5	1897	G	N1-C6-O6	9.09	125.36	119.90
36	1	2334	U	O5'-P-OP2	-9.09	97.52	105.70
36	5	2317	A	O5'-P-OP2	-9.08	97.53	105.70
36	5	2358	A	C8-N9-C4	9.08	109.43	105.80
36	5	1152	G	N1-C6-O6	9.06	125.34	119.90
36	5	1333	C	C6-N1-C2	-9.06	116.68	120.30
1	6	337	G	N3-C4-N9	9.03	131.42	126.00
36	1	439	C	C2-N1-C1'	9.01	128.72	118.80
1	6	1634	C	C2-N1-C1'	9.00	128.70	118.80
36	5	2308	C	N1-C2-O2	-8.99	113.50	118.90
37	7	101	G	N1-C6-O6	8.99	125.29	119.90
36	1	3095	U	O5'-P-OP1	-8.98	97.61	105.70
36	5	1390	A	N9-C4-C5	8.98	109.39	105.80
36	1	718	G	C4-C5-N7	8.98	114.39	110.80
36	5	366	A	N1-C6-N6	8.97	123.98	118.60
36	1	2827	U	N1-C2-N3	8.95	120.27	114.90
36	1	2868	U	N3-C2-O2	-8.95	115.94	122.20
36	5	877	C	N3-C4-C5	8.95	125.48	121.90
36	5	2281	A	C8-N9-C4	8.94	109.38	105.80
36	1	627	U	N3-C2-O2	8.94	128.46	122.20
36	1	2885	C	C6-N1-C2	8.94	123.88	120.30
36	5	2943	G	C6-C5-N7	-8.92	125.05	130.40
1	2	453	U	N3-C2-O2	-8.92	115.96	122.20
36	1	2700	G	N1-C6-O6	8.92	125.25	119.90
36	1	1389	G	C5-C6-O6	-8.91	123.25	128.60
1	2	1280	C	N3-C4-C5	-8.91	118.33	121.90
36	1	1428	A	O5'-P-OP2	-8.91	97.68	105.70
36	1	802	C	O5'-P-OP2	8.90	121.38	110.70
36	5	2954	U	C2-N1-C1'	8.90	128.38	117.70
36	5	1592	G	C8-N9-C4	-8.89	102.84	106.40
36	1	1154	A	O5'-P-OP1	-8.87	97.72	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3050	U	C5-C4-O4	8.87	131.22	125.90
36	5	2878	G	N1-C6-O6	-8.87	114.58	119.90
36	1	637	C	C6-N1-C2	8.86	123.84	120.30
38	4	103	G	C8-N9-C4	-8.86	102.86	106.40
36	1	2369	G	O5'-P-OP1	-8.86	97.73	105.70
36	5	57	A	N1-C6-N6	8.86	123.92	118.60
36	5	2945	G	O5'-P-OP2	-8.86	97.73	105.70
1	2	453	U	C2-N1-C1'	8.85	128.32	117.70
36	1	939	U	O5'-P-OP2	-8.84	97.74	105.70
36	5	1452	A	N9-C4-C5	-8.84	102.26	105.80
36	5	2377	G	C8-N9-C4	8.84	109.94	106.40
36	1	350	C	C6-N1-C2	-8.84	116.77	120.30
36	1	716	A	C4-C5-N7	8.83	115.12	110.70
36	5	1010	G	O5'-P-OP2	-8.83	97.75	105.70
36	5	670	C	C6-N1-C2	-8.83	116.77	120.30
36	5	2815	G	C8-N9-C4	8.83	109.93	106.40
36	1	2846	U	N1-C2-O2	8.82	128.97	122.80
36	1	2617	U	N3-C2-O2	-8.81	116.03	122.20
36	5	2971	A	C2-N3-C4	8.80	115.00	110.60
36	1	2764	C	C6-N1-C2	-8.79	116.78	120.30
36	5	2726	C	N3-C4-N4	-8.78	111.86	118.00
36	1	2422	C	O5'-P-OP1	-8.77	97.81	105.70
36	1	2610	G	N1-C6-O6	8.77	125.16	119.90
36	1	830	A	C5-C6-N6	-8.76	116.69	123.70
36	1	1138	U	N3-C2-O2	-8.75	116.07	122.20
36	1	651	G	N3-C4-N9	8.75	131.25	126.00
36	1	1896	A	O5'-P-OP1	-8.74	97.83	105.70
38	4	32	C	N3-C4-C5	8.74	125.40	121.90
1	6	1121	C	O5'-P-OP2	-8.74	97.83	105.70
36	1	111	C	C6-N1-C2	8.74	123.80	120.30
36	1	2756	C	C6-N1-C2	-8.73	116.81	120.30
36	1	716	A	C5-C6-N6	-8.73	116.72	123.70
1	6	119	A	C2-N3-C4	-8.73	106.24	110.60
36	1	1371	G	C8-N9-C4	8.71	109.89	106.40
36	5	86	G	O5'-P-OP2	-8.71	97.86	105.70
36	5	3245	A	N1-C6-N6	8.67	123.80	118.60
36	1	2169	G	N1-C6-O6	-8.67	114.70	119.90
36	1	1365	G	C8-N9-C4	-8.66	102.94	106.40
36	1	2283	G	N1-C6-O6	8.66	125.10	119.90
36	5	121	A	N1-C6-N6	8.66	123.79	118.60
1	2	639	U	N1-C2-O2	8.65	128.86	122.80
36	1	939	U	N3-C2-O2	8.65	128.26	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	979	U	N3-C2-O2	-8.65	116.15	122.20
36	1	2659	G	N1-C6-O6	8.64	125.08	119.90
36	1	979	U	C6-N1-C2	-8.62	115.83	121.00
36	5	2366	C	C5-C6-N1	8.62	125.31	121.00
36	1	776	U	C4-C5-C6	8.61	124.86	119.70
36	1	1343	A	N1-C6-N6	8.59	123.76	118.60
36	5	580	C	C6-N1-C2	-8.59	116.86	120.30
36	1	3214	U	N3-C2-O2	-8.59	116.19	122.20
36	5	2345	A	N1-C6-N6	8.58	123.75	118.60
36	5	645	A	N1-C2-N3	8.56	133.58	129.30
36	5	2211	U	N3-C2-O2	-8.56	116.21	122.20
36	5	875	G	N1-C6-O6	-8.55	114.77	119.90
36	5	1117	G	O5'-P-OP1	-8.55	98.01	105.70
38	8	16	G	N1-C6-O6	8.54	125.03	119.90
36	1	1911	A	N1-C6-N6	8.51	123.70	118.60
1	6	339	C	N1-C2-O2	-8.50	113.80	118.90
36	5	2354	C	N1-C2-O2	-8.50	113.80	118.90
36	1	1484	U	P-O3'-C3'	8.50	129.90	119.70
36	5	2191	U	N1-C2-O2	8.50	128.75	122.80
36	1	2404	A	C2-N3-C4	8.49	114.84	110.60
36	1	286	U	N3-C2-O2	-8.48	116.26	122.20
1	6	310	C	N1-C2-O2	-8.48	113.81	118.90
36	1	1367	G	N1-C6-O6	8.48	124.99	119.90
36	5	2341	A	C8-N9-C4	8.48	109.19	105.80
36	5	2426	U	N3-C2-O2	-8.47	116.27	122.20
36	1	2636	A	C8-N9-C4	-8.46	102.41	105.80
36	1	3057	U	N3-C2-O2	-8.46	116.27	122.20
36	1	640	U	C5-C4-O4	-8.46	120.83	125.90
1	6	1137	A	C8-N9-C4	8.45	109.18	105.80
1	6	65	A	C2-N3-C4	-8.45	106.37	110.60
36	5	1311	G	O5'-P-OP2	-8.45	98.09	105.70
36	1	1307	G	N1-C6-O6	-8.45	114.83	119.90
36	5	1116	G	O5'-P-OP1	-8.44	98.10	105.70
36	5	3006	A	N1-C2-N3	8.44	133.52	129.30
36	5	719	U	N1-C2-O2	8.41	128.69	122.80
36	1	3175	U	O5'-P-OP2	-8.41	98.13	105.70
47	M0	24	ARG	NE-CZ-NH1	8.41	124.50	120.30
36	5	1390	A	C8-N9-C4	-8.40	102.44	105.80
36	1	2339	C	O5'-P-OP2	-8.38	98.15	105.70
36	1	65	A	P-O3'-C3'	8.37	129.74	119.70
36	1	282	G	C8-N9-C4	-8.37	103.05	106.40
36	5	578	A	N1-C6-N6	8.36	123.62	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2630	C	N1-C2-O2	-8.36	113.88	118.90
36	1	1157	G	N3-C2-N2	-8.36	114.05	119.90
36	5	2257	C	C6-N1-C2	-8.35	116.96	120.30
36	1	3306	U	N3-C2-O2	-8.34	116.36	122.20
36	1	1001	G	C5-C6-O6	-8.34	123.60	128.60
36	1	3001	C	C6-N1-C2	8.33	123.63	120.30
36	5	2858	U	C6-N1-C2	-8.33	116.00	121.00
36	1	802	C	O5'-P-OP1	-8.32	98.21	105.70
36	1	3306	U	C5-C4-O4	8.32	130.89	125.90
36	5	2354	C	C6-N1-C2	8.32	123.63	120.30
36	5	38	U	O5'-P-OP2	-8.31	98.22	105.70
36	5	1164	G	O5'-P-OP2	-8.31	98.22	105.70
36	5	2996	U	N1-C2-O2	8.31	128.62	122.80
36	5	41	G	C5-C6-O6	-8.30	123.62	128.60
36	1	645	A	C5-C6-N1	8.30	121.85	117.70
1	6	630	A	N1-C6-N6	8.30	123.58	118.60
36	1	2351	U	O5'-P-OP2	8.29	120.65	110.70
1	2	402	C	C6-N1-C2	8.29	123.62	120.30
36	5	65	A	O5'-P-OP2	-8.29	98.24	105.70
36	5	1410	U	O5'-P-OP2	-8.28	98.24	105.70
1	6	1537	C	C6-N1-C1'	8.28	130.74	120.80
36	1	1148	G	C8-N9-C4	8.28	109.71	106.40
36	1	2700	G	C6-C5-N7	-8.28	125.43	130.40
36	5	2619	G	C5-C6-O6	-8.28	123.63	128.60
40	l3	275	ARG	NE-CZ-NH1	-8.28	116.16	120.30
36	5	41	G	N1-C6-O6	8.27	124.86	119.90
36	5	1513	G	N7-C8-N9	8.27	117.23	113.10
36	1	1389	G	N9-C4-C5	-8.26	102.10	105.40
36	5	2693	C	N3-C4-C5	8.25	125.20	121.90
36	1	439	C	N1-C2-O2	8.25	123.85	118.90
36	5	3056	U	N1-C2-O2	-8.24	117.03	122.80
36	5	404	G	O5'-P-OP2	-8.23	98.29	105.70
36	5	2272	G	O4'-C1'-N9	8.23	114.78	108.20
1	6	438	A	O5'-P-OP1	-8.23	98.30	105.70
36	1	347	G	C4-C5-N7	8.22	114.09	110.80
36	1	2938	G	O5'-P-OP1	-8.22	98.30	105.70
36	5	1099	A	N1-C6-N6	8.22	123.53	118.60
36	1	1103	A	O5'-P-OP2	8.21	120.56	110.70
36	1	860	G	C5-C6-O6	-8.21	123.67	128.60
36	1	3207	U	C2-N1-C1'	-8.21	107.85	117.70
36	1	1157	G	N9-C4-C5	8.20	108.68	105.40
1	2	1600	A	C2-N3-C4	-8.19	106.50	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3140	G	C5-C6-O6	-8.19	123.68	128.60
36	1	1130	A	N1-C6-N6	8.19	123.51	118.60
36	1	2618	G	C5-C6-N1	8.19	115.59	111.50
36	5	2758	A	C8-N9-C4	-8.19	102.52	105.80
36	5	727	G	O5'-P-OP1	-8.19	98.33	105.70
36	5	2858	U	N3-C2-O2	-8.19	116.47	122.20
36	1	817	A	C8-N9-C4	-8.18	102.53	105.80
1	6	1100	G	N3-C4-N9	8.18	130.91	126.00
36	1	1891	A	C8-N9-C4	8.18	109.07	105.80
36	1	2870	C	N3-C4-C5	8.18	125.17	121.90
36	1	406	G	O5'-P-OP2	-8.17	98.34	105.70
37	7	110	G	O5'-P-OP2	-8.17	98.35	105.70
38	4	40	A	N1-C6-N6	8.17	123.50	118.60
36	5	2913	C	N1-C2-O2	-8.16	114.01	118.90
36	5	952	A	O5'-P-OP2	-8.14	98.37	105.70
36	5	2881	C	C6-N1-C2	8.14	123.56	120.30
1	6	609	U	C5-C4-O4	8.14	130.78	125.90
36	5	2396	G	N9-C4-C5	8.13	108.65	105.40
36	1	2387	A	C8-N9-C4	8.13	109.05	105.80
36	1	2572	C	C2-N1-C1'	8.13	127.74	118.80
36	5	2116	G	N1-C6-O6	8.13	124.78	119.90
36	1	1316	C	N1-C2-O2	-8.13	114.02	118.90
36	1	1428	A	C5-N7-C8	-8.13	99.84	103.90
36	1	3344	A	O4'-C1'-N9	8.13	114.70	108.20
36	5	2700	G	C5-C6-O6	-8.13	123.72	128.60
36	1	1365	G	C6-N1-C2	-8.13	120.22	125.10
1	2	1200	G	N1-C6-O6	8.12	124.77	119.90
36	1	2624	G	N1-C6-O6	8.12	124.77	119.90
36	5	437	G	N3-C4-N9	-8.11	121.13	126.00
36	5	2147	A	C5-C6-N6	-8.11	117.21	123.70
36	5	2987	A	O5'-P-OP1	-8.11	98.41	105.70
1	6	1634	C	C6-N1-C2	-8.10	117.06	120.30
36	5	2249	G	C8-N9-C4	-8.10	103.16	106.40
36	1	2821	C	O5'-P-OP1	-8.10	98.41	105.70
36	1	939	U	N3-C4-O4	8.09	125.06	119.40
36	5	2147	A	C4-C5-N7	8.09	114.74	110.70
37	7	101	G	C6-C5-N7	-8.09	125.55	130.40
36	1	2165	G	C6-C5-N7	-8.08	125.55	130.40
36	5	1416	C	N1-C2-O2	8.08	123.75	118.90
36	5	2211	U	C4-C5-C6	8.07	124.55	119.70
36	1	1307	G	C5-C6-O6	8.06	133.44	128.60
36	1	1507	G	O5'-P-OP2	-8.06	98.44	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	648	C	C2-N1-C1'	8.06	127.67	118.80
36	1	1368	U	O5'-P-OP1	-8.06	98.45	105.70
36	1	59	G	N1-C6-O6	8.06	124.73	119.90
37	3	94	C	N1-C2-O2	-8.06	114.06	118.90
36	1	1510	G	C6-C5-N7	-8.06	125.57	130.40
36	5	1483	G	O4'-C1'-N9	8.05	114.64	108.20
36	1	933	A	C4-C5-C6	8.05	121.03	117.00
36	1	2878	G	C5-C6-O6	-8.05	123.77	128.60
1	6	337	G	C4-N9-C1'	8.05	136.96	126.50
36	5	411	U	O5'-P-OP2	-8.04	98.46	105.70
36	5	2866	U	N3-C2-O2	-8.04	116.57	122.20
36	1	701	G	N1-C6-O6	8.04	124.72	119.90
36	5	806	A	C8-N9-C4	8.04	109.02	105.80
36	5	2385	G	N3-C4-C5	8.04	132.62	128.60
41	14	233	LEU	CA-CB-CG	8.04	133.79	115.30
36	5	3196	U	O5'-P-OP1	-8.03	98.47	105.70
36	5	1365	G	C6-C5-N7	-8.03	125.58	130.40
36	1	2379	U	N1-C2-O2	-8.03	117.18	122.80
36	1	343	U	N1-C2-N3	8.02	119.72	114.90
36	5	831	G	C5-C6-O6	-8.02	123.79	128.60
1	2	1560	U	N3-C2-O2	-8.02	116.59	122.20
36	1	3298	C	C6-N1-C2	8.02	123.51	120.30
36	5	406	G	O4'-C1'-N9	8.02	114.61	108.20
1	2	75	U	N1-C2-O2	8.02	128.41	122.80
38	4	103	G	N3-C4-C5	-8.02	124.59	128.60
36	1	49	A	C5-C6-N1	-8.01	113.69	117.70
36	5	2352	A	N1-C2-N3	8.01	133.30	129.30
37	7	93	C	O5'-P-OP1	8.01	120.31	110.70
36	5	2943	G	C4-C5-N7	8.01	114.00	110.80
41	14	339	LEU	CA-CB-CG	8.00	133.70	115.30
38	4	140	G	C8-N9-C4	-7.99	103.20	106.40
36	5	1075	A	C8-N9-C4	7.99	108.99	105.80
1	6	272	U	P-O3'-C3'	7.98	129.28	119.70
36	5	2363	A	N1-C6-N6	7.98	123.39	118.60
36	5	1131	G	C2-N3-C4	-7.98	107.91	111.90
36	5	1331	U	C5-C6-N1	-7.98	118.71	122.70
36	5	2372	A	P-O3'-C3'	7.98	129.27	119.70
36	1	1445	U	C2-N1-C1'	-7.97	108.13	117.70
1	6	163	G	N3-C2-N2	-7.97	114.32	119.90
36	1	3178	A	N1-C6-N6	7.97	123.38	118.60
36	1	922	U	N1-C2-O2	7.97	128.38	122.80
36	5	3218	A	C6-C5-N7	-7.96	126.72	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	709	A	C8-N9-C4	7.96	108.98	105.80
1	6	1634	C	C5-C6-N1	7.96	124.98	121.00
38	8	8	C	C6-N1-C2	-7.96	117.12	120.30
36	1	2884	C	C6-N1-C2	7.95	123.48	120.30
36	1	3181	C	C5-C4-N4	7.95	125.77	120.20
36	5	40	A	N1-C6-N6	7.95	123.37	118.60
38	4	44	A	N9-C4-C5	-7.95	102.62	105.80
36	1	3201	C	C6-N1-C2	-7.94	117.12	120.30
36	5	3216	G	N1-C6-O6	7.94	124.67	119.90
36	5	2929	C	C2-N3-C4	-7.94	115.93	119.90
36	5	3123	A	O5'-P-OP1	-7.94	98.56	105.70
36	1	1578	C	C2-N1-C1'	7.93	127.53	118.80
37	7	87	G	N1-C6-O6	7.93	124.66	119.90
36	1	2397	A	C5-C6-N6	-7.93	117.35	123.70
1	6	987	G	C5-C6-O6	-7.93	123.84	128.60
36	5	1837	U	O5'-P-OP1	-7.93	98.56	105.70
38	4	113	U	C5-C6-N1	-7.93	118.74	122.70
36	5	339	C	C6-N1-C2	-7.93	117.13	120.30
36	1	3306	U	N3-C4-O4	-7.92	113.85	119.40
1	6	337	G	N3-C4-C5	-7.92	124.64	128.60
1	2	992	A	C2-N3-C4	-7.92	106.64	110.60
36	1	1428	A	C6-C5-N7	-7.92	126.76	132.30
1	6	337	G	C6-C5-N7	-7.91	125.65	130.40
36	5	2572	C	N1-C2-O2	7.91	123.65	118.90
36	1	356	C	O5'-P-OP2	-7.91	98.58	105.70
36	1	950	G	C4-C5-N7	7.91	113.96	110.80
36	1	1741	A	N1-C6-N6	7.91	123.34	118.60
36	5	911	C	C6-N1-C2	7.91	123.46	120.30
36	5	2758	A	N9-C4-C5	7.90	108.96	105.80
36	1	701	G	N3-C2-N2	-7.89	114.37	119.90
36	1	2846	U	N3-C4-O4	-7.89	113.87	119.40
36	5	1189	C	N1-C2-O2	-7.89	114.16	118.90
1	2	970	A	N1-C6-N6	7.89	123.34	118.60
36	5	942	U	N3-C4-O4	7.89	124.92	119.40
36	5	1657	C	N1-C2-O2	7.89	123.63	118.90
36	1	1104	G	O5'-P-OP1	-7.89	98.60	105.70
36	5	3012	A	C8-N9-C4	7.88	108.95	105.80
37	7	66	A	O5'-P-OP1	-7.87	98.61	105.70
36	5	1879	A	N1-C6-N6	7.86	123.32	118.60
36	1	958	C	N3-C4-C5	7.86	125.04	121.90
36	5	907	G	O5'-P-OP1	-7.86	98.63	105.70
36	5	1846	C	N3-C4-C5	7.85	125.04	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2923	U	O5'-P-OP1	-7.85	98.63	105.70
36	1	2550	U	N3-C2-O2	-7.85	116.70	122.20
36	1	1506	A	N1-C6-N6	-7.85	113.89	118.60
36	5	922	U	C2-N3-C4	-7.85	122.29	127.00
36	1	2400	G	N9-C4-C5	-7.84	102.26	105.40
36	5	2684	C	C6-N1-C2	-7.84	117.16	120.30
1	6	371	G	N3-C4-N9	7.84	130.71	126.00
36	1	2419	A	OP1-P-OP2	-7.84	107.84	119.60
36	5	1192	C	N1-C2-O2	7.83	123.60	118.90
1	6	647	G	N3-C4-N9	-7.83	121.30	126.00
1	2	576	G	C5-C6-O6	-7.83	123.90	128.60
36	1	85	A	C2-N3-C4	-7.82	106.69	110.60
36	5	2698	G	C8-N9-C4	7.82	109.53	106.40
36	1	1604	G	C4-N9-C1'	7.82	136.66	126.50
36	5	954	U	O5'-P-OP1	-7.81	98.67	105.70
36	5	2965	U	N3-C2-O2	7.80	127.66	122.20
36	1	2758	A	C8-N9-C4	7.80	108.92	105.80
1	6	1025	A	N1-C6-N6	7.80	123.28	118.60
36	5	3154	C	C2-N1-C1'	7.80	127.38	118.80
36	1	29	C	C6-N1-C2	7.79	123.42	120.30
36	1	1349	G	N3-C4-N9	7.79	130.67	126.00
36	5	917	A	O5'-P-OP2	-7.79	98.69	105.70
36	5	2753	G	C8-N9-C4	-7.78	103.29	106.40
1	6	1782	A	C8-N9-C4	-7.78	102.69	105.80
36	5	2816	G	C5-C6-O6	-7.77	123.94	128.60
36	1	1367	G	O5'-P-OP1	-7.77	98.71	105.70
36	1	3278	C	N3-C2-O2	-7.77	116.46	121.90
36	5	2708	C	N1-C2-O2	-7.76	114.24	118.90
36	1	369	A	C8-N9-C4	-7.76	102.70	105.80
36	1	2371	G	O5'-P-OP2	-7.76	98.72	105.70
36	5	95	A	C5-C6-N6	-7.76	117.49	123.70
36	5	776	U	N1-C2-N3	7.76	119.56	114.90
36	1	2996	U	N1-C2-O2	7.75	128.23	122.80
36	5	907	G	N9-C4-C5	-7.75	102.30	105.40
36	5	1152	G	N1-C2-N3	7.75	128.55	123.90
36	5	2872	A	C2-N3-C4	-7.75	106.72	110.60
36	1	2719	U	N1-C2-O2	-7.75	117.38	122.80
1	6	542	A	C6-C5-N7	-7.75	126.88	132.30
46	L9	91	ARG	NE-CZ-NH2	7.74	124.17	120.30
36	1	348	A	N1-C6-N6	7.73	123.24	118.60
1	2	1600	A	C5-C6-N1	-7.73	113.83	117.70
15	C3	22	ALA	C-N-CD	-7.73	103.59	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	716	A	C6-C5-N7	-7.73	126.89	132.30
36	5	211	A	N1-C6-N6	-7.73	113.96	118.60
36	5	92	G	C5-C6-N1	7.72	115.36	111.50
36	1	616	G	C5-C6-O6	-7.72	123.97	128.60
36	5	586	C	N3-C4-C5	7.72	124.99	121.90
36	1	2975	U	N1-C2-O2	7.71	128.20	122.80
36	1	3277	U	N3-C2-O2	-7.71	116.80	122.20
36	5	2944	U	N3-C2-O2	-7.71	116.81	122.20
36	5	2283	G	O5'-P-OP2	-7.70	98.77	105.70
1	2	830	U	N3-C2-O2	-7.70	116.81	122.20
36	5	1879	A	C4-C5-N7	7.69	114.54	110.70
36	5	63	A	C5-C6-N6	-7.69	117.55	123.70
36	1	3181	C	N3-C4-N4	-7.68	112.62	118.00
36	1	2413	A	C8-N9-C4	7.68	108.87	105.80
36	1	2404	A	N1-C6-N6	-7.68	113.99	118.60
36	5	1429	G	N1-C2-N2	-7.68	109.29	116.20
36	1	1117	G	N1-C6-O6	7.68	124.51	119.90
36	5	2726	C	N1-C2-N3	7.68	124.57	119.20
36	1	933	A	N1-C2-N3	7.67	133.14	129.30
36	5	347	G	N3-C4-N9	-7.67	121.39	126.00
36	5	1513	G	N3-C4-C5	-7.67	124.76	128.60
36	5	2981	U	C2-N1-C1'	7.67	126.91	117.70
36	5	1152	G	C5-C6-N1	-7.67	107.67	111.50
36	1	1307	G	C4-C5-N7	-7.67	107.73	110.80
1	6	453	U	C2-N1-C1'	7.67	126.90	117.70
36	1	934	G	O5'-P-OP1	-7.66	98.80	105.70
36	5	607	A	N1-C6-N6	-7.66	114.01	118.60
36	1	958	C	C2-N3-C4	-7.66	116.07	119.90
36	5	672	A	N1-C6-N6	7.66	123.19	118.60
36	1	3006	A	N1-C6-N6	7.65	123.19	118.60
1	6	858	G	O4'-C1'-N9	7.65	114.32	108.20
36	5	337	G	N3-C4-C5	-7.65	124.77	128.60
36	1	3055	U	C5-C4-O4	-7.65	121.31	125.90
36	5	2799	A	O5'-P-OP2	-7.65	98.81	105.70
36	1	25	U	N3-C4-O4	7.65	124.75	119.40
36	5	63	A	C6-C5-N7	-7.65	126.95	132.30
36	5	1300	G	N1-C6-O6	7.65	124.49	119.90
36	5	41	G	N3-C4-C5	7.64	132.42	128.60
36	5	2191	U	N3-C2-O2	-7.64	116.85	122.20
36	5	2954	U	O4'-C1'-N1	7.64	114.31	108.20
36	1	412	G	O5'-P-OP2	-7.64	98.83	105.70
36	1	2407	C	C4-C5-C6	7.64	121.22	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	895	A	C2-N3-C4	-7.63	106.78	110.60
38	4	53	A	C2-N3-C4	7.63	114.42	110.60
38	8	26	U	O5'-P-OP2	-7.63	98.83	105.70
36	5	3093	C	C5-C6-N1	-7.63	117.19	121.00
36	1	3229	G	N1-C6-O6	7.62	124.47	119.90
36	5	3092	C	C6-N1-C2	7.62	123.35	120.30
36	1	334	A	C8-N9-C4	-7.62	102.75	105.80
36	1	54	C	C6-N1-C2	7.62	123.35	120.30
36	1	358	G	C5-C6-O6	-7.62	124.03	128.60
63	n7	5	LEU	CB-CG-CD1	-7.62	98.05	111.00
36	1	1489	A	N9-C4-C5	-7.61	102.76	105.80
36	5	2730	G	C5-C6-O6	-7.61	124.03	128.60
36	1	2812	C	C6-N1-C2	7.61	123.34	120.30
36	1	699	A	C2-N3-C4	-7.60	106.80	110.60
36	5	2889	C	C2-N3-C4	-7.60	116.10	119.90
1	6	1117	U	N3-C4-O4	7.60	124.72	119.40
1	6	1560	U	N3-C2-O2	-7.60	116.88	122.20
36	1	2138	A	C8-N9-C4	-7.60	102.76	105.80
36	1	3001	C	C5-C6-N1	-7.60	117.20	121.00
36	5	2893	C	N3-C4-C5	-7.60	118.86	121.90
36	5	1931	U	C2-N1-C1'	-7.59	108.59	117.70
36	5	1179	A	O5'-P-OP1	-7.59	98.87	105.70
36	5	2364	G	C5-C6-O6	7.58	133.15	128.60
1	6	459	G	N1-C6-O6	7.58	124.45	119.90
36	1	1389	G	C6-C5-N7	-7.58	125.85	130.40
36	1	2550	U	C5-C4-O4	7.58	130.45	125.90
36	1	3215	A	C8-N9-C4	7.58	108.83	105.80
36	1	288	C	N1-C2-O2	-7.58	114.35	118.90
36	5	102	C	N3-C4-N4	7.57	123.30	118.00
36	1	2636	A	N7-C8-N9	7.57	117.59	113.80
1	2	553	G	C5-C6-O6	-7.56	124.06	128.60
36	5	882	A	C8-N9-C4	7.56	108.82	105.80
1	2	507	U	C2-N1-C1'	7.56	126.77	117.70
1	6	1119	G	O5'-P-OP2	-7.56	98.90	105.70
36	5	2180	G	C8-N9-C4	7.56	109.42	106.40
36	5	2389	C	C6-N1-C2	7.55	123.32	120.30
36	1	148	G	N1-C6-O6	7.55	124.43	119.90
36	1	859	G	C8-N9-C4	7.55	109.42	106.40
36	1	2808	A	C5-C6-N1	-7.55	113.93	117.70
36	5	2198	A	O5'-P-OP2	-7.55	98.91	105.70
36	5	981	U	C6-N1-C2	-7.54	116.47	121.00
36	5	95	A	N1-C6-N6	7.54	123.12	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2343	C	N3-C4-C5	7.54	124.92	121.90
36	5	1180	A	O4'-C1'-N9	-7.54	102.17	108.20
36	5	776	U	C4-C5-C6	7.54	124.22	119.70
36	5	2699	G	C4-C5-N7	7.54	113.81	110.80
36	1	120	G	C8-N9-C4	7.53	109.41	106.40
1	6	272	U	N3-C2-O2	-7.53	116.93	122.20
36	5	2965	U	N1-C2-O2	-7.53	117.53	122.80
36	1	909	G	C8-N9-C4	7.52	109.41	106.40
36	5	3209	A	O4'-C1'-N9	7.52	114.22	108.20
36	1	608	A	N1-C6-N6	7.52	123.11	118.60
36	1	2153	U	C6-N1-C2	-7.51	116.49	121.00
36	5	670	C	N3-C2-O2	-7.51	116.64	121.90
36	5	2271	A	C8-N9-C4	7.51	108.80	105.80
36	5	2831	G	C5-C6-N1	7.51	115.26	111.50
38	8	84	C	C6-N1-C2	-7.51	117.30	120.30
36	5	1452	A	C4-C5-N7	7.51	114.45	110.70
36	1	1000	C	C6-N1-C1'	-7.51	111.79	120.80
36	5	1047	A	N1-C6-N6	7.51	123.10	118.60
36	1	2946	A	N1-C6-N6	7.50	123.10	118.60
36	5	2366	C	C6-N1-C2	-7.50	117.30	120.30
36	1	2996	U	C5-C6-N1	7.49	126.45	122.70
38	4	58	G	C5-C6-O6	-7.49	124.11	128.60
36	1	49	A	C8-N9-C4	7.49	108.80	105.80
36	1	716	A	C2-N3-C4	-7.49	106.85	110.60
1	6	756	A	OP1-P-OP2	-7.49	108.36	119.60
36	5	646	A	N1-C6-N6	-7.49	114.11	118.60
36	5	2879	C	C6-N1-C2	7.49	123.30	120.30
36	5	1897	G	C4-C5-N7	7.49	113.80	110.80
38	8	4	C	N1-C2-O2	7.49	123.39	118.90
36	1	718	G	C5-N7-C8	-7.49	100.56	104.30
36	1	2222	A	C8-N9-C4	-7.49	102.81	105.80
36	1	2417	U	C2-N3-C4	-7.49	122.51	127.00
36	5	1445	U	N1-C2-O2	-7.48	117.56	122.80
36	1	28	C	C6-N1-C2	7.48	123.29	120.30
36	5	3195	U	OP1-P-O3'	7.48	121.66	105.20
36	1	2121	G	N1-C6-O6	-7.48	115.41	119.90
36	5	639	G	N1-C6-O6	7.48	124.39	119.90
36	5	1152	G	C4-C5-N7	7.47	113.79	110.80
1	2	1756	A	N1-C6-N6	7.47	123.08	118.60
36	5	1464	G	C8-N9-C4	7.47	109.39	106.40
36	1	2870	C	C6-N1-C1'	7.47	129.76	120.80
36	5	2372	A	N9-C4-C5	7.46	108.79	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1381	A	N1-C2-N3	7.46	133.03	129.30
1	6	610	G	C8-N9-C1'	-7.46	117.30	127.00
36	5	2116	G	C6-C5-N7	-7.46	125.92	130.40
1	6	1340	U	N3-C2-O2	-7.46	116.98	122.20
36	1	3344	A	C8-N9-C4	-7.46	102.82	105.80
36	5	2278	C	C4-C5-C6	-7.46	113.67	117.40
36	5	2797	C	N1-C2-O2	-7.46	114.43	118.90
1	2	577	G	N3-C4-N9	-7.46	121.53	126.00
36	1	2286	U	O5'-P-OP2	-7.45	99.00	105.70
1	2	577	G	N3-C4-C5	7.45	132.32	128.60
36	5	1181	U	C5-C6-N1	-7.45	118.98	122.70
36	1	2878	G	C8-N9-C4	7.44	109.38	106.40
36	5	1375	G	O5'-P-OP2	-7.44	99.00	105.70
36	5	1520	G	N3-C4-C5	-7.44	124.88	128.60
1	2	1761	U	C6-N1-C2	-7.43	116.54	121.00
36	1	645	A	C6-N1-C2	-7.43	114.14	118.60
36	5	3039	C	O5'-P-OP2	-7.43	99.01	105.70
36	1	2808	A	N9-C4-C5	-7.43	102.83	105.80
36	1	3207	U	C6-N1-C1'	7.43	131.60	121.20
1	6	1097	U	P-O3'-C3'	7.43	128.61	119.70
36	1	3207	U	C5-C4-O4	7.42	130.35	125.90
1	6	1643	U	C2-N3-C4	-7.42	122.55	127.00
36	5	838	G	C5-C6-O6	7.42	133.05	128.60
36	1	937	G	O5'-P-OP2	-7.41	99.03	105.70
36	1	1845	G	N9-C4-C5	7.41	108.36	105.40
36	5	2819	A	O5'-P-OP2	-7.41	99.03	105.70
36	5	62	A	O5'-P-OP2	-7.40	99.04	105.70
37	7	105	C	N3-C4-C5	-7.40	118.94	121.90
36	1	932	U	N1-C2-O2	-7.40	117.62	122.80
1	6	29	U	C5-C4-O4	7.40	130.34	125.90
1	6	542	A	N7-C8-N9	7.40	117.50	113.80
1	6	858	G	C4-C5-N7	7.40	113.76	110.80
1	6	371	G	C6-C5-N7	-7.39	125.97	130.40
36	5	1368	U	O5'-P-OP1	-7.39	99.05	105.70
36	5	53	G	O5'-P-OP2	-7.39	99.05	105.70
1	2	1773	C	N3-C4-C5	-7.38	118.95	121.90
36	1	1376	C	C4-C5-C6	7.38	121.09	117.40
36	1	2868	U	C2-N1-C1'	7.38	126.56	117.70
36	1	2830	G	N1-C6-O6	7.38	124.33	119.90
36	1	776	U	C5-C6-N1	-7.38	119.01	122.70
36	5	3245	A	C6-C5-N7	-7.38	127.13	132.30
36	1	2768	U	O5'-P-OP2	-7.37	99.07	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	77	G	N1-C6-O6	7.37	124.32	119.90
1	2	448	C	C6-N1-C2	-7.36	117.35	120.30
1	6	1361	U	C2-N1-C1'	7.36	126.54	117.70
36	1	860	G	N1-C6-O6	7.36	124.32	119.90
36	1	2944	U	N1-C2-O2	7.36	127.95	122.80
36	1	3344	A	N7-C8-N9	7.36	117.48	113.80
36	1	651	G	N3-C4-C5	-7.36	124.92	128.60
36	5	1504	A	C2-N3-C4	-7.36	106.92	110.60
38	4	40	A	C5-C6-N6	-7.35	117.82	123.70
36	1	1320	C	C6-N1-C2	-7.35	117.36	120.30
37	3	75	G	O5'-P-OP1	-7.35	99.09	105.70
36	1	1157	G	C4-C5-N7	-7.34	107.86	110.80
36	1	3216	G	N9-C4-C5	7.34	108.34	105.40
36	1	2624	G	N7-C8-N9	7.34	116.77	113.10
36	5	366	A	C4-C5-N7	7.34	114.37	110.70
36	1	1345	G	O5'-P-OP2	-7.34	99.10	105.70
37	7	93	C	N1-C2-O2	7.34	123.30	118.90
73	o7	65	ARG	NE-CZ-NH1	7.34	123.97	120.30
38	4	111	A	N1-C6-N6	7.34	123.00	118.60
36	5	3060	C	N1-C2-O2	-7.33	114.50	118.90
36	5	3197	G	N3-C4-N9	-7.33	121.60	126.00
1	2	1273	G	O4'-C1'-N9	7.33	114.06	108.20
36	5	1147	G	N3-C2-N2	-7.33	114.77	119.90
36	5	2821	C	N3-C2-O2	7.33	127.03	121.90
36	1	2147	A	O5'-P-OP1	-7.32	99.11	105.70
36	1	1838	G	C5-C6-O6	-7.32	124.21	128.60
1	6	542	A	N1-C6-N6	7.32	122.99	118.60
37	3	94	C	N3-C2-O2	7.31	127.02	121.90
36	5	1305	U	N1-C2-N3	-7.31	110.51	114.90
36	1	963	G	C5-C6-O6	-7.31	124.21	128.60
36	5	3126	C	N3-C4-C5	7.30	124.82	121.90
36	5	2950	G	O4'-C1'-N9	7.30	114.04	108.20
36	5	367	A	C8-N9-C4	7.30	108.72	105.80
1	2	448	C	N3-C4-C5	-7.30	118.98	121.90
36	1	1175	C	O5'-P-OP1	-7.30	99.13	105.70
36	1	298	U	O5'-P-OP2	-7.29	99.14	105.70
36	1	859	G	C6-C5-N7	-7.29	126.03	130.40
36	5	1847	A	C2-N3-C4	-7.29	106.95	110.60
36	5	2978	U	C4-C5-C6	7.29	124.07	119.70
36	5	3218	A	C4-C5-N7	7.28	114.34	110.70
36	5	873	C	O5'-P-OP2	-7.28	99.15	105.70
36	5	2140	U	N1-C2-N3	7.28	119.27	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	900	G	C8-N9-C4	7.28	109.31	106.40
36	5	3006	A	C2-N3-C4	-7.27	106.97	110.60
1	6	29	U	N3-C2-O2	-7.26	117.11	122.20
36	5	1437	C	C6-N1-C2	-7.26	117.39	120.30
38	8	23	U	N1-C2-N3	7.26	119.26	114.90
36	1	1377	G	C4-C5-N7	7.26	113.70	110.80
36	5	2211	U	C5-C4-O4	7.26	130.26	125.90
36	5	3218	A	C5-N7-C8	-7.26	100.27	103.90
36	1	30	G	N1-C6-O6	-7.26	115.55	119.90
36	1	2209	U	C5-C6-N1	7.25	126.33	122.70
1	2	75	U	N3-C2-O2	-7.25	117.12	122.20
36	5	1181	U	C4-C5-C6	7.25	124.05	119.70
36	1	940	G	O5'-P-OP1	-7.25	99.18	105.70
36	1	1180	A	O4'-C1'-N9	-7.24	102.41	108.20
36	5	2145	A	N1-C6-N6	-7.24	114.25	118.60
36	1	2700	G	C4-C5-N7	7.24	113.69	110.80
36	1	343	U	C6-N1-C2	-7.24	116.66	121.00
36	5	1416	C	N3-C2-O2	-7.24	116.83	121.90
36	5	1452	A	C5-C6-N6	-7.24	117.91	123.70
52	m6	94	ARG	NE-CZ-NH1	-7.24	116.68	120.30
36	5	1200	A	C4-C5-C6	7.23	120.62	117.00
1	2	287	G	O4'-C1'-N9	7.23	113.98	108.20
36	1	2153	U	N1-C2-N3	7.23	119.24	114.90
1	6	103	A	P-O3'-C3'	7.23	128.38	119.70
36	5	2932	U	C2-N3-C4	-7.23	122.67	127.00
36	1	1425	U	N1-C2-N3	7.22	119.23	114.90
36	5	651	G	C5-C6-O6	-7.22	124.27	128.60
36	5	1902	G	C6-C5-N7	-7.22	126.07	130.40
36	5	3216	G	C5-C6-O6	-7.22	124.27	128.60
36	1	1192	C	C2-N1-C1'	7.22	126.74	118.80
36	5	2981	U	N3-C2-O2	-7.22	117.15	122.20
36	5	2821	C	C2-N1-C1'	-7.22	110.86	118.80
36	1	639	G	C5-C6-O6	-7.22	124.27	128.60
36	5	2393	G	C5-C6-O6	-7.22	124.27	128.60
36	5	2278	C	C5-C6-N1	7.21	124.61	121.00
36	5	2361	A	OP2-P-O3'	7.21	121.06	105.20
36	1	2572	C	N3-C2-O2	-7.21	116.85	121.90
36	1	2865	U	OP2-P-O3'	7.21	121.06	105.20
37	3	91	G	N1-C6-O6	7.21	124.22	119.90
36	5	1430	U	O5'-P-OP1	-7.21	99.21	105.70
36	5	2412	G	C5-C6-N1	7.21	115.10	111.50
36	1	2621	G	N3-C2-N2	-7.20	114.86	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1113	G	C2-N3-C4	-7.20	108.30	111.90
36	5	827	A	O5'-P-OP1	-7.20	99.22	105.70
38	4	9	A	O5'-P-OP2	-7.20	99.22	105.70
36	1	1130	A	C5-C6-N6	-7.20	117.94	123.70
36	1	3004	C	O5'-P-OP1	-7.20	99.22	105.70
36	5	3143	C	N3-C2-O2	7.20	126.94	121.90
36	5	1866	C	C5-C6-N1	7.19	124.60	121.00
36	5	966	U	C2-N1-C1'	7.19	126.33	117.70
36	5	2883	U	O5'-P-OP2	-7.19	99.23	105.70
36	5	1433	A	C8-N9-C4	-7.18	102.93	105.80
36	1	2827	U	N3-C4-O4	-7.18	114.38	119.40
36	5	2343	C	C6-N1-C2	7.18	123.17	120.30
36	1	1158	A	N1-C6-N6	7.17	122.90	118.60
36	1	2351	U	C5-C6-N1	7.17	126.29	122.70
36	1	2384	A	C6-C5-N7	-7.17	127.28	132.30
36	1	2351	U	O5'-P-OP1	-7.17	99.25	105.70
36	5	2396	G	N3-C2-N2	-7.17	114.88	119.90
36	5	3140	G	N1-C6-O6	7.17	124.20	119.90
38	8	43	A	C8-N9-C4	-7.17	102.93	105.80
1	6	826	U	C5-C6-N1	7.17	126.28	122.70
36	1	1307	G	C8-N9-C4	-7.17	103.53	106.40
36	5	924	G	N1-C6-O6	7.17	124.20	119.90
36	1	2816	G	O4'-C1'-N9	7.16	113.93	108.20
36	5	2392	C	C2-N3-C4	-7.16	116.32	119.90
36	1	881	C	N1-C2-O2	7.16	123.19	118.90
36	5	2899	C	C6-N1-C2	-7.16	117.44	120.30
1	6	308	C	C5-C6-N1	-7.15	117.42	121.00
36	5	3000	A	N1-C6-N6	7.15	122.89	118.60
36	5	200	C	N3-C4-N4	7.15	123.00	118.00
36	5	2411	U	O5'-P-OP2	-7.15	99.27	105.70
36	1	350	C	N3-C2-O2	-7.14	116.90	121.90
36	5	645	A	C6-N1-C2	-7.14	114.31	118.60
36	5	2271	A	N7-C8-N9	-7.14	110.23	113.80
36	1	1303	A	C8-N9-C4	7.14	108.66	105.80
1	2	794	U	N3-C2-O2	-7.14	117.20	122.20
70	O4	51	LEU	CA-CB-CG	7.13	131.71	115.30
36	1	2610	G	C6-C5-N7	-7.13	126.12	130.40
37	3	57	G	N1-C6-O6	-7.13	115.62	119.90
36	1	2808	A	C4-C5-N7	7.13	114.26	110.70
36	5	1846	C	C6-N1-C2	7.13	123.15	120.30
36	5	1139	G	C8-N9-C4	7.12	109.25	106.40
36	5	3078	U	N3-C2-O2	-7.12	117.22	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2234	G	C5-C6-O6	-7.12	124.33	128.60
36	1	635	G	C5-C6-N1	7.12	115.06	111.50
1	2	831	U	C6-N1-C2	-7.12	116.73	121.00
36	1	1313	G	C5-C6-O6	-7.12	124.33	128.60
1	6	163	G	C2-N3-C4	-7.12	108.34	111.90
1	2	1458	G	N9-C4-C5	-7.11	102.56	105.40
36	5	965	A	O5'-P-OP2	-7.11	99.30	105.70
36	5	2320	A	C2-N3-C4	-7.11	107.05	110.60
1	6	75	U	C2-N1-C1'	7.11	126.23	117.70
36	5	3195	U	P-O3'-C3'	7.10	128.22	119.70
1	2	453	U	N1-C2-O2	7.10	127.77	122.80
36	5	283	G	C4-C5-N7	7.10	113.64	110.80
36	1	2756	C	N3-C4-C5	-7.10	119.06	121.90
36	5	2726	C	N3-C4-C5	-7.10	119.06	121.90
36	1	363	G	N1-C6-O6	7.10	124.16	119.90
36	1	2187	G	C6-C5-N7	-7.10	126.14	130.40
36	1	25	U	N3-C4-C5	-7.10	110.34	114.60
36	5	54	C	N1-C2-O2	-7.10	114.64	118.90
36	5	929	A	C8-N9-C4	7.10	108.64	105.80
35	SM	167	PRO	N-CA-CB	7.09	111.81	103.30
36	1	949	C	C6-N1-C2	-7.09	117.46	120.30
36	5	3143	C	N1-C2-O2	-7.09	114.64	118.90
36	5	835	G	O4'-C1'-N9	7.09	113.87	108.20
36	1	2827	U	N3-C2-O2	-7.09	117.23	122.20
38	4	40	A	N9-C4-C5	-7.09	102.96	105.80
1	6	542	A	O4'-C1'-N9	7.09	113.87	108.20
36	5	699	A	C2-N3-C4	-7.09	107.05	110.60
36	5	1003	A	C8-N9-C4	7.09	108.64	105.80
36	1	718	G	C2-N3-C4	-7.09	108.36	111.90
36	1	1467	A	N9-C4-C5	7.09	108.64	105.80
36	5	1696	A	O5'-P-OP2	-7.09	99.32	105.70
36	5	3335	A	N1-C6-N6	7.08	122.85	118.60
1	6	1773	C	N1-C2-O2	-7.08	114.65	118.90
36	5	945	C	C6-N1-C2	7.08	123.13	120.30
36	5	3206	C	N3-C2-O2	-7.08	116.94	121.90
1	6	957	G	N1-C6-O6	7.08	124.15	119.90
36	1	2873	U	N3-C2-O2	-7.07	117.25	122.20
38	4	113	U	C5-C4-O4	7.07	130.15	125.90
36	5	1300	G	OP1-P-O3'	7.07	120.76	105.20
36	5	3154	C	N1-C2-O2	7.07	123.14	118.90
36	1	1156	C	C5-C6-N1	-7.07	117.47	121.00
36	1	1422	G	O5'-P-OP1	-7.07	99.34	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	337	G	N3-C2-N2	7.07	124.85	119.90
37	7	112	G	C8-N9-C4	-7.07	103.57	106.40
36	5	1500	G	C8-N9-C4	7.06	109.22	106.40
36	5	3306	U	O5'-P-OP2	-7.06	99.35	105.70
36	1	329	U	N1-C2-O2	-7.06	117.86	122.80
36	1	3151	U	O5'-P-OP2	-7.05	99.35	105.70
36	5	2915	U	C6-N1-C2	7.05	125.23	121.00
1	2	1745	G	C5-C6-O6	-7.05	124.37	128.60
36	1	939	U	O5'-P-OP1	7.05	119.16	110.70
36	5	1897	G	C5-C6-O6	-7.05	124.37	128.60
36	1	2831	G	N1-C6-O6	7.05	124.13	119.90
36	5	719	U	N3-C2-O2	-7.05	117.27	122.20
36	5	1306	G	C5-C6-O6	-7.05	124.37	128.60
36	5	2758	A	C2-N3-C4	7.05	114.12	110.60
36	5	2848	G	C6-C5-N7	-7.05	126.17	130.40
36	5	424	G	C5-C6-O6	-7.05	124.37	128.60
36	5	2396	G	C8-N9-C4	-7.05	103.58	106.40
36	5	2295	A	C5-C6-N6	-7.04	118.06	123.70
36	5	819	U	N3-C4-C5	-7.04	110.38	114.60
36	1	890	C	C6-N1-C2	-7.04	117.48	120.30
36	5	581	U	C5-C6-N1	7.04	126.22	122.70
36	1	2397	A	N9-C4-C5	-7.04	102.99	105.80
36	5	3211	C	C6-N1-C2	7.03	123.11	120.30
36	1	24	G	N9-C4-C5	-7.03	102.59	105.40
36	1	2359	C	O5'-P-OP2	-7.03	99.37	105.70
36	5	2400	G	C4-C5-N7	7.03	113.61	110.80
38	4	32	C	C4-C5-C6	-7.02	113.89	117.40
38	4	99	C	C6-N1-C2	7.02	123.11	120.30
36	5	3362	A	O4'-C1'-N9	7.02	113.82	108.20
36	5	1528	G	C4-C5-N7	7.02	113.61	110.80
36	1	901	G	N1-C6-O6	7.01	124.11	119.90
36	1	1133	A	O5'-P-OP2	-7.01	99.39	105.70
36	5	2411	U	N3-C4-C5	7.01	118.81	114.60
36	5	2830	G	N1-C2-N3	7.01	128.11	123.90
36	1	2811	A	C8-N9-C4	-7.01	103.00	105.80
36	5	2142	A	OP1-P-O3'	7.01	120.62	105.20
36	1	1556	C	P-O3'-C3'	7.01	128.11	119.70
36	5	2943	G	C5-C6-O6	-7.00	124.40	128.60
36	1	2376	G	C5-C6-O6	-7.00	124.40	128.60
36	5	691	A	C2-N3-C4	-7.00	107.10	110.60
36	1	2605	G	N1-C6-O6	7.00	124.10	119.90
36	1	339	C	C5-C4-N4	7.00	125.10	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1368	U	C5-C4-O4	-7.00	121.70	125.90
36	5	861	C	C6-N1-C2	7.00	123.10	120.30
36	5	1190	A	C8-N9-C4	-7.00	103.00	105.80
36	1	2165	G	O5'-P-OP2	-6.99	99.41	105.70
36	5	1208	U	C5-C4-O4	6.99	130.10	125.90
36	1	2836	C	C5-C4-N4	6.99	125.09	120.20
36	1	2373	A	C8-N9-C4	-6.99	103.00	105.80
36	5	651	G	N1-C6-O6	6.99	124.09	119.90
36	1	1489	A	C5-C6-N6	-6.99	118.11	123.70
36	1	2954	U	C6-N1-C2	6.99	125.19	121.00
36	5	3179	U	O5'-P-OP1	-6.99	99.41	105.70
36	1	639	G	N3-C2-N2	-6.99	115.01	119.90
36	5	3200	G	N1-C6-O6	6.99	124.09	119.90
36	5	1131	G	N1-C2-N3	6.98	128.09	123.90
36	5	1208	U	N1-C2-N3	6.98	119.09	114.90
36	5	3154	C	C6-N1-C2	-6.98	117.51	120.30
36	1	909	G	O5'-P-OP1	-6.98	99.42	105.70
36	1	895	A	C6-C5-N7	-6.98	127.42	132.30
36	1	2138	A	N1-C2-N3	6.98	132.79	129.30
36	5	2836	C	C4-C5-C6	6.98	120.89	117.40
1	2	553	G	C6-C5-N7	-6.98	126.21	130.40
36	5	2618	G	C5-C6-O6	-6.98	124.41	128.60
36	1	908	G	O4'-C1'-N9	-6.97	102.62	108.20
36	5	1419	A	O5'-P-OP2	-6.97	99.42	105.70
36	1	400	G	C5-C6-O6	-6.97	124.42	128.60
36	5	2314	U	C5-C4-O4	-6.97	121.72	125.90
36	1	2343	C	N3-C4-C5	6.97	124.69	121.90
1	6	136	C	C2-N1-C1'	6.97	126.47	118.80
36	1	2995	A	C8-N9-C4	6.97	108.59	105.80
36	1	1151	U	N3-C4-O4	6.96	124.28	119.40
36	1	2808	A	C5-N7-C8	-6.96	100.42	103.90
36	1	1192	C	N3-C2-O2	-6.96	117.03	121.90
38	4	14	C	N3-C4-C5	6.96	124.68	121.90
36	5	1858	A	O4'-C1'-N9	6.96	113.77	108.20
36	1	816	A	N9-C4-C5	6.96	108.58	105.80
36	5	3075	G	N1-C6-O6	6.96	124.08	119.90
36	1	2764	C	C5-C6-N1	6.96	124.48	121.00
36	5	871	U	C5-C4-O4	6.96	130.07	125.90
36	5	2148	U	C2-N1-C1'	-6.96	109.35	117.70
36	5	640	U	N3-C2-O2	6.96	127.07	122.20
1	2	558	U	C2-N1-C1'	6.95	126.04	117.70
36	1	410	U	N1-C2-O2	-6.95	117.93	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2898	G	O4'-C1'-N9	-6.95	102.64	108.20
36	1	1133	A	N9-C4-C5	-6.95	103.02	105.80
36	1	1547	G	C8-N9-C4	6.95	109.18	106.40
36	5	2302	G	N1-C6-O6	-6.95	115.73	119.90
36	5	2550	U	C5-C4-O4	6.95	130.07	125.90
1	2	571	G	N3-C4-N9	-6.95	121.83	126.00
36	1	2978	U	O4'-C1'-N1	6.95	113.76	108.20
1	6	858	G	C6-C5-N7	-6.95	126.23	130.40
36	1	627	U	C2-N1-C1'	-6.94	109.37	117.70
1	2	1431	C	C6-N1-C2	6.94	123.08	120.30
36	1	2130	G	N1-C6-O6	-6.94	115.73	119.90
36	5	2709	C	N3-C4-C5	6.94	124.68	121.90
36	1	2159	U	C6-N1-C2	6.94	125.16	121.00
36	1	2343	C	C6-N1-C2	6.94	123.08	120.30
36	1	3209	A	N1-C6-N6	6.94	122.76	118.60
36	1	3268	A	C4-C5-C6	6.94	120.47	117.00
36	1	648	C	C6-N1-C1'	-6.93	112.48	120.80
36	5	1848	G	C4-C5-N7	6.93	113.57	110.80
36	5	2379	U	C5-C6-N1	-6.93	119.23	122.70
51	m5	98	LEU	CA-CB-CG	6.93	131.25	115.30
36	5	1881	A	N1-C6-N6	6.93	122.76	118.60
36	5	1060	U	N3-C4-O4	-6.93	114.55	119.40
36	1	835	G	O4'-C1'-N9	6.93	113.74	108.20
36	1	2403	G	O5'-P-OP2	-6.93	99.46	105.70
36	1	28	C	N3-C4-C5	6.93	124.67	121.90
36	1	2679	A	C2-N3-C4	-6.93	107.14	110.60
36	5	2943	G	N9-C4-C5	-6.92	102.63	105.40
36	1	2836	C	N3-C2-O2	-6.92	117.05	121.90
36	5	2887	A	O5'-P-OP1	-6.92	99.47	105.70
44	17	229	PHE	CB-CG-CD1	6.92	125.65	120.80
36	1	93	C	C6-N1-C2	-6.92	117.53	120.30
36	1	942	U	N3-C4-O4	6.92	124.25	119.40
36	1	1365	G	N3-C4-N9	6.92	130.15	126.00
36	1	2257	C	C6-N1-C2	-6.92	117.53	120.30
36	1	3362	A	C6-C5-N7	-6.92	127.46	132.30
36	5	2385	G	N3-C4-N9	-6.92	121.85	126.00
36	5	1462	A	C2-N3-C4	-6.91	107.14	110.60
36	1	1149	G	N9-C4-C5	6.91	108.17	105.40
36	5	3209	A	N7-C8-N9	6.91	117.26	113.80
36	1	1001	G	C6-C5-N7	-6.91	126.25	130.40
36	1	785	G	N3-C4-C5	-6.91	125.15	128.60
38	4	79	A	C8-N9-C4	-6.91	103.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1116	G	C8-N9-C4	-6.91	103.64	106.40
36	5	2351	U	C6-N1-C2	-6.91	116.86	121.00
36	1	2836	C	C4-C5-C6	6.91	120.85	117.40
36	5	3287	U	N1-C2-O2	6.91	127.64	122.80
36	1	2975	U	N3-C2-O2	-6.91	117.37	122.20
36	5	838	G	N1-C6-O6	-6.91	115.76	119.90
36	1	808	A	C6-N1-C2	-6.90	114.46	118.60
36	1	1294	A	C2-N3-C4	6.90	114.05	110.60
1	6	68	A	N1-C6-N6	6.90	122.74	118.60
1	6	377	G	C6-C5-N7	6.90	134.54	130.40
36	5	217	U	C5-C6-N1	-6.90	119.25	122.70
36	5	361	A	N1-C6-N6	-6.90	114.46	118.60
36	1	2944	U	N3-C4-C5	6.90	118.74	114.60
36	5	2231	C	O4'-C1'-N1	6.90	113.72	108.20
1	2	794	U	N1-C2-O2	6.89	127.62	122.80
36	1	2798	C	N1-C2-O2	-6.89	114.76	118.90
36	5	55	G	C8-N9-C4	6.89	109.16	106.40
36	5	609	G	O5'-P-OP2	-6.89	99.50	105.70
36	1	670	C	C4-C5-C6	6.89	120.84	117.40
36	5	146	U	C5-C6-N1	-6.89	119.25	122.70
36	5	718	G	C8-N9-C4	-6.89	103.64	106.40
36	5	2915	U	N3-C4-C5	6.89	118.73	114.60
36	5	1149	G	C5-C6-O6	-6.89	124.47	128.60
36	5	1592	G	C5-C6-N1	-6.88	108.06	111.50
36	5	2897	A	N1-C6-N6	6.88	122.73	118.60
36	1	1391	C	C5-C4-N4	-6.88	115.38	120.20
24	d2	93	LEU	CA-CB-CG	6.88	131.13	115.30
1	6	1581	C	C6-N1-C2	6.88	123.05	120.30
36	1	2726	C	N3-C4-N4	-6.88	113.19	118.00
1	6	1000	C	N3-C2-O2	-6.88	117.09	121.90
36	5	1524	A	C8-N9-C4	6.88	108.55	105.80
36	1	640	U	OP2-P-O3'	6.87	120.32	105.20
36	5	2666	C	O5'-P-OP2	-6.87	99.51	105.70
1	2	694	U	C2-N1-C1'	6.87	125.95	117.70
36	5	1116	G	N9-C4-C5	6.87	108.15	105.40
36	5	2841	G	C4-C5-N7	6.87	113.55	110.80
36	5	2954	U	C6-N1-C1'	-6.87	111.58	121.20
36	5	1426	C	N1-C2-O2	-6.87	114.78	118.90
52	m6	84	LEU	CB-CG-CD1	-6.87	99.32	111.00
36	5	2421	U	N1-C2-O2	-6.87	117.99	122.80
36	1	3181	C	C6-N1-C2	-6.87	117.55	120.30
36	1	386	A	N1-C6-N6	6.86	122.72	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	217	U	OP1-P-O3'	6.86	120.30	105.20
36	1	1458	U	C5-C6-N1	-6.86	119.27	122.70
37	7	101	G	N9-C4-C5	-6.86	102.66	105.40
1	2	434	G	O5'-P-OP2	-6.86	99.53	105.70
36	1	948	C	N1-C2-O2	-6.86	114.78	118.90
36	1	2855	U	N3-C4-O4	-6.86	114.60	119.40
36	1	918	C	N1-C2-O2	-6.85	114.79	118.90
36	1	937	G	C8-N9-C4	6.85	109.14	106.40
36	1	1376	C	N3-C4-C5	-6.85	119.16	121.90
1	6	795	U	N3-C2-O2	-6.85	117.40	122.20
36	1	3362	A	N1-C6-N6	6.85	122.71	118.60
36	5	651	G	C6-C5-N7	-6.85	126.29	130.40
36	1	2417	U	C5-C6-N1	-6.85	119.28	122.70
1	6	359	A	C6-N1-C2	6.85	122.71	118.60
36	5	1169	A	N1-C2-N3	6.85	132.72	129.30
36	1	24	G	C8-N9-C4	6.85	109.14	106.40
1	6	1340	U	N1-C2-O2	6.85	127.59	122.80
36	1	2808	A	O4'-C1'-N9	-6.84	102.72	108.20
1	2	966	A	N1-C6-N6	6.84	122.71	118.60
36	1	284	A	C8-N9-C4	-6.84	103.06	105.80
1	6	362	G	C8-N9-C1'	-6.84	118.11	127.00
36	5	2887	A	O4'-C1'-N9	-6.84	102.73	108.20
36	5	2941	A	O4'-C1'-N9	-6.84	102.73	108.20
36	5	2395	G	O5'-P-OP2	-6.84	99.54	105.70
36	5	1412	G	C8-N9-C4	-6.84	103.67	106.40
36	1	2173	U	N1-C2-O2	-6.84	118.01	122.80
36	1	1920	U	N3-C2-O2	-6.83	117.42	122.20
36	1	895	A	C4-C5-N7	6.83	114.12	110.70
36	1	2434	U	C5-C4-O4	6.83	130.00	125.90
36	1	3362	A	N7-C8-N9	6.83	117.22	113.80
36	5	1419	A	O5'-P-OP1	6.83	118.90	110.70
36	5	2928	C	N3-C4-N4	6.83	122.78	118.00
1	6	858	G	C4-N9-C1'	6.83	135.38	126.50
36	5	2632	G	O5'-P-OP1	-6.83	99.55	105.70
36	5	2993	G	C4-C5-N7	6.83	113.53	110.80
36	1	1849	C	N3-C2-O2	6.83	126.68	121.90
36	5	997	A	C8-N9-C4	-6.83	103.07	105.80
36	1	590	G	C4-C5-N7	6.83	113.53	110.80
36	1	882	A	O5'-P-OP2	-6.83	99.56	105.70
36	1	340	C	N3-C2-O2	-6.83	117.12	121.90
36	1	2400	G	C8-N9-C4	6.83	109.13	106.40
36	5	1191	U	O5'-P-OP1	-6.83	99.56	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1328	C	C4-C5-C6	6.83	120.81	117.40
36	5	2765	C	N3-C4-N4	6.83	122.78	118.00
38	4	38	U	N3-C2-O2	-6.82	117.42	122.20
36	5	1165	A	O5'-P-OP2	-6.82	99.56	105.70
36	1	280	U	N1-C2-O2	-6.82	118.03	122.80
36	1	2585	G	N3-C4-C5	-6.82	125.19	128.60
36	1	3078	U	N1-C2-O2	6.82	127.57	122.80
36	5	2211	U	N1-C2-N3	6.82	118.99	114.90
1	6	1568	C	C6-N1-C2	-6.82	117.57	120.30
36	5	2231	C	C2-N1-C1'	6.82	126.30	118.80
20	c8	116	LEU	CA-CB-CG	6.82	130.98	115.30
36	5	1874	A	C8-N9-C4	6.82	108.53	105.80
36	5	2356	A	C2-N3-C4	-6.82	107.19	110.60
36	1	2937	G	C8-N9-C4	6.82	109.13	106.40
36	5	1532	C	C6-N1-C2	6.82	123.03	120.30
36	5	92	G	N3-C4-C5	-6.81	125.19	128.60
36	5	3018	C	O5'-P-OP2	-6.81	99.57	105.70
36	1	2883	U	C5-C6-N1	6.81	126.11	122.70
36	1	1506	A	N9-C4-C5	6.81	108.52	105.80
36	1	2358	A	C8-N9-C4	6.81	108.52	105.80
36	5	2283	G	C5-C6-O6	-6.81	124.52	128.60
36	1	439	C	C6-N1-C1'	-6.80	112.64	120.80
36	1	877	C	N3-C4-C5	6.80	124.62	121.90
1	6	20	G	N1-C6-O6	6.80	123.98	119.90
36	5	881	C	N3-C2-O2	-6.80	117.14	121.90
12	C0	88	PRO	N-CA-CB	6.80	111.46	103.30
36	1	609	G	O5'-P-OP2	-6.80	99.58	105.70
36	5	1375	G	C2-N3-C4	6.80	115.30	111.90
36	5	1321	G	N1-C6-O6	6.79	123.98	119.90
1	6	1058	U	OP1-P-O3'	6.79	120.15	105.20
36	5	586	C	C6-N1-C2	6.79	123.02	120.30
36	1	2192	C	O5'-P-OP2	-6.79	99.59	105.70
36	1	2827	U	C5-C6-N1	-6.79	119.30	122.70
1	6	1767	G	C8-N9-C4	6.79	109.11	106.40
36	5	1115	G	C4-N9-C1'	6.79	135.33	126.50
36	5	2377	G	N7-C8-N9	-6.79	109.70	113.10
36	1	1144	U	C5-C6-N1	-6.79	119.31	122.70
36	1	2719	U	C2-N1-C1'	-6.79	109.56	117.70
36	5	2572	C	C2-N1-C1'	6.79	126.26	118.80
36	1	1510	G	N3-C4-N9	6.78	130.07	126.00
36	1	2147	A	C8-N9-C4	6.78	108.51	105.80
36	5	644	G	C8-N9-C4	-6.78	103.69	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	874	U	O5'-P-OP1	-6.78	99.60	105.70
36	1	636	C	O5'-P-OP1	-6.78	99.60	105.70
36	1	1797	A	O5'-P-OP1	-6.78	99.60	105.70
36	5	640	U	C5-C4-O4	-6.78	121.83	125.90
36	5	1495	U	N3-C4-C5	-6.78	110.53	114.60
36	1	1117	G	C5-C6-O6	-6.78	124.53	128.60
36	1	3057	U	N1-C2-N3	6.78	118.97	114.90
36	5	1520	G	C8-N9-C4	-6.78	103.69	106.40
36	5	1799	A	N1-C6-N6	6.78	122.67	118.60
36	5	2295	A	C2-N3-C4	6.78	113.99	110.60
1	2	576	G	N1-C6-O6	6.77	123.96	119.90
36	1	1316	C	C2-N3-C4	-6.77	116.51	119.90
36	1	2361	A	C5-N7-C8	6.77	107.29	103.90
36	1	654	C	C6-N1-C2	6.77	123.01	120.30
36	5	776	U	C2-N3-C4	-6.77	122.94	127.00
36	1	2231	C	C6-N1-C2	6.77	123.01	120.30
1	6	1773	C	C6-N1-C2	-6.77	117.59	120.30
36	5	2983	C	N3-C4-C5	-6.77	119.19	121.90
1	6	65	A	C5-C6-N1	-6.77	114.32	117.70
1	6	542	A	O5'-P-OP1	-6.77	99.61	105.70
36	5	2147	A	C6-C5-N7	-6.77	127.56	132.30
36	5	2413	A	C2-N3-C4	-6.77	107.22	110.60
1	6	139	C	C6-N1-C2	-6.77	117.59	120.30
36	5	1847	A	C8-N9-C4	6.77	108.51	105.80
1	2	1389	C	N1-C2-O2	6.76	122.96	118.90
1	6	610	G	C4-N9-C1'	6.76	135.29	126.50
36	1	1604	G	C8-N9-C1'	-6.76	118.22	127.00
37	3	98	C	N1-C2-O2	-6.76	114.85	118.90
36	5	2765	C	C5-C6-N1	6.76	124.38	121.00
36	5	2944	U	C6-N1-C2	-6.76	116.95	121.00
36	5	2699	G	C6-C5-N7	-6.75	126.35	130.40
36	5	1848	G	C5-C6-O6	-6.75	124.55	128.60
36	5	92	G	O5'-P-OP1	-6.75	99.62	105.70
36	1	86	G	C4-C5-N7	-6.75	108.10	110.80
36	5	1300	G	C5-C6-O6	-6.75	124.55	128.60
36	5	217	U	OP1-P-O3'	6.75	120.04	105.20
36	5	639	G	C5-C6-N1	-6.75	108.13	111.50
36	1	2958	A	C5-C6-N1	6.75	121.07	117.70
36	1	2293	C	C5-C4-N4	-6.74	115.48	120.20
36	5	1556	C	C6-N1-C2	-6.74	117.60	120.30
36	5	3028	G	N3-C2-N2	6.74	124.62	119.90
36	1	2893	C	N3-C4-C5	6.74	124.59	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	337	G	C8-N9-C1'	-6.74	118.24	127.00
36	1	943	U	N3-C2-O2	-6.74	117.48	122.20
36	1	3215	A	N1-C6-N6	6.74	122.64	118.60
1	6	90	C	C2-N3-C4	-6.74	116.53	119.90
36	5	2345	A	C4-C5-C6	6.74	120.37	117.00
36	1	421	G	N3-C4-N9	6.73	130.04	126.00
36	5	2796	G	O5'-P-OP2	-6.73	99.64	105.70
36	5	1433	A	C6-N1-C2	-6.73	114.56	118.60
36	1	200	C	C2-N3-C4	-6.73	116.54	119.90
36	1	282	G	N1-C6-O6	-6.73	115.86	119.90
36	5	1194	G	N1-C6-O6	-6.73	115.86	119.90
36	5	2412	G	N3-C4-C5	-6.73	125.24	128.60
36	1	2601	A	C5-C6-N1	6.73	121.06	117.70
36	5	2764	C	C2-N3-C4	6.73	123.26	119.90
36	1	2417	U	N1-C2-O2	-6.72	118.09	122.80
36	5	1200	A	C6-C5-N7	-6.72	127.60	132.30
1	6	1749	A	N1-C6-N6	6.72	122.63	118.60
36	5	1161	G	C5-C6-N1	6.72	114.86	111.50
73	O7	65	ARG	NE-CZ-NH1	6.72	123.66	120.30
36	5	824	C	C6-N1-C2	-6.72	117.61	120.30
36	5	1879	A	C6-C5-N7	-6.72	127.60	132.30
36	1	2873	U	C5-C4-O4	6.71	129.93	125.90
36	5	2341	A	N7-C8-N9	-6.71	110.44	113.80
36	5	2988	C	C5-C6-N1	-6.71	117.64	121.00
36	1	1313	G	C4-C5-N7	6.71	113.48	110.80
1	6	609	U	N3-C4-O4	-6.71	114.70	119.40
36	5	3362	A	C2-N3-C4	-6.71	107.24	110.60
36	5	347	G	N9-C4-C5	6.71	108.08	105.40
36	5	1795	U	O5'-P-OP2	6.71	118.75	110.70
1	2	831	U	C2-N1-C1'	6.71	125.75	117.70
36	1	44	U	N1-C2-O2	-6.71	118.11	122.80
36	1	1907	C	O5'-P-OP2	-6.71	99.66	105.70
36	1	2197	C	N1-C2-N3	-6.71	114.51	119.20
36	1	2983	C	O4'-C1'-N1	6.71	113.56	108.20
36	1	2403	G	OP1-P-O3'	6.71	119.95	105.20
36	5	779	G	O5'-P-OP2	-6.70	99.67	105.70
36	5	881	C	C5-C6-N1	6.70	124.35	121.00
37	7	101	G	C4-C5-N7	6.70	113.48	110.80
36	1	930	U	C5-C6-N1	-6.70	119.35	122.70
36	5	2191	U	N3-C4-O4	-6.70	114.71	119.40
36	1	793	C	N3-C2-O2	6.70	126.59	121.90
36	1	1897	G	C5-C6-O6	-6.70	124.58	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2366	C	C2-N3-C4	6.70	123.25	119.90
36	5	180	C	N3-C2-O2	-6.70	117.21	121.90
36	1	2647	A	C6-N1-C2	-6.70	114.58	118.60
36	1	3215	A	N9-C4-C5	-6.70	103.12	105.80
36	5	1868	G	N1-C6-O6	6.70	123.92	119.90
36	5	2872	A	N3-C4-C5	6.69	131.49	126.80
1	2	1773	C	C6-N1-C2	-6.69	117.62	120.30
36	5	1116	G	N3-C4-C5	-6.69	125.25	128.60
36	1	1331	U	O4'-C1'-N1	-6.69	102.85	108.20
36	1	2731	U	N1-C2-O2	-6.69	118.12	122.80
36	5	1389	G	C5-C6-O6	-6.69	124.59	128.60
36	1	595	G	C5-C6-N1	-6.69	108.16	111.50
36	5	389	A	N1-C6-N6	-6.69	114.59	118.60
36	1	661	G	C8-N9-C4	-6.69	103.72	106.40
36	5	1390	A	C5-C6-N6	6.69	129.05	123.70
36	1	1506	A	C5-C6-N6	6.69	129.05	123.70
38	4	51	G	C5-C6-O6	-6.69	124.59	128.60
36	1	1166	G	N1-C6-O6	6.68	123.91	119.90
36	5	1420	C	C2-N1-C1'	-6.68	111.45	118.80
36	5	1701	C	C6-N1-C2	-6.68	117.63	120.30
36	5	1879	A	O5'-P-OP1	6.68	118.71	110.70
36	5	2271	A	N1-C6-N6	-6.68	114.59	118.60
36	1	785	G	N3-C4-N9	6.68	130.01	126.00
36	5	1490	A	C8-N9-C4	-6.68	103.13	105.80
36	1	2121	G	N3-C4-C5	-6.67	125.26	128.60
36	1	895	A	C5-N7-C8	-6.67	100.56	103.90
36	5	1868	G	N9-C4-C5	-6.67	102.73	105.40
1	2	57	G	O5'-P-OP2	-6.67	99.69	105.70
36	1	3368	U	C2-N1-C1'	-6.67	109.70	117.70
36	1	3362	A	O4'-C1'-N9	6.66	113.53	108.20
36	1	2165	G	C4-C5-N7	6.66	113.46	110.80
36	1	2177	G	N3-C4-C5	-6.66	125.27	128.60
41	L4	206	LEU	CA-CB-CG	6.66	130.62	115.30
36	1	280	U	C5-C4-O4	-6.66	121.91	125.90
36	5	1848	G	N1-C6-O6	6.66	123.89	119.90
36	5	3112	G	C4-C5-N7	6.66	113.46	110.80
36	5	3277	U	N3-C2-O2	-6.66	117.54	122.20
36	5	2871	G	O5'-P-OP2	-6.65	99.71	105.70
1	2	1596	C	N3-C2-O2	-6.65	117.24	121.90
36	1	2247	G	N1-C6-O6	6.65	123.89	119.90
36	5	2808	A	C8-N9-C4	6.65	108.46	105.80
36	5	2349	U	OP1-P-O3'	6.65	119.83	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	658	G	C4-N9-C1'	6.65	135.14	126.50
36	5	3197	G	N9-C4-C5	6.65	108.06	105.40
36	1	2384	A	C5-C6-N6	-6.64	118.39	123.70
36	5	2134	G	N9-C4-C5	-6.64	102.74	105.40
37	7	101	G	C5-C6-O6	-6.64	124.61	128.60
36	5	216	G	C4-C5-N7	6.64	113.46	110.80
36	5	424	G	C4-C5-N7	6.64	113.46	110.80
38	4	15	G	C5-C6-O6	-6.64	124.62	128.60
1	6	371	G	C4-N9-C1'	6.64	135.13	126.50
36	5	2400	G	C4-N9-C1'	-6.64	117.87	126.50
1	6	815	G	C6-C5-N7	-6.63	126.42	130.40
36	5	39	A	N1-C6-N6	6.63	122.58	118.60
36	1	2144	A	C5-C6-N1	6.63	121.02	117.70
36	1	2756	C	N3-C4-N4	6.63	122.64	118.00
36	5	3287	U	N3-C2-O2	-6.63	117.56	122.20
36	1	1381	A	N1-C6-N6	6.63	122.58	118.60
1	6	558	U	C2-N1-C1'	6.63	125.65	117.70
36	5	3006	A	C8-N9-C4	-6.62	103.15	105.80
36	5	934	G	C4-N9-C1'	6.62	135.11	126.50
36	1	1520	G	N7-C8-N9	-6.62	109.79	113.10
36	1	1416	C	N3-C4-C5	6.62	124.55	121.90
36	5	1488	G	N1-C6-O6	-6.62	115.93	119.90
36	5	3362	A	N1-C2-N3	6.62	132.61	129.30
36	5	1449	A	C4-C5-C6	6.62	120.31	117.00
36	5	2815	G	N7-C8-N9	-6.62	109.79	113.10
1	6	1662	G	C8-N9-C4	6.62	109.05	106.40
36	5	1192	C	N3-C2-O2	-6.62	117.27	121.90
36	1	785	G	O5'-P-OP2	-6.61	99.75	105.70
36	1	907	G	O4'-C1'-N9	6.61	113.49	108.20
36	1	1295	G	O5'-P-OP1	-6.61	99.75	105.70
36	1	2358	A	C2-N3-C4	-6.61	107.29	110.60
1	6	1125	A	C2-N3-C4	-6.61	107.29	110.60
36	1	2130	G	C5-C6-O6	6.61	132.57	128.60
36	5	2176	U	N3-C2-O2	-6.61	117.57	122.20
36	5	2708	C	N3-C2-O2	6.61	126.53	121.90
36	1	3382	U	N1-C2-O2	6.61	127.42	122.80
36	1	2148	U	N3-C2-O2	6.61	126.82	122.20
36	1	2875	U	P-O3'-C3'	-6.61	111.77	119.70
36	5	2870	C	N3-C4-C5	6.61	124.54	121.90
36	1	2816	G	C5-C6-O6	-6.60	124.64	128.60
36	1	867	G	N3-C2-N2	-6.60	115.28	119.90
36	1	2283	G	C5-C6-O6	-6.60	124.64	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	924	G	C5-C6-N1	-6.60	108.20	111.50
36	5	3188	G	N3-C4-C5	-6.60	125.30	128.60
1	6	1782	A	N9-C4-C5	6.60	108.44	105.80
36	5	1200	A	C5-C6-N6	-6.60	118.42	123.70
36	5	2944	U	C5-C6-N1	6.59	126.00	122.70
36	5	2899	C	N3-C2-O2	-6.59	117.28	121.90
36	5	1316	C	N1-C2-O2	-6.59	114.94	118.90
36	1	1604	G	N3-C4-C5	-6.59	125.31	128.60
36	5	3362	A	C5-N7-C8	-6.59	100.61	103.90
36	1	2944	U	O5'-P-OP1	-6.59	99.77	105.70
1	6	144	U	N1-C2-O2	6.59	127.41	122.80
36	5	636	C	O5'-P-OP2	-6.59	99.77	105.70
36	1	1792	C	N1-C2-O2	-6.58	114.95	118.90
36	1	49	A	C2-N3-C4	-6.58	107.31	110.60
36	5	2145	A	N3-C4-C5	-6.58	122.19	126.80
36	5	2349	U	N3-C2-O2	-6.58	117.59	122.20
1	6	1700	C	N1-C2-O2	6.58	122.85	118.90
36	1	2714	G	C4-C5-C6	-6.58	114.85	118.80
36	5	1512	U	O5'-P-OP1	-6.58	99.78	105.70
36	1	3141	A	C8-N9-C4	6.58	108.43	105.80
36	5	806	A	C4-C5-C6	-6.58	113.71	117.00
36	5	1429	G	N3-C2-N2	6.58	124.50	119.90
1	2	1486	G	C5-N7-C8	-6.58	101.01	104.30
36	1	2812	C	O5'-P-OP1	-6.58	99.78	105.70
36	5	877	C	C5-C4-N4	-6.58	115.60	120.20
1	2	388	G	C5-C6-O6	-6.57	124.66	128.60
36	5	1124	U	N3-C4-O4	-6.57	114.80	119.40
36	5	1879	A	C5-N7-C8	-6.57	100.61	103.90
36	5	2849	C	N3-C2-O2	6.57	126.50	121.90
36	1	658	G	C8-N9-C1'	-6.57	118.46	127.00
36	1	917	A	O5'-P-OP2	-6.57	99.79	105.70
36	5	890	C	C4-C5-C6	6.57	120.69	117.40
36	1	1405	U	C6-N1-C2	6.57	124.94	121.00
36	5	366	A	C2-N3-C4	-6.57	107.32	110.60
36	5	2169	G	N9-C4-C5	6.57	108.03	105.40
36	1	634	C	C2-N1-C1'	-6.57	111.58	118.80
36	1	3326	G	C8-N9-C4	6.57	109.03	106.40
36	5	3059	G	C8-N9-C4	6.57	109.03	106.40
1	2	1120	U	C5-C4-O4	6.56	129.84	125.90
36	1	56	G	C5-C6-O6	-6.56	124.66	128.60
36	1	2935	U	C5-C6-N1	6.56	125.98	122.70
1	6	404	G	N3-C2-N2	-6.56	115.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	504	A	C8-N9-C4	6.56	108.43	105.80
1	2	380	U	N3-C2-O2	-6.56	117.61	122.20
36	1	1343	A	C5-C6-N6	-6.56	118.45	123.70
1	6	377	G	C8-N9-C1'	6.56	135.53	127.00
1	2	1560	U	C5-C4-O4	6.56	129.84	125.90
10	S8	29	LEU	CA-CB-CG	6.56	130.39	115.30
36	1	776	U	N1-C2-N3	6.56	118.83	114.90
36	1	885	U	C5-C6-N1	-6.56	119.42	122.70
36	1	2159	U	C5-C6-N1	-6.56	119.42	122.70
36	1	1307	G	OP1-P-O3'	6.56	119.62	105.20
36	1	2601	A	C8-N9-C4	6.56	108.42	105.80
36	5	2231	C	C6-N1-C2	-6.56	117.68	120.30
36	1	2679	A	O4'-C1'-N9	6.55	113.44	108.20
36	5	665	A	N1-C6-N6	6.55	122.53	118.60
36	5	662	U	O5'-P-OP1	-6.55	99.80	105.70
36	1	1902	G	N9-C4-C5	-6.55	102.78	105.40
36	1	2606	G	N3-C4-N9	6.55	129.93	126.00
36	5	41	G	N9-C4-C5	-6.55	102.78	105.40
36	1	54	C	C2-N1-C1'	-6.55	111.60	118.80
36	5	911	C	C2-N3-C4	-6.55	116.63	119.90
36	5	1846	C	C2-N3-C4	-6.55	116.63	119.90
36	1	2625	C	N1-C2-O2	-6.54	114.97	118.90
36	1	1007	U	C5-C4-O4	-6.54	121.97	125.90
1	6	558	U	P-O3'-C3'	6.54	127.55	119.70
1	6	1700	C	C2-N1-C1'	6.54	126.00	118.80
36	1	1489	A	C6-C5-N7	-6.54	127.72	132.30
36	5	1859	A	O5'-P-OP2	-6.54	99.81	105.70
36	1	2606	G	C6-C5-N7	-6.54	126.48	130.40
36	5	1528	G	C6-C5-N7	-6.54	126.48	130.40
36	1	1198	C	C6-N1-C2	-6.54	117.69	120.30
36	1	614	C	C6-N1-C2	6.54	122.92	120.30
36	1	2147	A	C5-C6-N1	6.54	120.97	117.70
1	6	1631	A	N1-C6-N6	-6.54	114.68	118.60
36	5	1130	A	C2-N3-C4	6.54	113.87	110.60
36	1	304	G	N9-C4-C5	6.53	108.01	105.40
36	1	1405	U	N3-C2-O2	6.53	126.77	122.20
36	5	800	G	N3-C4-N9	6.53	129.92	126.00
36	5	216	G	C5-C6-O6	-6.53	124.68	128.60
36	5	1548	C	N1-C2-O2	-6.53	114.98	118.90
36	1	1547	G	N7-C8-N9	-6.53	109.84	113.10
1	6	1726	G	OP2-P-O3'	6.53	119.56	105.20
36	1	1124	U	N3-C4-C5	6.53	118.52	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3112	G	OP1-P-O3'	6.53	119.56	105.20
36	5	425	G	C2-N3-C4	-6.53	108.64	111.90
36	5	2314	U	N3-C4-O4	6.53	123.97	119.40
36	1	2213	A	N1-C6-N6	-6.53	114.69	118.60
36	5	911	C	C4-C5-C6	6.53	120.66	117.40
40	l3	196	ARG	NE-CZ-NH1	6.52	123.56	120.30
36	1	1897	G	N1-C6-O6	6.52	123.81	119.90
36	1	2355	G	C6-C5-N7	-6.52	126.49	130.40
1	6	371	G	C8-N9-C1'	-6.52	118.52	127.00
36	5	647	A	C2-N3-C4	-6.52	107.34	110.60
36	1	944	C	C5-C6-N1	6.52	124.26	121.00
36	5	2184	U	N3-C4-C5	6.52	118.51	114.60
1	2	728	U	C2-N1-C1'	6.51	125.52	117.70
1	6	287	G	C5-C6-O6	-6.51	124.69	128.60
36	5	3183	A	N1-C6-N6	6.51	122.51	118.60
36	1	709	A	N7-C8-N9	-6.51	110.55	113.80
36	1	1099	A	N1-C6-N6	6.51	122.51	118.60
36	1	1414	G	N1-C6-O6	6.51	123.81	119.90
36	1	1794	G	O5'-P-OP2	-6.51	99.84	105.70
36	5	907	G	C8-N9-C4	6.51	109.00	106.40
38	4	40	A	C4-C5-N7	6.51	113.95	110.70
36	5	562	C	C2-N1-C1'	6.50	125.95	118.80
1	6	696	C	O4'-C1'-N1	6.50	113.40	108.20
36	5	1408	G	N3-C2-N2	-6.50	115.35	119.90
36	5	3035	A	C8-N9-C4	6.50	108.40	105.80
36	5	326	U	O5'-P-OP2	-6.50	99.85	105.70
36	5	2395	G	C4-C5-N7	6.50	113.40	110.80
36	5	2735	U	C5-C6-N1	6.50	125.95	122.70
40	l3	4	ARG	NE-CZ-NH1	6.50	123.55	120.30
36	1	347	G	C5-C6-O6	-6.50	124.70	128.60
36	5	2110	G	C4-C5-N7	6.50	113.40	110.80
1	2	1196	A	P-O3'-C3'	6.50	127.49	119.70
75	O9	36	ARG	NE-CZ-NH1	6.50	123.55	120.30
36	5	2693	C	C2-N3-C4	-6.50	116.65	119.90
36	1	1101	G	C5-C6-O6	6.49	132.50	128.60
36	5	3181	C	C2-N1-C1'	6.49	125.94	118.80
36	1	2714	G	C4-N9-C1'	-6.49	118.06	126.50
36	1	2633	U	N3-C2-O2	-6.49	117.66	122.20
36	1	1838	G	C6-C5-N7	-6.49	126.51	130.40
36	5	1329	U	C2-N3-C4	-6.48	123.11	127.00
36	5	2346	C	N3-C4-N4	6.48	122.54	118.00
36	5	3362	A	N7-C8-N9	6.48	117.04	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1365	G	C2-N3-C4	6.48	115.14	111.90
36	1	2856	G	C8-N9-C4	6.48	108.99	106.40
36	5	816	A	N9-C4-C5	6.48	108.39	105.80
36	5	1335	C	C5-C4-N4	-6.48	115.66	120.20
36	1	1308	A	C4-C5-C6	6.48	120.24	117.00
36	5	803	C	C5-C4-N4	-6.48	115.66	120.20
36	5	2414	G	N1-C6-O6	6.48	123.79	119.90
36	1	1177	G	C5-C6-O6	-6.48	124.71	128.60
36	5	3046	A	O5'-P-OP2	-6.47	99.87	105.70
36	1	86	G	N9-C4-C5	6.47	107.99	105.40
36	1	2976	A	C5-C6-N6	-6.47	118.52	123.70
36	1	965	A	OP1-P-O3'	6.47	119.43	105.20
36	1	2959	C	N3-C4-C5	6.47	124.49	121.90
36	1	3368	U	C6-N1-C1'	6.47	130.26	121.20
1	2	425	A	N1-C6-N6	6.47	122.48	118.60
1	6	1119	G	C8-N9-C4	-6.47	103.81	106.40
36	1	627	U	N1-C2-O2	-6.47	118.27	122.80
36	1	3183	A	C5-C6-N6	-6.47	118.53	123.70
36	5	767	U	O4'-C1'-N1	6.47	113.37	108.20
36	5	3014	U	C5-C4-O4	-6.47	122.02	125.90
49	M3	85	LEU	CA-CB-CG	6.46	130.16	115.30
36	5	2601	A	N1-C6-N6	-6.46	114.72	118.60
36	1	3217	C	C2-N1-C1'	6.46	125.90	118.80
36	1	1140	G	N3-C2-N2	6.46	124.42	119.90
36	1	2176	U	N3-C2-O2	-6.46	117.68	122.20
36	1	2406	C	C6-N1-C2	6.46	122.88	120.30
36	5	1303	A	C5-C6-N6	-6.46	118.53	123.70
36	5	3195	U	O4'-C1'-N1	6.46	113.36	108.20
36	1	2836	C	N1-C2-N3	6.45	123.72	119.20
36	5	2156	C	C6-N1-C2	6.45	122.88	120.30
36	5	2980	U	N1-C2-N3	6.45	118.77	114.90
1	2	572	C	O5'-P-OP1	-6.45	99.89	105.70
36	1	694	C	N3-C4-C5	6.45	124.48	121.90
36	1	1798	A	C2-N3-C4	-6.45	107.38	110.60
36	1	859	G	C4-C5-N7	6.45	113.38	110.80
36	1	2610	G	C5-C6-O6	-6.45	124.73	128.60
1	6	308	C	C2-N1-C1'	-6.45	111.71	118.80
1	6	1091	A	C2-N3-C4	-6.45	107.38	110.60
36	1	3178	A	C4-C5-C6	6.45	120.22	117.00
36	5	1912	U	N3-C2-O2	6.45	126.71	122.20
36	1	1820	U	P-O3'-C3'	6.44	127.43	119.70
36	5	637	C	O5'-P-OP2	-6.44	99.90	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1869	C	O5'-P-OP2	-6.44	99.90	105.70
36	1	2693	C	N3-C4-C5	6.44	124.48	121.90
36	1	3078	U	N3-C2-O2	-6.44	117.69	122.20
36	1	2381	G	C5-C6-O6	6.44	132.46	128.60
36	5	3136	G	N1-C2-N2	-6.44	110.40	116.20
36	1	1466	G	N3-C2-N2	6.44	124.41	119.90
36	1	895	A	N1-C6-N6	6.44	122.46	118.60
36	5	95	A	C4-C5-N7	6.44	113.92	110.70
36	5	824	C	N3-C2-O2	-6.44	117.39	121.90
36	1	2617	U	N3-C4-O4	-6.44	114.89	119.40
1	2	507	U	N1-C2-O2	6.43	127.30	122.80
36	1	931	C	C2-N3-C4	-6.43	116.68	119.90
36	5	1420	C	OP2-P-O3'	6.43	119.36	105.20
38	4	44	A	C6-C5-N7	-6.43	127.80	132.30
36	5	2757	U	N1-C2-N3	6.43	118.76	114.90
1	6	542	A	C5-N7-C8	-6.43	100.69	103.90
36	1	227	G	N1-C6-O6	6.43	123.76	119.90
36	1	718	G	C6-C5-N7	-6.42	126.55	130.40
36	5	1449	A	N1-C6-N6	6.42	122.45	118.60
36	5	1834	U	N3-C4-C5	-6.42	110.75	114.60
36	1	645	A	N3-C4-C5	-6.42	122.31	126.80
36	1	2693	C	C6-N1-C2	6.42	122.87	120.30
36	1	1344	G	N9-C4-C5	-6.42	102.83	105.40
36	1	637	C	C5-C6-N1	-6.42	117.79	121.00
36	1	2725	U	C5-C6-N1	-6.42	119.49	122.70
36	5	2406	C	N1-C2-O2	-6.42	115.05	118.90
36	1	801	A	N1-C2-N3	-6.41	126.09	129.30
1	6	630	A	N9-C4-C5	-6.41	103.23	105.80
36	5	419	G	N3-C2-N2	6.41	124.39	119.90
36	1	24	G	C8-N9-C1'	-6.41	118.67	127.00
1	6	65	A	N3-C4-C5	6.41	131.29	126.80
36	5	694	C	N3-C2-O2	-6.41	117.42	121.90
36	5	2164	A	C4-C5-C6	6.41	120.20	117.00
36	1	669	U	C6-N1-C2	6.41	124.84	121.00
36	1	2177	G	N3-C4-N9	6.40	129.84	126.00
36	1	2794	G	N9-C4-C5	6.40	107.96	105.40
36	1	2222	A	N9-C4-C5	6.40	108.36	105.80
36	1	2302	G	C5-C6-O6	6.40	132.44	128.60
1	6	448	C	C6-N1-C2	-6.40	117.74	120.30
1	6	451	A	O5'-P-OP1	-6.40	99.94	105.70
35	sM	167	PRO	N-CA-CB	6.40	110.98	103.30
36	5	1369	A	N1-C6-N6	6.40	122.44	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	140	G	C5-C6-N1	-6.40	108.30	111.50
36	5	612	U	O5'-P-OP1	-6.40	99.94	105.70
36	5	2412	G	C8-N9-C4	-6.40	103.84	106.40
36	1	1407	A	C5-N7-C8	6.40	107.10	103.90
36	5	2975	U	N1-C2-O2	6.40	127.28	122.80
36	5	1799	A	C5-C6-N6	-6.40	118.58	123.70
36	5	2830	G	C2-N3-C4	-6.39	108.70	111.90
36	1	2384	A	N9-C4-C5	-6.39	103.24	105.80
36	1	3006	A	C2-N3-C4	-6.39	107.40	110.60
48	M1	112	LEU	CA-CB-CG	6.39	130.00	115.30
36	5	1364	C	OP2-P-O3'	6.39	119.26	105.20
36	5	3140	G	C4-C5-N7	6.39	113.36	110.80
36	5	1184	A	N1-C6-N6	-6.39	114.77	118.60
36	5	2953	U	N3-C4-O4	6.39	123.87	119.40
1	2	1761	U	P-O3'-C3'	6.39	127.37	119.70
36	1	148	G	C5-C6-O6	-6.39	124.77	128.60
36	1	1433	A	C5-C6-N6	-6.39	118.59	123.70
36	1	2621	G	N1-C6-O6	6.39	123.73	119.90
36	1	3266	G	N9-C4-C5	6.39	107.96	105.40
36	5	83	U	N3-C2-O2	-6.39	117.73	122.20
36	5	2816	G	C6-N1-C2	-6.39	121.27	125.10
41	14	327	LEU	CA-CB-CG	6.39	130.00	115.30
1	2	590	C	C2-N1-C1'	6.39	125.83	118.80
36	1	1589	A	C5-C6-N6	-6.39	118.59	123.70
36	5	886	C	C6-N1-C2	-6.39	117.75	120.30
36	5	2403	G	O5'-P-OP1	6.39	118.36	110.70
36	1	1929	G	N9-C4-C5	-6.38	102.85	105.40
1	2	425	A	C5-N7-C8	-6.38	100.71	103.90
36	1	590	G	C5-C6-O6	-6.38	124.77	128.60
36	5	3079	U	C5-C4-O4	6.38	129.73	125.90
36	1	2714	G	C5-N7-C8	-6.38	101.11	104.30
36	1	2976	A	C6-N1-C2	-6.38	114.77	118.60
36	5	2957	G	C5-C6-O6	-6.38	124.77	128.60
36	1	1904	C	C5-C6-N1	6.38	124.19	121.00
36	5	103	G	N1-C6-O6	-6.38	116.07	119.90
36	1	2305	G	C5-C6-O6	-6.38	124.77	128.60
37	3	74	C	O5'-P-OP1	-6.38	99.96	105.70
1	6	371	G	N3-C4-C5	-6.38	125.41	128.60
36	1	320	G	O5'-P-OP2	-6.38	99.96	105.70
36	1	350	C	N3-C4-C5	-6.38	119.35	121.90
36	1	3041	U	N1-C2-O2	-6.38	118.34	122.80
36	5	57	A	C5-C6-N6	-6.38	118.60	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	859	G	C4-C5-N7	6.38	113.35	110.80
36	5	1369	A	C5-C6-N6	-6.38	118.60	123.70
36	5	1909	A	C8-N9-C4	6.38	108.35	105.80
36	1	2943	G	N1-C6-O6	6.38	123.72	119.90
36	1	1849	C	C5-C4-N4	-6.37	115.74	120.20
36	5	2186	U	O5'-P-OP2	-6.37	99.96	105.70
36	1	1495	U	C5-C4-O4	6.37	129.72	125.90
36	1	2952	G	C8-N9-C1'	-6.37	118.72	127.00
36	1	3204	C	C6-N1-C2	-6.37	117.75	120.30
36	5	200	C	N3-C4-C5	-6.37	119.35	121.90
36	5	2897	A	C5-C6-N6	-6.37	118.61	123.70
36	1	3227	A	O5'-P-OP2	-6.37	99.97	105.70
36	5	121	A	C5-C6-N6	-6.37	118.61	123.70
36	5	3330	A	C6-N1-C2	-6.37	114.78	118.60
45	18	69	LEU	CA-CB-CG	6.37	129.94	115.30
36	1	2605	G	C5-C6-O6	-6.36	124.78	128.60
36	1	2874	G	C5-C6-O6	6.36	132.42	128.60
1	6	1765	A	O5'-P-OP1	-6.36	99.97	105.70
1	2	986	G	N3-C4-C5	-6.36	125.42	128.60
36	1	3079	U	C2-N1-C1'	-6.36	110.07	117.70
1	6	377	G	C4-N9-C1'	-6.36	118.23	126.50
36	5	3078	U	N1-C2-O2	6.36	127.25	122.80
36	1	1385	C	N3-C2-O2	6.36	126.35	121.90
36	1	2954	U	N3-C2-O2	6.36	126.65	122.20
36	5	1188	U	N1-C2-N3	6.36	118.72	114.90
36	1	1154	A	C4-C5-C6	6.36	120.18	117.00
36	5	1047	A	C6-C5-N7	-6.36	127.85	132.30
36	5	1519	G	N1-C6-O6	6.35	123.71	119.90
36	1	1520	G	C5-N7-C8	6.35	107.48	104.30
36	5	1437	C	C2-N1-C1'	6.35	125.79	118.80
1	6	1740	A	C8-N9-C4	6.35	108.34	105.80
36	5	2345	A	C6-C5-N7	-6.35	127.86	132.30
36	5	1305	U	O5'-P-OP1	-6.35	99.99	105.70
36	5	1595	U	N3-C2-O2	6.35	126.64	122.20
36	1	1103	A	N9-C4-C5	-6.34	103.26	105.80
36	1	1133	A	C6-C5-N7	-6.34	127.86	132.30
38	4	47	C	N3-C2-O2	-6.34	117.46	121.90
37	7	11	A	C5-N7-C8	-6.34	100.73	103.90
1	2	323	A	C8-N9-C4	-6.34	103.26	105.80
36	1	363	G	C6-C5-N7	-6.34	126.59	130.40
36	1	363	G	C4-C5-N7	6.34	113.34	110.80
36	1	3181	C	N1-C2-N3	6.34	123.64	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1051	U	N1-C2-O2	-6.34	118.36	122.80
36	1	2620	G	C8-N9-C4	6.34	108.94	106.40
36	5	1595	U	N1-C2-O2	-6.34	118.36	122.80
36	5	2978	U	N1-C2-N3	6.34	118.70	114.90
36	1	3132	C	O5'-P-OP1	6.33	118.30	110.70
10	S8	172	ARG	NE-CZ-NH1	6.33	123.47	120.30
36	1	25	U	C4-C5-C6	6.33	123.50	119.70
36	1	149	U	N3-C4-O4	6.33	123.83	119.40
36	1	939	U	C2-N3-C4	-6.33	123.20	127.00
36	1	1578	C	C6-N1-C2	-6.33	117.77	120.30
53	M7	56	ARG	NE-CZ-NH2	-6.33	117.13	120.30
36	5	2134	G	N3-C2-N2	6.33	124.33	119.90
1	2	321	C	N1-C2-O2	6.33	122.70	118.90
36	1	2403	G	N3-C4-N9	6.33	129.80	126.00
1	6	14	C	O5'-P-OP2	-6.33	100.00	105.70
1	2	1747	G	C2-N3-C4	-6.33	108.73	111.90
36	1	1741	A	C2-N3-C4	-6.33	107.44	110.60
36	5	2584	G	C4-N9-C1'	6.33	134.73	126.50
36	5	145	G	N3-C4-N9	-6.33	122.20	126.00
36	5	1303	A	N1-C6-N6	6.33	122.40	118.60
36	1	1133	A	C6-N1-C2	-6.33	114.80	118.60
1	2	1462	G	N9-C4-C5	-6.33	102.87	105.40
36	1	343	U	N3-C4-C5	-6.33	110.80	114.60
36	1	945	C	O5'-P-OP2	-6.33	100.01	105.70
36	1	1344	G	C8-N9-C4	6.33	108.93	106.40
36	1	957	C	O5'-P-OP2	-6.32	100.01	105.70
36	1	984	G	N1-C2-N2	-6.32	110.51	116.20
36	1	1339	C	N1-C2-O2	-6.32	115.11	118.90
1	2	848	C	C6-N1-C2	-6.32	117.77	120.30
36	1	776	U	C5-C4-O4	6.32	129.69	125.90
36	5	2393	G	N1-C6-O6	6.32	123.69	119.90
36	5	3204	C	O5'-P-OP2	-6.32	100.01	105.70
36	1	639	G	C5-C6-N1	-6.32	108.34	111.50
36	1	2144	A	C2-N3-C4	6.32	113.76	110.60
36	1	2256	A	O5'-P-OP2	-6.32	100.01	105.70
36	5	2659	G	N1-C6-O6	6.32	123.69	119.90
37	7	103	A	N1-C6-N6	6.32	122.39	118.60
36	1	2726	C	N1-C2-O2	6.32	122.69	118.90
36	1	3275	U	C5-C6-N1	6.32	125.86	122.70
36	5	922	U	N3-C4-O4	-6.32	114.98	119.40
1	2	1386	G	C8-N9-C4	6.31	108.93	106.40
36	1	14	U	O5'-P-OP2	-6.31	100.02	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	697	A	C8-N9-C4	6.31	108.33	105.80
36	1	1158	A	C5-C6-N6	-6.31	118.65	123.70
36	1	1407	A	N7-C8-N9	-6.31	110.64	113.80
36	1	2714	G	C8-N9-C1'	6.31	135.21	127.00
36	1	2726	C	C5-C4-N4	6.31	124.62	120.20
36	1	510	G	N3-C2-N2	-6.31	115.48	119.90
36	1	808	A	N1-C2-N3	6.31	132.45	129.30
36	1	1003	A	N1-C6-N6	6.31	122.39	118.60
36	1	1097	G	O5'-P-OP2	-6.31	100.02	105.70
1	6	687	G	N3-C2-N2	-6.31	115.48	119.90
36	5	718	G	O4'-C1'-N9	6.31	113.25	108.20
36	1	821	U	C5-C4-O4	6.31	129.68	125.90
36	1	979	U	O4'-C1'-N1	6.31	113.25	108.20
36	1	2870	C	N3-C4-N4	-6.31	113.58	118.00
36	1	2401	A	C8-N9-C4	-6.30	103.28	105.80
1	6	1100	G	C2-N3-C4	6.30	115.05	111.90
36	5	1365	G	C4-C5-N7	6.30	113.32	110.80
36	5	2283	G	N1-C6-O6	6.30	123.68	119.90
36	5	2372	A	N7-C8-N9	6.30	116.95	113.80
36	1	2367	A	N1-C6-N6	6.30	122.38	118.60
36	5	250	U	C5-C6-N1	6.30	125.85	122.70
1	2	864	U	N3-C2-O2	-6.30	117.79	122.20
36	1	943	U	N1-C2-O2	6.30	127.21	122.80
1	6	1780	G	N3-C2-N2	6.30	124.31	119.90
36	5	2116	G	N3-C4-N9	6.30	129.78	126.00
36	5	3137	C	N3-C4-N4	-6.30	113.59	118.00
37	7	108	A	N1-C6-N6	6.30	122.38	118.60
36	1	3053	G	N1-C6-O6	-6.30	116.12	119.90
36	1	3362	A	C5-N7-C8	-6.30	100.75	103.90
1	6	308	C	C2-N3-C4	-6.30	116.75	119.90
36	1	1466	G	N1-C2-N2	-6.30	110.53	116.20
36	5	3112	G	C5-C6-O6	-6.30	124.82	128.60
36	5	1464	G	N9-C4-C5	-6.30	102.88	105.40
36	5	3301	U	O5'-P-OP1	-6.30	100.03	105.70
36	5	1520	G	C6-C5-N7	-6.29	126.62	130.40
36	5	2838	A	O5'-P-OP1	6.29	118.25	110.70
36	5	2978	U	N3-C2-O2	-6.29	117.80	122.20
36	1	54	C	N3-C4-N4	-6.29	113.60	118.00
36	5	1476	G	N3-C4-C5	6.29	131.74	128.60
37	7	12	U	C5-C4-O4	-6.29	122.13	125.90
1	6	1000	C	C2-N1-C1'	6.29	125.72	118.80
1	6	1581	C	N3-C4-C5	6.29	124.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	77	G	C5-C6-O6	-6.29	124.83	128.60
36	5	2514	U	C5-C6-N1	6.28	125.84	122.70
1	6	425	A	N1-C6-N6	-6.28	114.83	118.60
36	1	288	C	N3-C4-N4	6.28	122.40	118.00
36	1	304	G	N3-C2-N2	-6.28	115.50	119.90
1	6	359	A	N3-C4-C5	6.28	131.20	126.80
36	1	2411	U	N3-C4-O4	-6.28	115.00	119.40
36	1	3259	U	N1-C2-O2	-6.28	118.41	122.80
1	6	747	C	N1-C2-O2	-6.28	115.13	118.90
36	1	810	A	C8-N9-C4	-6.28	103.29	105.80
36	5	2770	G	C8-N9-C4	-6.28	103.89	106.40
1	2	647	G	N3-C2-N2	-6.27	115.51	119.90
36	1	830	A	C6-C5-N7	-6.27	127.91	132.30
38	4	85	G	N7-C8-N9	6.27	116.24	113.10
1	6	418	G	C4-C5-N7	6.27	113.31	110.80
36	1	797	U	OP2-P-O3'	6.27	119.00	105.20
36	1	1495	U	C2-N3-C4	-6.27	123.24	127.00
1	6	1100	G	C5-C6-N1	6.27	114.64	111.50
36	5	1770	G	C4-N9-C1'	6.27	134.65	126.50
36	5	1834	U	N1-C2-O2	-6.27	118.41	122.80
36	5	2112	U	C6-N1-C2	-6.27	117.24	121.00
36	5	2242	A	O5'-P-OP2	-6.27	100.05	105.70
36	1	1741	A	C6-C5-N7	-6.27	127.91	132.30
36	1	2397	A	O5'-P-OP2	-6.27	100.06	105.70
36	1	2878	G	N1-C6-O6	6.27	123.66	119.90
36	5	3142	A	O5'-P-OP1	-6.27	100.06	105.70
1	2	966	A	C5-C6-N6	-6.27	118.69	123.70
36	1	227	G	N3-C2-N2	-6.27	115.51	119.90
36	1	1792	C	C4-C5-C6	6.27	120.53	117.40
36	5	3004	C	N1-C2-O2	-6.27	115.14	118.90
36	5	1468	A	N1-C6-N6	6.26	122.36	118.60
36	5	207	U	N1-C2-O2	-6.26	118.42	122.80
36	1	213	A	N1-C6-N6	6.26	122.36	118.60
1	6	609	U	N3-C2-O2	-6.26	117.82	122.20
1	6	1036	A	O5'-P-OP2	-6.26	100.06	105.70
1	2	647	G	N3-C4-N9	-6.26	122.25	126.00
36	5	3277	U	N1-C2-O2	6.26	127.18	122.80
1	6	1742	U	O5'-P-OP2	-6.26	100.07	105.70
36	1	979	U	N1-C2-N3	6.26	118.65	114.90
36	1	2295	A	N1-C6-N6	6.26	122.35	118.60
36	5	1175	C	N3-C4-C5	6.26	124.40	121.90
36	5	2838	A	N1-C6-N6	6.26	122.35	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2983	C	C6-N1-C2	-6.26	117.80	120.30
36	5	3084	C	C6-N1-C2	6.25	122.80	120.30
36	1	2132	C	O5'-P-OP2	-6.25	100.07	105.70
36	5	38	U	C5-C6-N1	-6.25	119.57	122.70
36	1	719	U	O5'-P-OP1	-6.25	100.07	105.70
36	5	1426	C	N3-C2-O2	6.25	126.28	121.90
36	5	2851	A	C2-N3-C4	-6.25	107.47	110.60
36	1	49	A	N1-C6-N6	6.25	122.35	118.60
36	1	968	G	N3-C4-C5	-6.25	125.47	128.60
36	5	2526	C	N1-C2-O2	6.25	122.65	118.90
36	5	819	U	N1-C2-O2	-6.25	118.43	122.80
61	n5	115	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	2	831	U	C5-C6-N1	6.25	125.82	122.70
36	5	2610	G	C5-C6-N1	-6.25	108.38	111.50
1	2	1202	A	C8-N9-C4	-6.24	103.30	105.80
36	1	350	C	C2-N1-C1'	6.24	125.67	118.80
36	1	816	A	C8-N9-C4	-6.24	103.30	105.80
1	6	136	C	N1-C2-O2	6.24	122.65	118.90
36	5	2911	A	N1-C6-N6	6.24	122.35	118.60
36	5	3378	C	C2-N3-C4	-6.24	116.78	119.90
1	6	75	U	N1-C2-O2	6.24	127.17	122.80
36	5	2286	U	N3-C2-O2	-6.24	117.83	122.20
36	5	2572	C	N3-C2-O2	-6.24	117.53	121.90
37	7	69	C	C6-N1-C2	6.24	122.80	120.30
36	1	1655	G	N9-C4-C5	-6.24	102.91	105.40
43	L6	78	ARG	NE-CZ-NH1	6.24	123.42	120.30
36	5	1200	A	OP1-P-O3'	6.24	118.92	105.20
36	5	1879	A	N9-C4-C5	-6.24	103.31	105.80
36	1	421	G	C8-N9-C4	6.24	108.89	106.40
36	5	2330	C	O5'-P-OP2	-6.24	100.09	105.70
1	2	1745	G	N3-C4-N9	6.24	129.74	126.00
36	1	395	A	C8-N9-C4	-6.24	103.31	105.80
36	5	3369	G	C2-N3-C4	6.24	115.02	111.90
36	5	810	A	C5-C6-N1	6.23	120.82	117.70
36	1	1467	A	C8-N9-C4	-6.23	103.31	105.80
36	5	810	A	C2-N3-C4	6.23	113.72	110.60
1	2	1291	G	N3-C4-N9	-6.23	122.26	126.00
36	5	922	U	C4-C5-C6	6.23	123.44	119.70
36	1	2376	G	N7-C8-N9	6.23	116.21	113.10
36	5	40	A	C6-C5-N7	-6.23	127.94	132.30
36	5	2283	G	C4-C5-N7	6.23	113.29	110.80
36	1	2860	U	O5'-P-OP1	-6.23	100.10	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	973	A	O5'-P-OP2	-6.22	100.10	105.70
36	1	2396	G	N9-C4-C5	6.22	107.89	105.40
36	5	1500	G	N7-C8-N9	-6.22	109.99	113.10
36	5	2400	G	N9-C4-C5	-6.22	102.91	105.40
36	1	859	G	N3-C2-N2	6.22	124.25	119.90
36	5	2928	C	C5-C4-N4	-6.22	115.84	120.20
36	1	1133	A	C8-N9-C4	6.22	108.29	105.80
36	1	2817	A	C5-C6-N6	-6.22	118.72	123.70
36	5	791	A	N1-C6-N6	6.22	122.33	118.60
36	5	1303	A	C8-N9-C4	6.22	108.29	105.80
36	5	2598	G	N1-C6-O6	6.22	123.63	119.90
36	5	2916	U	C4-C5-C6	6.22	123.43	119.70
36	5	3188	G	N1-C6-O6	-6.22	116.17	119.90
36	1	111	C	N3-C4-C5	6.21	124.39	121.90
36	1	2692	A	C8-N9-C4	-6.21	103.31	105.80
36	1	2935	U	N3-C4-C5	-6.21	110.87	114.60
36	1	2938	G	OP1-P-OP2	6.21	128.92	119.60
1	6	314	C	C6-N1-C2	-6.21	117.81	120.30
36	5	3153	U	N1-C2-O2	6.21	127.15	122.80
36	5	2411	U	C6-N1-C2	6.21	124.73	121.00
36	1	813	G	N3-C2-N2	6.21	124.25	119.90
1	6	158	U	P-O3'-C3'	6.21	127.15	119.70
36	5	1817	G	O4'-C1'-N9	6.21	113.17	108.20
36	5	3052	G	C5-C6-O6	6.21	132.33	128.60
36	1	702	C	N1-C2-O2	-6.21	115.17	118.90
36	1	1902	G	C5-N7-C8	-6.21	101.20	104.30
36	5	3026	G	C5-C6-O6	-6.21	124.88	128.60
36	1	3115	C	C6-N1-C2	6.21	122.78	120.30
36	1	3275	U	OP1-P-O3'	6.21	118.85	105.20
38	4	16	G	C8-N9-C4	6.21	108.88	106.40
36	5	2147	A	C5-N7-C8	-6.21	100.80	103.90
1	2	1463	C	C6-N1-C2	6.21	122.78	120.30
36	1	66	A	O5'-P-OP2	6.21	118.15	110.70
1	6	1766	A	C5-C6-N1	-6.21	114.60	117.70
36	5	661	G	C5-C6-O6	-6.20	124.88	128.60
36	5	1174	G	C8-N9-C1'	-6.20	118.93	127.00
36	5	1481	A	P-O3'-C3'	6.20	127.14	119.70
36	5	1511	U	C5-C6-N1	-6.20	119.60	122.70
36	1	400	G	N1-C6-O6	6.20	123.62	119.90
36	5	1131	G	OP1-P-OP2	6.20	128.90	119.60
36	5	2943	G	N3-C4-N9	6.20	129.72	126.00
38	4	85	G	C8-N9-C4	-6.20	103.92	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	92	G	N1-C6-O6	-6.20	116.18	119.90
36	5	2309	A	N1-C6-N6	-6.20	114.88	118.60
36	5	2874	G	C5-C6-O6	6.20	132.32	128.60
36	1	2406	C	N1-C2-O2	-6.20	115.18	118.90
36	5	1917	C	N1-C2-O2	-6.20	115.18	118.90
36	1	1339	C	C2-N3-C4	-6.20	116.80	119.90
36	5	1110	U	N1-C2-O2	6.20	127.14	122.80
36	1	1140	G	N1-C2-N2	-6.19	110.63	116.20
36	1	1520	G	C2-N3-C4	6.19	115.00	111.90
36	5	2285	C	C6-N1-C2	-6.19	117.82	120.30
1	2	555	A	C8-N9-C4	-6.19	103.32	105.80
36	1	2872	A	N1-C6-N6	-6.19	114.89	118.60
36	1	2899	C	C2-N1-C1'	6.19	125.61	118.80
21	c9	57	ARG	NE-CZ-NH2	-6.19	117.20	120.30
36	5	145	G	N3-C4-C5	6.19	131.69	128.60
36	5	639	G	N3-C2-N2	-6.19	115.57	119.90
36	1	1442	U	N1-C2-O2	-6.19	118.47	122.80
36	1	2937	G	O5'-P-OP1	-6.19	100.13	105.70
1	6	362	G	C4-N9-C1'	6.19	134.54	126.50
36	1	2188	A	N1-C6-N6	-6.19	114.89	118.60
36	1	298	U	O5'-P-OP1	6.18	118.12	110.70
36	5	1161	G	C2-N3-C4	6.18	114.99	111.90
36	1	2709	C	N3-C4-C5	6.18	124.37	121.90
36	1	2314	U	O5'-P-OP2	-6.18	100.14	105.70
36	1	2812	C	C5-C6-N1	-6.18	117.91	121.00
36	5	102	C	C5-C4-N4	-6.18	115.88	120.20
36	5	1872	C	N3-C2-O2	-6.18	117.58	121.90
36	5	3215	A	N1-C6-N6	6.18	122.31	118.60
36	1	989	A	C8-N9-C4	6.18	108.27	105.80
36	1	2541	U	C2-N1-C1'	6.18	125.11	117.70
36	1	2800	G	N1-C2-N3	6.18	127.61	123.90
36	5	2359	C	C5-C6-N1	-6.18	117.91	121.00
36	1	69	C	N3-C4-C5	-6.17	119.43	121.90
36	5	1902	G	O5'-P-OP1	-6.17	100.14	105.70
36	5	1902	G	N3-C4-N9	6.17	129.70	126.00
36	1	148	G	C6-C5-N7	-6.17	126.70	130.40
36	1	1655	G	C5-C6-O6	-6.17	124.90	128.60
36	5	41	G	C8-N9-C4	6.17	108.87	106.40
36	5	816	A	O5'-P-OP2	-6.17	100.15	105.70
38	8	25	G	O5'-P-OP2	-6.17	100.15	105.70
36	1	2830	G	N3-C2-N2	-6.17	115.58	119.90
36	5	2287	C	C6-N1-C2	-6.17	117.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2942	C	N1-C2-O2	-6.17	115.20	118.90
36	5	2903	A	C2-N3-C4	-6.17	107.52	110.60
36	1	3208	G	N1-C6-O6	-6.16	116.20	119.90
36	5	890	C	O5'-P-OP2	-6.16	100.16	105.70
36	5	1663	C	O5'-P-OP2	-6.16	100.16	105.70
1	2	1746	A	N1-C2-N3	-6.16	126.22	129.30
36	5	1305	U	C6-N1-C2	6.16	124.69	121.00
36	5	3315	G	N3-C4-C5	-6.16	125.52	128.60
36	1	1360	C	C6-N1-C2	6.16	122.76	120.30
36	1	3143	C	C5-C6-N1	-6.16	117.92	121.00
1	6	453	U	N3-C2-O2	-6.16	117.89	122.20
36	5	931	C	C2-N3-C4	-6.16	116.82	119.90
1	2	1568	C	P-O3'-C3'	6.16	127.09	119.70
36	5	2623	G	N9-C4-C5	-6.15	102.94	105.40
36	1	1349	G	N9-C4-C5	-6.15	102.94	105.40
36	5	427	C	N3-C4-C5	6.15	124.36	121.90
36	5	1116	G	OP2-P-O3'	6.15	118.73	105.20
36	5	1866	C	C2-N1-C1'	6.15	125.56	118.80
1	6	1463	C	C6-N1-C2	6.15	122.76	120.30
36	1	131	C	C6-N1-C2	-6.15	117.84	120.30
36	1	348	A	C5-C6-N6	-6.15	118.78	123.70
36	1	635	G	N3-C4-N9	6.15	129.69	126.00
36	1	644	G	C8-N9-C4	-6.15	103.94	106.40
36	1	1445	U	N3-C4-O4	-6.15	115.10	119.40
1	6	3	U	C5-C6-N1	-6.15	119.63	122.70
1	6	1659	A	C2-N3-C4	-6.15	107.53	110.60
1	6	1641	C	N1-C2-O2	-6.14	115.21	118.90
36	5	646	A	C5-C6-N6	6.14	128.62	123.70
36	5	3190	C	C6-N1-C2	-6.14	117.84	120.30
36	1	1195	A	O5'-P-OP1	-6.14	100.17	105.70
36	1	2961	G	O5'-P-OP2	-6.14	100.17	105.70
36	5	788	C	OP2-P-O3'	6.14	118.71	105.20
36	5	2345	A	C8-N9-C4	6.14	108.26	105.80
36	5	366	A	C6-C5-N7	-6.14	128.00	132.30
36	5	1445	U	N3-C2-O2	6.14	126.50	122.20
36	1	616	G	N1-C6-O6	6.14	123.58	119.90
38	4	103	G	N7-C8-N9	6.14	116.17	113.10
36	1	364	G	N3-C4-N9	-6.14	122.32	126.00
1	6	1389	C	N1-C2-O2	6.14	122.58	118.90
36	5	2408	U	C5-C6-N1	-6.14	119.63	122.70
36	1	153	U	C6-N1-C2	-6.13	117.32	121.00
36	1	1134	G	C5-C6-O6	-6.13	124.92	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1199	C	N3-C2-O2	-6.13	117.61	121.90
36	1	1411	C	N3-C4-C5	6.13	124.35	121.90
1	6	609	U	C5-C6-N1	-6.13	119.63	122.70
36	5	2168	A	O5'-P-OP2	-6.13	100.18	105.70
36	5	2710	C	N1-C2-O2	-6.13	115.22	118.90
1	2	1096	C	N1-C2-O2	6.13	122.58	118.90
1	2	1202	A	N1-C6-N6	-6.13	114.92	118.60
36	1	660	A	O5'-P-OP1	-6.13	100.18	105.70
38	4	113	U	N3-C2-O2	-6.13	117.91	122.20
1	6	1535	U	N3-C2-O2	-6.13	117.91	122.20
36	1	1124	U	N1-C2-O2	6.13	127.09	122.80
36	5	2630	C	O5'-P-OP1	-6.13	100.18	105.70
1	2	1258	U	N3-C2-O2	-6.13	117.91	122.20
36	1	3266	G	C8-N9-C4	-6.13	103.95	106.40
36	5	1155	C	C2-N1-C1'	6.13	125.54	118.80
36	5	1587	A	C8-N9-C4	6.13	108.25	105.80
37	7	102	A	C8-N9-C4	6.13	108.25	105.80
1	2	581	U	C2-N1-C1'	6.13	125.05	117.70
36	1	702	C	C2-N3-C4	-6.13	116.84	119.90
36	1	3302	U	C5-C6-N1	-6.13	119.64	122.70
41	L4	182	LEU	CA-CB-CG	6.13	129.39	115.30
1	6	53	G	N3-C4-C5	-6.13	125.54	128.60
38	8	95	G	N3-C4-N9	-6.13	122.32	126.00
44	17	83	LEU	CA-CB-CG	6.13	129.39	115.30
1	6	317	C	N3-C4-C5	6.12	124.35	121.90
36	1	421	G	N9-C4-C5	-6.12	102.95	105.40
36	1	2894	C	N3-C4-C5	-6.12	119.45	121.90
36	5	828	A	N1-C6-N6	-6.12	114.93	118.60
36	5	2611	U	O5'-P-OP2	-6.12	100.19	105.70
36	1	1295	G	C4-C5-N7	-6.12	108.35	110.80
36	1	2245	C	N3-C2-O2	-6.12	117.62	121.90
36	1	2624	G	C6-C5-N7	-6.12	126.73	130.40
36	5	498	A	O5'-P-OP2	-6.12	100.19	105.70
36	5	578	A	O5'-P-OP2	6.12	118.05	110.70
36	5	1395	G	N1-C6-O6	6.12	123.57	119.90
1	2	1458	G	N3-C4-N9	6.12	129.67	126.00
36	1	609	G	C8-N9-C4	-6.12	103.95	106.40
36	1	1392	G	O4'-C1'-N9	6.12	113.09	108.20
36	5	1592	G	N7-C8-N9	6.12	116.16	113.10
1	6	362	G	N3-C4-N9	6.12	129.67	126.00
36	5	2333	C	C5-C4-N4	-6.12	115.92	120.20
36	5	195	U	N1-C2-N3	6.12	118.57	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	644	G	N3-C4-C5	-6.12	125.54	128.60
36	5	941	G	N1-C6-O6	-6.12	116.23	119.90
36	5	1124	U	OP1-P-O3'	6.12	118.65	105.20
36	5	2632	G	N1-C6-O6	-6.12	116.23	119.90
36	1	1136	A	C8-N9-C4	-6.11	103.36	105.80
36	1	2278	C	N3-C4-C5	6.11	124.35	121.90
36	5	792	G	C2-N3-C4	-6.11	108.84	111.90
37	7	49	G	C6-C5-N7	-6.11	126.73	130.40
1	2	137	U	N3-C2-O2	-6.11	117.92	122.20
36	1	1094	U	C5-C6-N1	6.11	125.75	122.70
36	5	1190	A	N7-C8-N9	6.11	116.86	113.80
36	5	1372	C	C6-N1-C2	6.11	122.74	120.30
1	2	1572	G	N9-C4-C5	-6.11	102.96	105.40
36	5	836	A	C5-C6-N1	6.11	120.75	117.70
36	1	618	C	N1-C2-O2	-6.11	115.24	118.90
36	1	1192	C	C6-N1-C1'	-6.11	113.47	120.80
1	6	1751	C	C6-N1-C2	6.11	122.74	120.30
36	5	405	U	C6-N1-C2	6.11	124.66	121.00
36	5	2134	G	C8-N9-C4	6.11	108.84	106.40
36	5	2295	A	C5-C6-N1	6.11	120.75	117.70
36	1	2827	U	C6-N1-C1'	6.10	129.74	121.20
36	5	1520	G	N3-C4-N9	6.10	129.66	126.00
36	1	933	A	C6-N1-C2	-6.10	114.94	118.60
36	5	635	G	N9-C4-C5	-6.10	102.96	105.40
36	5	701	G	C4-C5-N7	-6.10	108.36	110.80
36	1	1365	G	C5-C6-N1	6.10	114.55	111.50
36	5	92	G	N3-C4-N9	6.10	129.66	126.00
36	5	2363	A	C5-C6-N6	-6.10	118.82	123.70
36	1	282	G	O5'-P-OP2	6.10	118.02	110.70
1	6	542	A	C8-N9-C4	-6.10	103.36	105.80
38	4	14	C	C5-C6-N1	-6.09	117.95	121.00
1	6	1749	A	C2-N3-C4	-6.09	107.55	110.60
36	5	2888	U	C5-C4-O4	-6.09	122.24	125.90
36	1	2134	G	N3-C2-N2	6.09	124.17	119.90
36	5	437	G	C8-N9-C4	-6.09	103.96	106.40
36	1	1001	G	C4-C5-N7	6.09	113.24	110.80
36	1	2249	G	N3-C4-C5	-6.09	125.56	128.60
36	5	1099	A	C5-C6-N6	-6.09	118.83	123.70
36	5	1881	A	C5-C6-N6	-6.09	118.83	123.70
36	5	2164	A	C8-N9-C4	-6.09	103.36	105.80
36	5	2963	C	C6-N1-C2	6.09	122.73	120.30
36	1	644	G	C5-C6-N1	-6.09	108.46	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2177	G	C6-C5-N7	-6.09	126.75	130.40
36	1	2369	G	N3-C4-C5	-6.09	125.56	128.60
36	5	37	U	N1-C2-N3	6.09	118.55	114.90
36	5	2364	G	N1-C6-O6	-6.09	116.25	119.90
36	5	3172	A	C2-N3-C4	-6.09	107.56	110.60
36	1	1849	C	N3-C4-C5	6.08	124.33	121.90
69	o3	73	ARG	NE-CZ-NH2	-6.08	117.26	120.30
36	1	587	U	C2-N3-C4	-6.08	123.35	127.00
36	1	1859	A	C8-N9-C4	6.08	108.23	105.80
36	1	2385	G	N3-C4-C5	6.08	131.64	128.60
1	6	455	C	C5-C4-N4	-6.08	115.94	120.20
36	1	1520	G	C8-N9-C4	6.08	108.83	106.40
36	1	1911	A	C5-C6-N6	-6.08	118.83	123.70
36	5	1198	C	N3-C2-O2	-6.08	117.64	121.90
36	5	2531	C	N1-C2-O2	6.08	122.55	118.90
36	1	2410	U	N1-C2-O2	-6.08	118.54	122.80
36	1	2618	G	N1-C6-O6	-6.08	116.25	119.90
1	6	453	U	N1-C2-O2	6.08	127.06	122.80
36	5	424	G	C5-C6-N1	6.08	114.54	111.50
36	5	948	C	O5'-P-OP1	6.08	118.00	110.70
1	6	1637	C	N3-C2-O2	-6.08	117.65	121.90
1	2	830	U	N1-C2-O2	6.08	127.05	122.80
36	1	583	G	N3-C2-N2	-6.08	115.65	119.90
36	1	1318	A	C5-N7-C8	-6.08	100.86	103.90
36	1	3382	U	C2-N1-C1'	6.08	124.99	117.70
36	5	974	G	N3-C4-C5	-6.08	125.56	128.60
36	5	1932	A	C2-N3-C4	-6.08	107.56	110.60
36	1	2935	U	C6-N1-C2	-6.07	117.36	121.00
36	5	417	A	N7-C8-N9	-6.07	110.76	113.80
52	m6	128	ARG	N-CA-C	6.07	127.40	111.00
36	5	800	G	N1-C2-N2	-6.07	110.74	116.20
1	2	1202	A	C2-N3-C4	6.07	113.64	110.60
36	1	24	G	N1-C2-N2	-6.07	110.74	116.20
36	5	819	U	C4-C5-C6	6.07	123.34	119.70
36	5	2719	U	N1-C2-O2	-6.07	118.55	122.80
1	2	1782	A	C5-C6-N1	-6.07	114.67	117.70
36	5	2514	U	O5'-P-OP1	-6.07	100.24	105.70
36	1	357	A	C6-N1-C2	-6.07	114.96	118.60
1	6	144	U	O4'-C1'-N1	6.07	113.05	108.20
36	1	2373	A	O5'-P-OP1	-6.06	100.24	105.70
36	1	636	C	N3-C4-C5	6.06	124.33	121.90
36	1	1589	A	O4'-C1'-N9	-6.06	103.35	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2234	G	C8-N9-C4	6.06	108.82	106.40
36	5	3110	C	C5-C6-N1	-6.06	117.97	121.00
36	1	1198	C	N1-C2-O2	-6.06	115.26	118.90
36	1	2393	G	O5'-P-OP2	-6.06	100.25	105.70
36	5	2615	G	N1-C6-O6	6.06	123.53	119.90
36	5	2626	A	O4'-C1'-N9	-6.06	103.35	108.20
36	5	3056	U	N3-C2-O2	6.06	126.44	122.20
36	1	325	A	OP1-P-OP2	-6.06	110.52	119.60
36	1	1101	G	N1-C6-O6	-6.06	116.27	119.90
36	1	3201	C	N3-C2-O2	-6.06	117.66	121.90
36	1	1433	A	C2-N3-C4	6.05	113.63	110.60
36	1	1476	G	C5-C6-O6	6.05	132.23	128.60
1	6	1120	U	N3-C2-O2	-6.05	117.96	122.20
36	5	1716	U	P-O3'-C3'	6.05	126.96	119.70
36	1	644	G	C6-C5-N7	-6.05	126.77	130.40
36	1	1156	C	C4-C5-C6	6.05	120.42	117.40
36	5	1637	A	N1-C6-N6	-6.05	114.97	118.60
36	5	2941	A	N9-C4-C5	6.05	108.22	105.80
36	1	1307	G	N3-C4-N9	-6.05	122.37	126.00
36	1	2865	U	N3-C4-C5	6.05	118.23	114.60
36	1	2943	G	C5-C6-O6	-6.05	124.97	128.60
1	6	804	A	N1-C6-N6	6.05	122.23	118.60
36	5	2273	G	N1-C6-O6	-6.05	116.27	119.90
36	5	2808	A	N9-C4-C5	-6.05	103.38	105.80
36	5	2858	U	C5-C6-N1	6.05	125.72	122.70
36	5	3343	G	N3-C4-N9	6.05	129.63	126.00
36	1	2758	A	N7-C8-N9	-6.04	110.78	113.80
36	1	47	C	C6-N1-C2	6.04	122.72	120.30
36	1	1849	C	N1-C2-O2	-6.04	115.27	118.90
36	1	34	A	OP2-P-O3'	6.04	118.49	105.20
36	1	1000	C	C6-N1-C2	6.04	122.72	120.30
36	1	1351	U	N1-C2-O2	6.04	127.03	122.80
36	5	1301	A	N1-C6-N6	6.04	122.22	118.60
36	5	3136	G	C2-N3-C4	-6.04	108.88	111.90
37	7	49	G	C5-C6-O6	-6.04	124.97	128.60
36	5	2345	A	C8-N9-C1'	-6.04	116.83	127.70
1	2	380	U	N1-C2-O2	6.04	127.03	122.80
36	1	3143	C	C6-N1-C2	6.04	122.72	120.30
1	6	647	G	N3-C4-C5	6.04	131.62	128.60
36	5	588	G	OP1-P-OP2	6.04	128.66	119.60
1	6	1782	A	C5-C6-N6	6.04	128.53	123.70
36	1	120	G	N9-C4-C5	-6.04	102.99	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	785	G	C2-N3-C4	6.04	114.92	111.90
36	5	417	A	N1-C6-N6	-6.03	114.98	118.60
36	1	1174	G	C8-N9-C1'	-6.03	119.16	127.00
36	1	1556	C	N1-C2-O2	6.03	122.52	118.90
36	1	2832	C	C6-N1-C2	-6.03	117.89	120.30
36	1	1333	C	O5'-P-OP2	-6.03	100.27	105.70
36	1	1335	C	N3-C4-N4	-6.03	113.78	118.00
36	1	2884	C	C5-C4-N4	-6.03	115.98	120.20
36	1	3001	C	C2-N1-C1'	-6.03	112.17	118.80
36	5	2820	A	C8-N9-C4	-6.03	103.39	105.80
36	1	2856	G	O5'-P-OP2	6.03	117.93	110.70
52	M6	78	ARG	NE-CZ-NH2	-6.03	117.29	120.30
36	5	1495	U	C5-C6-N1	6.03	125.71	122.70
36	5	2249	G	N7-C8-N9	6.03	116.11	113.10
1	6	858	G	C5-N7-C8	-6.02	101.29	104.30
36	5	1844	C	C6-N1-C2	-6.02	117.89	120.30
36	1	2198	A	N1-C2-N3	6.02	132.31	129.30
36	5	869	G	C5-C6-N1	6.02	114.51	111.50
36	5	2870	C	C2-N1-C1'	-6.02	112.18	118.80
50	m4	106	ARG	NE-CZ-NH1	6.02	123.31	120.30
77	q1	21	ARG	NE-CZ-NH1	-6.02	117.29	120.30
38	4	31	G	OP2-P-O3'	6.02	118.45	105.20
1	6	1023	A	C5-C6-N6	-6.02	118.89	123.70
36	5	1179	A	C4-C5-C6	6.02	120.01	117.00
36	5	3374	U	C5-C6-N1	-6.02	119.69	122.70
36	1	2418	G	C2-N3-C4	6.02	114.91	111.90
36	5	640	U	N3-C4-O4	6.02	123.61	119.40
36	5	2616	C	C4-C5-C6	-6.02	114.39	117.40
1	2	1733	C	N3-C4-N4	6.02	122.21	118.00
36	1	2643	A	C8-N9-C4	6.02	108.21	105.80
1	2	931	C	C6-N1-C2	6.01	122.70	120.30
36	1	3242	G	C4-N9-C1'	-6.01	118.68	126.50
36	5	885	U	N1-C2-O2	-6.01	118.59	122.80
36	5	960	U	C2-N1-C1'	6.01	124.92	117.70
36	1	942	U	OP1-P-OP2	-6.01	110.58	119.60
36	1	2912	G	C5-C6-N1	6.01	114.51	111.50
36	5	1335	C	N1-C2-O2	-6.01	115.29	118.90
36	1	2406	C	N3-C2-O2	6.01	126.11	121.90
36	1	3006	A	O5'-P-OP1	-6.01	100.29	105.70
36	1	3046	A	O5'-P-OP2	-6.01	100.29	105.70
36	5	119	U	C5-C4-O4	6.01	129.51	125.90
36	5	2849	C	N3-C4-C5	-6.01	119.50	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2314	U	C5-C4-O4	-6.01	122.29	125.90
36	5	885	U	N3-C4-O4	6.01	123.61	119.40
37	7	81	U	N1-C2-O2	6.01	127.01	122.80
1	6	139	C	N3-C2-O2	-6.01	117.69	121.90
36	5	1151	U	N3-C2-O2	6.01	126.41	122.20
36	5	2236	G	C4-C5-N7	6.01	113.20	110.80
1	2	1600	A	N1-C6-N6	6.01	122.20	118.60
36	1	206	G	N7-C8-N9	-6.01	110.10	113.10
36	1	1445	U	C6-N1-C1'	6.01	129.61	121.20
70	O4	8	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	6	1737	G	N9-C4-C5	-6.01	103.00	105.40
36	5	2253	G	O5'-P-OP2	-6.01	100.29	105.70
36	1	900	G	N7-C8-N9	-6.00	110.10	113.10
37	3	38	U	N1-C2-O2	-6.00	118.60	122.80
36	5	3026	G	N1-C6-O6	6.00	123.50	119.90
1	2	966	A	N9-C4-C5	-6.00	103.40	105.80
36	1	1139	G	C2-N3-C4	-6.00	108.90	111.90
36	1	1343	A	C6-C5-N7	-6.00	128.10	132.30
36	5	1085	A	O5'-P-OP1	-6.00	100.30	105.70
36	5	1495	U	O4'-C1'-N1	6.00	113.00	108.20
36	5	2623	G	C8-N9-C4	6.00	108.80	106.40
36	5	2849	C	C5-C6-N1	6.00	124.00	121.00
36	1	153	U	N3-C4-C5	-6.00	111.00	114.60
36	1	1051	U	N1-C2-N3	6.00	118.50	114.90
59	n3	48	ARG	NE-CZ-NH1	6.00	123.30	120.30
36	1	1111	U	N3-C4-C5	6.00	118.20	114.60
36	1	1197	A	O5'-P-OP2	-6.00	100.30	105.70
1	6	543	C	C5-C6-N1	6.00	124.00	121.00
36	1	2355	G	C4-C5-C6	6.00	122.40	118.80
1	6	858	G	N7-C8-N9	6.00	116.10	113.10
68	o2	44	ARG	NE-CZ-NH2	6.00	123.30	120.30
36	1	1308	A	N9-C4-C5	6.00	108.20	105.80
38	4	14	C	C2-N3-C4	-6.00	116.90	119.90
36	5	75	G	N1-C6-O6	6.00	123.50	119.90
36	1	1142	G	C8-N9-C4	-5.99	104.00	106.40
1	2	1657	U	O4'-C1'-N1	5.99	112.99	108.20
36	5	1193	A	C2-N3-C4	-5.99	107.60	110.60
36	5	2383	C	C2-N3-C4	-5.99	116.90	119.90
36	5	3245	A	C5-C6-N1	-5.99	114.70	117.70
36	1	1174	G	C4-N9-C1'	5.99	134.29	126.50
36	5	928	C	N3-C2-O2	-5.99	117.71	121.90
1	6	1127	G	C6-C5-N7	-5.99	126.81	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	923	C	C6-N1-C2	5.99	122.69	120.30
36	5	3093	C	C2-N3-C4	-5.99	116.91	119.90
36	1	2993	G	N3-C4-N9	5.99	129.59	126.00
36	1	2361	A	OP2-P-O3'	5.99	118.37	105.20
36	5	1605	A	O4'-C1'-N9	5.99	112.99	108.20
36	5	2345	A	N9-C4-C5	-5.99	103.41	105.80
1	2	765	G	O4'-C1'-N9	-5.98	103.41	108.20
1	2	1280	C	C6-N1-C2	-5.98	117.91	120.30
36	1	2943	G	C4-C5-N7	5.98	113.19	110.80
36	5	57	A	N9-C4-C5	-5.98	103.41	105.80
36	1	793	C	N1-C2-O2	-5.98	115.31	118.90
1	6	1091	A	C5-C6-N1	-5.98	114.71	117.70
36	1	1467	A	N1-C6-N6	-5.97	115.02	118.60
1	6	83	G	N1-C6-O6	5.97	123.48	119.90
1	6	163	G	N9-C4-C5	5.97	107.79	105.40
1	6	959	U	C5-C4-O4	-5.97	122.32	125.90
1	6	1635	A	N1-C6-N6	5.97	122.19	118.60
36	5	2850	G	C5-C6-O6	-5.97	125.02	128.60
36	5	2890	A	C4-C5-C6	5.97	119.99	117.00
36	5	3207	U	C2-N1-C1'	-5.97	110.53	117.70
36	1	614	C	N3-C4-C5	5.97	124.29	121.90
36	5	997	A	OP2-P-O3'	5.97	118.34	105.20
1	2	1636	C	N3-C4-C5	-5.97	119.51	121.90
36	1	374	A	N1-C2-N3	-5.97	126.31	129.30
37	3	103	A	N1-C6-N6	5.97	122.18	118.60
1	6	1573	A	P-O3'-C3'	5.97	126.86	119.70
36	5	283	G	C6-C5-N7	-5.97	126.82	130.40
36	5	2148	U	N1-C2-O2	-5.97	118.62	122.80
36	5	2916	U	C5-C6-N1	-5.97	119.72	122.70
1	6	352	A	O5'-P-OP1	-5.97	100.33	105.70
6	s4	38	LEU	CA-CB-CG	5.97	129.03	115.30
36	5	361	A	C2-N3-C4	5.97	113.58	110.60
36	5	411	U	N1-C2-O2	-5.96	118.62	122.80
36	5	884	A	C2-N3-C4	-5.96	107.62	110.60
36	5	2327	U	C5-C6-N1	-5.96	119.72	122.70
47	m0	10	ARG	NE-CZ-NH1	-5.96	117.32	120.30
36	1	1307	G	P-O3'-C3'	5.96	126.85	119.70
36	1	2643	A	N1-C6-N6	5.96	122.18	118.60
36	5	1405	U	N1-C2-N3	5.96	118.47	114.90
36	5	3178	A	O5'-P-OP1	-5.96	100.34	105.70
36	5	1495	U	C6-N1-C2	-5.95	117.43	121.00
36	1	2585	G	N3-C4-N9	5.95	129.57	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2823	G	C4-C5-N7	-5.95	108.42	110.80
36	1	206	G	C8-N9-C4	5.95	108.78	106.40
36	1	1103	A	C8-N9-C4	5.95	108.18	105.80
36	1	3229	G	C5-C6-O6	-5.95	125.03	128.60
36	5	3164	C	O4'-C1'-N1	5.95	112.96	108.20
1	2	734	A	P-O3'-C3'	5.95	126.84	119.70
36	1	2409	G	N3-C4-C5	-5.95	125.62	128.60
37	3	33	U	N3-C2-O2	-5.95	118.04	122.20
37	3	88	G	N3-C4-C5	-5.95	125.63	128.60
36	5	1160	C	N1-C2-O2	-5.95	115.33	118.90
36	1	2134	G	C5-C6-N1	5.95	114.47	111.50
36	1	2212	C	C6-N1-C2	5.95	122.68	120.30
36	1	2815	G	C8-N9-C4	5.94	108.78	106.40
36	5	3188	G	C4-C5-N7	-5.94	108.42	110.80
1	2	370	A	N1-C6-N6	-5.94	115.03	118.60
1	2	794	U	C2-N1-C1'	5.94	124.83	117.70
36	5	3214	U	N3-C2-O2	-5.94	118.04	122.20
36	5	3335	A	C6-C5-N7	-5.94	128.14	132.30
36	1	2712	U	N3-C2-O2	-5.94	118.04	122.20
1	2	571	G	C4-C5-N7	-5.94	108.42	110.80
36	1	639	G	C6-C5-N7	-5.94	126.84	130.40
37	3	83	U	C5-C6-N1	-5.94	119.73	122.70
36	5	2524	A	C5-N7-C8	-5.94	100.93	103.90
36	1	1376	C	N1-C2-O2	-5.94	115.34	118.90
36	5	339	C	N1-C2-O2	-5.94	115.34	118.90
36	5	902	G	C5-C6-O6	-5.94	125.04	128.60
36	1	2176	U	N1-C2-O2	5.93	126.95	122.80
36	5	2616	C	OP2-P-O3'	5.93	118.25	105.20
36	5	2967	A	N1-C2-N3	5.93	132.27	129.30
36	1	1835	A	O5'-P-OP1	-5.93	100.36	105.70
36	5	3245	A	N3-C4-C5	5.93	130.95	126.80
66	o0	41	LEU	CA-CB-CG	5.93	128.95	115.30
36	1	2887	A	C8-N9-C4	-5.93	103.43	105.80
1	6	1000	C	C4-C5-C6	5.93	120.36	117.40
36	5	512	U	N3-C2-O2	-5.93	118.05	122.20
36	5	2308	C	N3-C2-O2	5.93	126.05	121.90
36	5	2325	G	N3-C2-N2	-5.93	115.75	119.90
36	1	803	C	O5'-P-OP1	5.93	117.81	110.70
36	1	1002	A	C8-N9-C4	5.93	108.17	105.80
1	6	1025	A	N9-C4-C5	-5.93	103.43	105.80
36	5	2163	C	C2-N3-C4	-5.93	116.94	119.90
36	5	2388	U	OP2-P-O3'	5.93	118.24	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	282	G	C2'-C3'-O3'	5.92	123.18	113.70
36	5	1507	G	C6-C5-N7	-5.92	126.85	130.40
36	5	1598	G	C8-N9-C4	5.92	108.77	106.40
36	5	3118	C	C6-N1-C2	-5.92	117.93	120.30
36	1	2952	G	C4-N9-C1'	5.92	134.20	126.50
36	1	2236	G	N1-C6-O6	5.92	123.45	119.90
36	5	43	A	N1-C6-N6	5.92	122.15	118.60
36	1	1154	A	C8-N9-C4	-5.92	103.43	105.80
37	3	91	G	C6-C5-N7	-5.92	126.85	130.40
36	5	661	G	OP1-P-O3'	5.92	118.22	105.20
1	2	316	A	C8-N9-C4	5.92	108.17	105.80
36	5	2123	G	O5'-P-OP1	-5.92	100.38	105.70
36	1	2656	A	N1-C6-N6	-5.91	115.05	118.60
36	1	2886	U	C5-C4-O4	-5.91	122.35	125.90
1	6	390	G	O5'-P-OP2	-5.91	100.38	105.70
36	5	970	A	C5-C6-N6	-5.91	118.97	123.70
36	5	2295	A	N1-C2-N3	-5.91	126.34	129.30
1	2	1560	U	C6-N1-C2	-5.91	117.45	121.00
36	5	2524	A	N7-C8-N9	5.91	116.75	113.80
36	1	1304	A	N1-C6-N6	-5.91	115.06	118.60
36	1	3143	C	N1-C2-O2	-5.91	115.36	118.90
1	6	1100	G	C6-N1-C2	-5.91	121.56	125.10
36	5	868	C	C6-N1-C2	5.91	122.66	120.30
36	5	2236	G	C6-C5-N7	-5.91	126.86	130.40
36	1	2624	G	C8-N9-C4	-5.90	104.04	106.40
1	2	694	U	N1-C2-O2	5.90	126.93	122.80
36	1	1103	A	P-O3'-C3'	5.90	126.78	119.70
45	L8	189	LEU	CA-CB-CG	5.90	128.88	115.30
1	6	1060	U	N3-C2-O2	-5.90	118.07	122.20
36	5	2366	C	C2-N1-C1'	5.90	125.29	118.80
36	1	1374	G	C6-C5-N7	-5.90	126.86	130.40
36	1	2375	G	C8-N9-C4	5.90	108.76	106.40
36	1	2905	U	N3-C2-O2	5.90	126.33	122.20
36	1	3058	U	OP1-P-OP2	5.90	128.45	119.60
36	1	3382	U	N3-C2-O2	-5.90	118.07	122.20
38	8	21	C	N1-C2-O2	-5.90	115.36	118.90
36	5	946	U	O5'-P-OP2	-5.90	100.39	105.70
36	1	75	G	C6-C5-N7	-5.90	126.86	130.40
1	6	459	G	C5-C6-O6	-5.90	125.06	128.60
36	5	1452	A	C6-C5-N7	-5.90	128.17	132.30
1	2	569	C	N3-C2-O2	-5.90	117.77	121.90
36	1	1448	U	OP2-P-O3'	5.89	118.17	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2257	C	N3-C2-O2	-5.89	117.77	121.90
36	1	2726	C	C6-N1-C2	-5.89	117.94	120.30
36	5	1206	G	C8-N9-C4	-5.89	104.04	106.40
36	5	2358	A	N3-C4-C5	5.89	130.93	126.80
37	7	94	C	C4-C5-C6	-5.89	114.45	117.40
1	2	1274	C	C5-C4-N4	5.89	124.32	120.20
36	1	2384	A	C4-C5-N7	5.89	113.65	110.70
36	5	2917	G	O5'-P-OP2	-5.89	100.40	105.70
36	1	659	G	C5-C6-O6	-5.89	125.07	128.60
38	4	113	U	C4-C5-C6	5.89	123.23	119.70
36	5	784	A	O5'-P-OP2	-5.89	100.40	105.70
1	6	1034	C	C4-C5-C6	5.89	120.34	117.40
36	1	938	C	C6-N1-C2	-5.89	117.94	120.30
36	1	1116	G	C8-N9-C4	-5.89	104.05	106.40
38	4	32	C	C2-N1-C1'	-5.89	112.32	118.80
36	5	1381	A	C2-N3-C4	-5.89	107.66	110.60
36	5	1876	U	N3-C4-C5	5.89	118.13	114.60
1	6	1031	U	C5-C6-N1	-5.88	119.76	122.70
1	2	425	A	C4-C5-N7	5.88	113.64	110.70
1	6	1001	A	N9-C4-C5	-5.88	103.45	105.80
36	5	2929	C	N3-C4-C5	5.88	124.25	121.90
38	4	116	G	N9-C4-C5	-5.88	103.05	105.40
36	5	3095	U	N3-C4-O4	-5.88	115.28	119.40
36	1	912	G	OP2-P-O3'	5.88	118.14	105.20
1	6	1092	A	N1-C6-N6	5.88	122.13	118.60
36	1	439	C	C5-C6-N1	5.88	123.94	121.00
36	1	1386	A	C6-N1-C2	-5.88	115.07	118.60
36	5	2838	A	C5-C6-N6	-5.88	119.00	123.70
38	8	3	A	C5-C6-N1	5.88	120.64	117.70
15	C3	22	ALA	C-N-CA	5.88	146.68	122.00
36	1	1907	C	N3-C4-C5	-5.88	119.55	121.90
36	1	3133	C	C5-C4-N4	-5.88	116.09	120.20
36	1	3303	G	O4'-C1'-N9	5.88	112.90	108.20
37	3	86	U	C2-N3-C4	-5.88	123.47	127.00
41	L4	327	LEU	CA-CB-CG	5.88	128.81	115.30
36	1	916	G	N1-C6-O6	-5.88	116.38	119.90
36	1	1351	U	N3-C2-O2	-5.88	118.09	122.20
36	5	516	A	N1-C6-N6	5.88	122.12	118.60
1	2	90	C	C6-N1-C2	-5.87	117.95	120.30
36	1	1166	G	C6-C5-N7	-5.87	126.88	130.40
36	5	1897	G	N3-C4-C5	5.87	131.54	128.60
36	5	2354	C	C5-C4-N4	-5.87	116.09	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1120	U	N3-C2-O2	-5.87	118.09	122.20
1	2	1462	G	C4-C5-N7	5.87	113.15	110.80
36	1	999	G	C5-C6-O6	-5.87	125.08	128.60
36	1	2134	G	N3-C4-N9	5.87	129.52	126.00
1	2	576	G	C4-C5-N7	5.87	113.15	110.80
36	5	1433	A	N9-C4-C5	5.87	108.15	105.80
36	5	3181	C	C6-N1-C1'	-5.87	113.76	120.80
36	1	1182	A	C8-N9-C4	5.87	108.15	105.80
36	1	1419	A	N1-C6-N6	5.87	122.12	118.60
36	1	1923	C	C6-N1-C2	5.87	122.65	120.30
36	1	2798	C	N3-C4-C5	-5.87	119.55	121.90
36	1	2936	A	N1-C6-N6	-5.87	115.08	118.60
1	6	795	U	N1-C2-O2	5.87	126.91	122.80
36	1	730	C	C6-N1-C2	5.87	122.65	120.30
36	1	2886	U	N3-C4-O4	5.87	123.51	119.40
36	5	966	U	O5'-P-OP2	-5.87	100.42	105.70
36	5	2339	C	O5'-P-OP1	-5.87	100.42	105.70
36	1	2525	G	N3-C4-N9	5.87	129.52	126.00
36	5	1445	U	C5-C4-O4	-5.87	122.38	125.90
36	5	1905	G	C2-N3-C4	5.87	114.83	111.90
38	8	16	G	C5-C6-O6	-5.87	125.08	128.60
36	1	1058	U	N1-C2-O2	5.86	126.91	122.80
36	1	1779	C	C6-N1-C2	-5.86	117.95	120.30
1	6	426	G	C4-N9-C1'	5.86	134.12	126.50
36	1	809	G	C5-C6-O6	-5.86	125.08	128.60
36	1	2142	A	C6-N1-C2	-5.86	115.08	118.60
1	6	901	G	N1-C6-O6	5.86	123.42	119.90
36	1	2276	G	C5-C6-O6	-5.86	125.08	128.60
36	1	2383	C	N3-C4-C5	5.86	124.24	121.90
36	1	2803	A	C2-N3-C4	5.86	113.53	110.60
36	1	2950	G	N1-C6-O6	-5.86	116.38	119.90
1	6	338	C	C5-C6-N1	5.86	123.93	121.00
1	6	1432	U	O4'-C1'-N1	5.86	112.89	108.20
36	5	1055	A	O5'-P-OP2	-5.86	100.43	105.70
36	5	1399	A	O5'-P-OP1	5.86	117.73	110.70
1	2	970	A	C4-C5-N7	5.86	113.63	110.70
36	1	611	A	O5'-P-OP1	5.86	117.73	110.70
36	5	665	A	C5-C6-N6	-5.86	119.01	123.70
36	5	2334	U	O5'-P-OP1	5.86	117.73	110.70
38	8	80	A	C4-C5-C6	5.86	119.93	117.00
36	1	941	G	OP1-P-O3'	5.86	118.09	105.20
36	1	2323	G	N3-C2-N2	5.86	124.00	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1634	C	N1-C2-O2	5.86	122.41	118.90
36	5	661	G	O5'-P-OP1	-5.86	100.43	105.70
36	5	934	G	C8-N9-C1'	-5.86	119.39	127.00
36	5	1338	C	N3-C4-N4	5.86	122.10	118.00
36	1	288	C	N3-C4-C5	-5.86	119.56	121.90
36	1	1507	G	C6-N1-C2	-5.86	121.59	125.10
36	1	3201	C	N3-C4-C5	-5.86	119.56	121.90
36	5	880	G	C8-N9-C4	5.86	108.74	106.40
36	5	970	A	N1-C6-N6	5.86	122.11	118.60
36	5	2383	C	C4-C5-C6	5.86	120.33	117.40
36	5	3048	A	C5-C6-N6	-5.86	119.02	123.70
1	2	334	G	C2-N3-C4	-5.85	108.97	111.90
36	1	950	G	N1-C6-O6	5.85	123.41	119.90
36	1	1157	G	OP2-P-O3'	5.85	118.07	105.20
36	1	2134	G	N1-C6-O6	-5.85	116.39	119.90
36	1	3055	U	N3-C4-C5	5.85	118.11	114.60
36	5	1902	G	N3-C2-N2	-5.85	115.80	119.90
36	5	2840	C	O5'-P-OP1	-5.85	100.43	105.70
36	1	1901	A	N1-C6-N6	-5.85	115.09	118.60
36	1	3039	C	O5'-P-OP2	-5.85	100.43	105.70
1	6	1280	C	N3-C4-C5	-5.85	119.56	121.90
36	5	989	A	C5-C6-N6	-5.85	119.02	123.70
5	S3	182	LEU	CA-CB-CG	5.85	128.75	115.30
36	1	1513	G	C6-N1-C2	-5.85	121.59	125.10
36	1	2329	C	O5'-P-OP2	-5.85	100.44	105.70
36	1	2893	C	C5-C6-N1	-5.85	118.08	121.00
1	6	1698	G	P-O3'-C3'	5.85	126.72	119.70
36	5	360	G	C5-C6-N1	-5.85	108.58	111.50
36	5	641	C	N3-C4-C5	5.85	124.24	121.90
36	5	889	U	OP2-P-O3'	5.85	118.07	105.20
1	2	388	G	N1-C6-O6	5.85	123.41	119.90
36	1	668	G	C5-N7-C8	5.85	107.22	104.30
36	1	1495	U	N1-C2-O2	-5.85	118.71	122.80
36	5	1903	U	N3-C4-O4	5.85	123.49	119.40
36	5	2849	C	N1-C2-O2	-5.85	115.39	118.90
37	3	57	G	C5-C6-O6	5.85	132.11	128.60
36	1	874	U	N1-C2-N3	5.84	118.41	114.90
36	1	2134	G	C2-N3-C4	5.84	114.82	111.90
36	1	2185	G	P-O3'-C3'	5.84	126.71	119.70
36	1	2307	G	O4'-C1'-N9	5.84	112.88	108.20
1	6	315	A	C2-N3-C4	5.84	113.52	110.60
1	6	350	U	N1-C2-N3	5.84	118.41	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1316	C	N3-C4-N4	5.84	122.09	118.00
36	5	1476	G	N3-C4-N9	-5.84	122.49	126.00
36	5	2639	G	C6-C5-N7	-5.84	126.89	130.40
36	5	3216	G	C6-C5-N7	-5.84	126.89	130.40
36	1	1796	G	C8-N9-C4	-5.84	104.06	106.40
36	1	3193	C	C6-N1-C2	-5.84	117.96	120.30
36	5	2772	C	P-O3'-C3'	5.84	126.71	119.70
36	5	1433	A	O5'-P-OP1	-5.84	100.44	105.70
1	2	334	G	N3-C4-C5	5.84	131.52	128.60
36	5	2375	G	N1-C6-O6	-5.84	116.40	119.90
36	5	3195	U	C2-N1-C1'	5.84	124.71	117.70
36	1	2699	G	C6-C5-N7	-5.84	126.90	130.40
36	1	83	U	C5-C4-O4	-5.84	122.40	125.90
36	1	96	G	N3-C4-C5	5.84	131.52	128.60
36	1	345	G	OP1-P-O3'	5.84	118.04	105.20
64	N8	34	MET	CG-SD-CE	5.84	109.54	100.20
36	5	1452	A	C2-N3-C4	-5.84	107.68	110.60
38	8	96	A	C8-N9-C4	5.84	108.14	105.80
36	5	1721	U	O5'-P-OP1	-5.83	100.45	105.70
36	1	3050	U	N1-C2-O2	5.83	126.88	122.80
36	5	63	A	C4-C5-C6	5.83	119.92	117.00
36	5	216	G	N1-C6-O6	5.83	123.40	119.90
36	5	2366	C	N3-C4-N4	5.83	122.08	118.00
36	5	3049	A	C8-N9-C4	5.83	108.13	105.80
36	1	1589	A	N1-C6-N6	5.83	122.10	118.60
36	1	1516	C	N1-C2-O2	-5.83	115.40	118.90
36	1	2855	U	C5-C6-N1	-5.83	119.79	122.70
38	4	20	U	N1-C2-O2	-5.83	118.72	122.80
36	5	1047	A	C5-C6-N6	-5.83	119.04	123.70
36	5	2422	C	N3-C4-C5	5.83	124.23	121.90
36	5	2764	C	C5-C4-N4	5.83	124.28	120.20
36	1	1307	G	C6-C5-N7	5.83	133.90	130.40
36	1	2709	C	C2-N3-C4	-5.83	116.99	119.90
36	5	2105	G	C5-C6-O6	-5.83	125.10	128.60
1	2	499	U	P-O3'-C3'	5.83	126.69	119.70
38	4	116	G	C8-N9-C4	5.83	108.73	106.40
36	5	48	A	N9-C4-C5	5.83	108.13	105.80
36	5	1496	C	C2-N1-C1'	5.83	125.21	118.80
36	5	3048	A	O5'-P-OP2	-5.83	100.46	105.70
68	O2	27	ARG	NE-CZ-NH1	-5.82	117.39	120.30
36	5	406	G	N1-C6-O6	-5.82	116.41	119.90
36	5	1387	G	N1-C2-N2	5.82	121.44	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1829	G	C4-C5-N7	-5.82	108.47	110.80
36	1	421	G	C5-C6-N1	5.82	114.41	111.50
36	1	957	C	O5'-P-OP1	5.82	117.69	110.70
36	1	2369	G	C5-C6-N1	5.82	114.41	111.50
36	5	2145	A	C4-N9-C1'	5.82	136.78	126.30
1	2	73	U	O4'-C1'-N1	5.82	112.86	108.20
36	1	155	G	N1-C6-O6	-5.82	116.41	119.90
36	1	196	G	C5-C6-O6	-5.82	125.11	128.60
36	5	1205	A	C6-N1-C2	-5.82	115.11	118.60
37	7	41	G	N1-C6-O6	5.82	123.39	119.90
36	5	1328	C	N3-C4-C5	-5.82	119.57	121.90
36	5	2389	C	C2-N3-C4	-5.82	116.99	119.90
1	2	734	A	OP1-P-O3'	5.82	118.00	105.20
38	4	138	A	N1-C6-N6	-5.82	115.11	118.60
1	6	599	A	C8-N9-C4	-5.82	103.47	105.80
38	4	25	G	C5-C6-O6	5.82	132.09	128.60
1	6	1730	A	N1-C2-N3	5.82	132.21	129.30
36	5	339	C	C5-C4-N4	5.82	124.27	120.20
36	5	514	G	C5-C6-O6	-5.82	125.11	128.60
36	5	806	A	N3-C4-C5	5.82	130.87	126.80
36	1	648	C	C5-C4-N4	-5.81	116.13	120.20
36	1	1474	A	C2-N3-C4	-5.81	107.69	110.60
1	6	421	A	N1-C6-N6	5.81	122.09	118.60
36	5	2293	C	N3-C4-C5	5.81	124.22	121.90
36	5	3223	A	C5-C6-N1	5.81	120.61	117.70
36	5	1478	C	N3-C4-C5	-5.81	119.58	121.90
36	5	1904	C	C6-N1-C2	5.81	122.62	120.30
36	1	590	G	N1-C6-O6	5.81	123.38	119.90
1	6	1164	G	C5-C6-N1	5.81	114.40	111.50
36	5	2408	U	N1-C2-N3	5.81	118.38	114.90
36	5	3028	G	N9-C4-C5	-5.81	103.08	105.40
36	1	812	G	C4-C5-N7	-5.80	108.48	110.80
36	1	1891	A	N7-C8-N9	-5.80	110.90	113.80
36	5	931	C	N3-C4-C5	5.80	124.22	121.90
36	5	630	A	C2-N3-C4	-5.80	107.70	110.60
36	1	709	A	O5'-P-OP1	-5.80	100.48	105.70
36	1	1420	C	C5-C4-N4	5.80	124.26	120.20
36	1	3266	G	N3-C4-N9	-5.80	122.52	126.00
1	6	901	G	C6-C5-N7	-5.80	126.92	130.40
36	5	56	G	N1-C6-O6	-5.80	116.42	119.90
36	1	1156	C	C2-N3-C4	-5.80	117.00	119.90
36	5	1180	A	N9-C4-C5	5.80	108.12	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	297	U	C5-C6-N1	5.80	125.60	122.70
36	5	1496	C	O5'-P-OP1	5.80	117.66	110.70
1	2	1131	A	C8-N9-C4	5.80	108.12	105.80
36	1	1866	C	C6-N1-C2	5.80	122.62	120.30
36	1	2169	G	C5-C6-N1	5.80	114.40	111.50
36	1	3375	A	N1-C2-N3	5.80	132.20	129.30
1	6	1087	A	C2-N3-C4	-5.80	107.70	110.60
69	o3	73	ARG	NE-CZ-NH1	5.80	123.20	120.30
36	1	2379	U	N3-C4-O4	5.79	123.46	119.40
36	1	3278	C	C2-N1-C1'	5.79	125.17	118.80
38	4	16	G	N9-C4-C5	-5.79	103.08	105.40
36	1	1796	G	N9-C4-C5	5.79	107.72	105.40
1	6	1596	C	N3-C2-O2	-5.79	117.84	121.90
36	5	2134	G	N3-C4-N9	5.79	129.48	126.00
36	5	2967	A	C2-N3-C4	-5.79	107.70	110.60
1	2	460	A	N1-C6-N6	-5.79	115.12	118.60
36	1	666	A	C5-C6-N1	5.79	120.60	117.70
1	6	805	U	C6-N1-C2	-5.79	117.53	121.00
36	5	1803	C	C6-N1-C2	5.79	122.62	120.30
36	5	366	A	N9-C4-C5	-5.79	103.48	105.80
36	5	3305	A	N1-C6-N6	5.79	122.07	118.60
38	4	38	U	N1-C2-O2	5.79	126.85	122.80
36	5	1316	C	N3-C4-C5	-5.79	119.58	121.90
36	5	1837	U	N3-C2-O2	5.79	126.25	122.20
36	5	2185	G	OP2-P-O3'	5.79	117.93	105.20
1	2	1486	G	C4-C5-N7	5.79	113.11	110.80
15	C3	114	ARG	NE-CZ-NH1	5.79	123.19	120.30
36	5	79	U	C6-N1-C2	-5.79	117.53	121.00
36	5	192	C	O5'-P-OP2	-5.79	100.49	105.70
1	2	1432	U	O4'-C1'-N1	5.79	112.83	108.20
36	1	2798	C	C6-N1-C2	-5.79	117.99	120.30
1	2	507	U	N3-C2-O2	-5.78	118.15	122.20
36	1	357	A	N1-C2-N3	5.78	132.19	129.30
36	1	382	U	N1-C2-O2	-5.78	118.75	122.80
42	L5	115	LEU	CA-CB-CG	5.78	128.60	115.30
1	6	868	G	C5-C6-N1	5.78	114.39	111.50
36	5	70	A	C8-N9-C4	-5.78	103.49	105.80
36	5	2983	C	O5'-P-OP1	-5.78	100.50	105.70
36	5	931	C	C5-C6-N1	-5.78	118.11	121.00
36	5	1194	G	N3-C4-C5	-5.78	125.71	128.60
1	2	1653	C	N3-C4-C5	-5.78	119.59	121.90
36	1	2620	G	N3-C2-N2	-5.78	115.85	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1	U	C2-N1-C1'	5.78	124.64	117.70
36	1	1346	G	C5-C6-N1	-5.78	108.61	111.50
36	1	2642	A	C6-N1-C2	5.78	122.07	118.60
36	5	96	G	N3-C4-C5	5.78	131.49	128.60
36	1	148	G	C4-C5-N7	5.78	113.11	110.80
36	1	435	C	C6-N1-C2	5.78	122.61	120.30
36	1	1489	A	C8-N9-C4	5.78	108.11	105.80
54	M8	180	ARG	NE-CZ-NH1	5.78	123.19	120.30
36	5	1906	G	C8-N9-C4	5.78	108.71	106.40
37	7	71	G	OP2-P-O3'	5.78	117.91	105.20
1	2	1200	G	C5-C6-O6	-5.78	125.13	128.60
36	1	2620	G	N1-C6-O6	5.78	123.36	119.90
36	1	3189	G	N1-C6-O6	5.78	123.36	119.90
1	6	858	G	C8-N9-C1'	-5.78	119.49	127.00
36	5	2126	A	C5-C6-N6	-5.78	119.08	123.70
36	5	2664	C	C5-C4-N4	-5.78	116.16	120.20
36	1	3079	U	C6-N1-C1'	5.77	129.28	121.20
36	1	866	A	O5'-P-OP1	-5.77	100.50	105.70
36	1	2869	U	N1-C2-O2	-5.77	118.76	122.80
1	6	1139	A	N1-C6-N6	-5.77	115.14	118.60
36	5	1394	A	C8-N9-C4	5.77	108.11	105.80
36	5	2374	C	N3-C4-C5	5.77	124.21	121.90
1	6	989	U	O5'-P-OP2	-5.77	100.51	105.70
36	1	2943	G	C6-C5-N7	-5.77	126.94	130.40
36	5	1430	U	C6-N1-C2	5.77	124.46	121.00
36	5	2113	A	C8-N9-C4	5.77	108.11	105.80
36	5	2830	G	N1-C6-O6	5.77	123.36	119.90
68	o2	44	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	6	192	U	N3-C2-O2	-5.77	118.16	122.20
36	5	912	G	C4-C5-N7	-5.77	108.49	110.80
36	1	3224	G	N3-C2-N2	-5.77	115.86	119.90
36	5	2426	U	N3-C4-O4	-5.77	115.36	119.40
1	6	1309	C	C6-N1-C2	-5.76	118.00	120.30
36	5	388	G	O5'-P-OP2	-5.76	100.51	105.70
36	1	1349	G	C8-N9-C1'	-5.76	119.51	127.00
37	7	98	C	O5'-P-OP2	-5.76	100.51	105.70
36	1	1326	A	C8-N9-C4	5.76	108.11	105.80
36	5	399	A	C5-C6-N6	-5.76	119.09	123.70
1	2	1636	C	N3-C4-N4	5.76	122.03	118.00
36	1	3242	G	C8-N9-C4	5.76	108.70	106.40
25	d3	32	ARG	NE-CZ-NH2	-5.76	117.42	120.30
36	5	641	C	C2-N3-C4	-5.76	117.02	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L2	122	ASP	CB-CG-OD2	5.76	123.48	118.30
36	1	819	U	C5-C6-N1	-5.76	119.82	122.70
36	1	3022	G	O4'-C1'-N9	5.76	112.81	108.20
36	5	1171	G	C4-C5-N7	5.76	113.10	110.80
37	7	93	C	N3-C2-O2	-5.76	117.87	121.90
36	5	1194	G	C5-C6-N1	5.75	114.38	111.50
36	5	2178	A	C8-N9-C4	5.75	108.10	105.80
36	5	2911	A	O5'-P-OP2	-5.75	100.52	105.70
1	2	308	C	C2-N1-C1'	-5.75	112.47	118.80
36	5	3184	A	C8-N9-C4	5.75	108.10	105.80
36	5	3206	C	O4'-C1'-N1	-5.75	103.60	108.20
36	1	2101	C	P-O3'-C3'	5.75	126.60	119.70
36	5	819	U	N3-C4-O4	5.75	123.43	119.40
36	5	1293	U	N1-C2-O2	-5.75	118.77	122.80
36	1	832	G	C8-N9-C4	5.75	108.70	106.40
1	6	1124	A	C4-C5-N7	5.75	113.58	110.70
36	5	2700	G	O5'-P-OP2	-5.75	100.53	105.70
36	1	859	G	N3-C4-N9	5.75	129.45	126.00
36	1	2289	U	C6-N1-C2	-5.75	117.55	121.00
36	5	652	G	O5'-P-OP1	-5.75	100.53	105.70
36	5	776	U	C5-C4-O4	5.75	129.35	125.90
36	5	1205	A	C5-C6-N1	5.75	120.57	117.70
1	2	322	G	N9-C4-C5	5.75	107.70	105.40
1	2	453	U	C6-N1-C1'	-5.75	113.16	121.20
1	6	351	C	C2-N1-C1'	5.75	125.12	118.80
36	5	1847	A	N3-C4-C5	5.75	130.82	126.80
36	5	2921	U	N1-C2-N3	5.75	118.35	114.90
36	1	2608	G	N3-C4-C5	5.75	131.47	128.60
36	5	355	A	C2-N3-C4	-5.75	107.73	110.60
36	5	2363	A	N9-C4-C5	-5.75	103.50	105.80
1	2	720	G	OP1-P-O3'	5.74	117.84	105.20
36	1	1199	C	N1-C2-O2	5.74	122.35	118.90
36	5	349	A	N1-C6-N6	-5.74	115.15	118.60
38	8	18	U	O5'-P-OP2	-5.74	100.53	105.70
36	1	2305	G	C6-C5-N7	-5.74	126.95	130.40
36	1	2801	A	C4-N9-C1'	-5.74	115.96	126.30
36	1	3309	G	C8-N9-C4	-5.74	104.10	106.40
36	5	2323	G	C8-N9-C4	-5.74	104.10	106.40
36	5	2405	C	C6-N1-C2	-5.74	118.00	120.30
36	5	2417	U	N3-C4-O4	5.74	123.42	119.40
36	5	2707	C	C6-N1-C2	5.74	122.60	120.30
41	14	187	LEU	CA-CB-CG	5.74	128.50	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	397	A	C5-C6-N1	5.74	120.57	117.70
36	1	967	A	C2-N3-C4	-5.74	107.73	110.60
36	1	2917	G	C5-C6-O6	-5.74	125.16	128.60
1	6	1634	C	C6-N1-C1'	-5.74	113.91	120.80
36	5	3327	G	OP2-P-O3'	5.74	117.83	105.20
36	5	889	U	N1-C2-N3	-5.74	111.46	114.90
36	5	1086	C	C6-N1-C2	5.74	122.59	120.30
36	5	1834	U	N1-C2-N3	5.74	118.34	114.90
36	5	2281	A	N7-C8-N9	-5.74	110.93	113.80
1	2	1486	G	N7-C8-N9	5.73	115.97	113.10
36	5	635	G	C8-N9-C4	5.73	108.69	106.40
36	5	2385	G	N1-C6-O6	5.73	123.34	119.90
1	6	440	U	N1-C2-N3	5.73	118.34	114.90
36	5	886	C	C4-C5-C6	5.73	120.27	117.40
36	5	2180	G	N9-C4-C5	-5.73	103.11	105.40
36	5	2930	A	O4'-C1'-N9	5.73	112.79	108.20
36	5	3309	G	C8-N9-C4	-5.73	104.11	106.40
36	1	972	A	C8-N9-C4	5.73	108.09	105.80
36	1	1392	G	N7-C8-N9	-5.73	110.23	113.10
36	5	41	G	C5-N7-C8	-5.73	101.44	104.30
36	5	987	U	N1-C2-N3	5.73	118.34	114.90
36	5	2937	G	N1-C6-O6	5.73	123.34	119.90
36	1	636	C	C2-N3-C4	-5.73	117.04	119.90
36	1	788	C	C2-N1-C1'	-5.73	112.50	118.80
1	6	351	C	N3-C4-N4	5.73	122.01	118.00
1	6	542	A	C4-N9-C1'	5.73	136.61	126.30
1	6	1697	G	N3-C4-C5	-5.73	125.74	128.60
36	1	949	C	C2-N1-C1'	5.73	125.10	118.80
36	1	2426	U	C5-C4-O4	5.73	129.34	125.90
36	5	2290	C	N3-C4-C5	5.73	124.19	121.90
36	1	1795	U	C2-N1-C1'	5.73	124.57	117.70
36	1	3001	C	N3-C4-C5	5.73	124.19	121.90
36	5	337	G	C8-N9-C4	-5.73	104.11	106.40
1	6	1382	A	O4'-C1'-N9	5.72	112.78	108.20
36	5	2824	G	C5-C6-O6	-5.72	125.17	128.60
36	5	3184	A	N9-C4-C5	-5.72	103.51	105.80
36	1	734	C	C2-N1-C1'	5.72	125.09	118.80
9	s7	131	PHE	C-N-CD	5.72	140.42	128.40
36	5	1064	A	P-O3'-C3'	5.72	126.57	119.70
36	1	3001	C	C2-N3-C4	-5.72	117.04	119.90
1	6	609	U	N1-C2-N3	5.72	118.33	114.90
1	6	1023	A	N1-C6-N6	5.72	122.03	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1205	A	C5-C6-N6	-5.72	119.12	123.70
36	5	2169	G	C4-C5-N7	-5.72	108.51	110.80
36	5	2352	A	C6-N1-C2	-5.72	115.17	118.60
1	6	194	U	C2-N1-C1'	5.72	124.56	117.70
1	6	1537	C	O4'-C1'-N1	5.72	112.78	108.20
1	2	1782	A	C5-C6-N6	5.72	128.27	123.70
36	1	105	C	C5-C4-N4	-5.72	116.20	120.20
36	1	1490	A	C8-N9-C4	-5.72	103.51	105.80
36	1	2115	G	C6-C5-N7	-5.72	126.97	130.40
1	6	416	A	C2-N3-C4	-5.72	107.74	110.60
36	5	2976	A	N1-C6-N6	-5.72	115.17	118.60
38	8	106	C	C6-N1-C2	5.72	122.59	120.30
36	5	1463	U	N3-C2-O2	5.71	126.20	122.20
36	5	2948	C	N1-C2-O2	5.71	122.33	118.90
36	5	2349	U	C5-C4-O4	5.71	129.33	125.90
36	5	1131	G	O5'-P-OP2	-5.71	100.56	105.70
36	5	1452	A	C5-N7-C8	-5.71	101.04	103.90
36	1	1712	G	N1-C6-O6	5.71	123.33	119.90
36	1	2213	A	N9-C4-C5	5.71	108.08	105.80
36	5	1413	G	N1-C2-N3	5.71	127.33	123.90
38	4	113	U	N1-C2-N3	5.71	118.33	114.90
36	5	1308	A	C5-N7-C8	5.71	106.75	103.90
36	5	1917	C	C5-C4-N4	-5.71	116.20	120.20
36	1	3184	A	C8-N9-C4	5.71	108.08	105.80
39	L2	191	LEU	CA-CB-CG	-5.71	102.17	115.30
1	6	1641	C	C5-C4-N4	-5.71	116.20	120.20
36	5	2732	G	O5'-P-OP2	-5.71	100.56	105.70
36	5	2825	C	C6-N1-C2	5.71	122.58	120.30
36	1	2572	C	C6-N1-C1'	-5.71	113.95	120.80
36	1	2816	G	N1-C6-O6	5.71	123.32	119.90
36	1	822	G	N1-C6-O6	5.70	123.32	119.90
36	1	3133	C	N3-C4-N4	5.70	121.99	118.00
36	1	3269	U	C5-C4-O4	5.70	129.32	125.90
36	5	1331	U	C6-N1-C2	5.70	124.42	121.00
36	5	2392	C	C5-C6-N1	-5.70	118.15	121.00
37	7	81	U	N3-C2-O2	-5.70	118.21	122.20
36	1	785	G	C5-C6-N1	5.70	114.35	111.50
36	1	1437	C	C6-N1-C2	-5.70	118.02	120.30
36	5	1141	C	C4-C5-C6	-5.70	114.55	117.40
36	5	2384	A	C5-C6-N6	-5.70	119.14	123.70
36	1	188	U	C5-C6-N1	-5.70	119.85	122.70
36	1	276	U	N3-C2-O2	5.70	126.19	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	429	U	N1-C2-O2	5.70	126.79	122.80
36	1	2869	U	O5'-P-OP1	-5.70	100.57	105.70
1	6	405	C	C6-N1-C2	5.70	122.58	120.30
1	6	1111	G	C6-C5-N7	-5.70	126.98	130.40
37	7	28	C	C6-N1-C2	-5.70	118.02	120.30
1	6	536	C	C2-N1-C1'	5.70	125.07	118.80
36	5	1156	C	C5-C4-N4	-5.70	116.21	120.20
36	5	1484	U	C5-C6-N1	-5.70	119.85	122.70
36	1	2144	A	N7-C8-N9	-5.70	110.95	113.80
36	1	2983	C	O5'-P-OP1	-5.70	100.57	105.70
36	5	1588	A	C8-N9-C4	5.70	108.08	105.80
36	5	3060	C	N3-C2-O2	5.70	125.89	121.90
1	2	638	U	C2-N1-C1'	5.69	124.53	117.70
36	1	339	C	C2-N3-C4	-5.69	117.05	119.90
36	1	583	G	N3-C4-N9	-5.69	122.58	126.00
36	1	634	C	C6-N1-C2	5.69	122.58	120.30
36	1	1906	G	C6-C5-N7	-5.69	126.98	130.40
36	1	2754	G	C8-N9-C4	5.69	108.68	106.40
36	1	3207	U	O4'-C1'-N1	5.69	112.75	108.20
36	5	35	A	C2-N3-C4	-5.69	107.75	110.60
36	5	928	C	N3-C4-N4	-5.69	114.02	118.00
36	5	2937	G	C6-C5-N7	-5.69	126.98	130.40
36	1	2937	G	N7-C8-N9	-5.69	110.25	113.10
36	5	797	U	OP2-P-O3'	5.69	117.72	105.20
36	5	1119	C	N1-C2-O2	-5.69	115.48	118.90
36	5	1837	U	N1-C2-O2	-5.69	118.82	122.80
36	1	997	A	C4-C5-C6	5.69	119.84	117.00
1	6	978	A	N9-C4-C5	5.69	108.08	105.80
36	5	437	G	N1-C2-N2	5.69	121.32	116.20
36	1	2606	G	C8-N9-C1'	-5.69	119.61	127.00
1	6	638	U	N3-C2-O2	-5.69	118.22	122.20
36	5	1528	G	N3-C4-N9	5.69	129.41	126.00
37	7	78	U	N3-C2-O2	-5.69	118.22	122.20
36	1	156	G	N3-C4-N9	5.68	129.41	126.00
36	1	2776	C	C5-C4-N4	-5.68	116.22	120.20
36	5	1428	A	O5'-P-OP1	-5.68	100.58	105.70
36	5	2134	G	N1-C2-N2	-5.68	111.08	116.20
1	6	957	G	N3-C2-N2	-5.68	115.92	119.90
36	5	1902	G	C4-C5-C6	5.68	122.21	118.80
36	1	156	G	N3-C4-C5	-5.68	125.76	128.60
36	1	3050	U	N3-C2-O2	-5.68	118.22	122.20
36	5	644	G	C4-C5-C6	5.68	122.21	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	124	U	N3-C4-O4	-5.68	115.42	119.40
36	1	2621	G	C4-C5-C6	5.68	122.21	118.80
37	3	88	G	N1-C6-O6	-5.68	116.49	119.90
36	1	416	A	OP2-P-O3'	5.68	117.69	105.20
36	1	1138	U	N1-C2-O2	5.68	126.77	122.80
36	1	2409	G	C6-C5-N7	-5.68	126.99	130.40
36	1	2608	G	N1-C6-O6	5.68	123.31	119.90
36	5	800	G	C8-N9-C1'	-5.68	119.62	127.00
36	5	1665	C	N3-C4-N4	-5.68	114.03	118.00
36	5	1927	G	C5-C6-N1	-5.68	108.66	111.50
36	5	2363	A	C6-C5-N7	-5.68	128.33	132.30
36	1	1177	G	N3-C2-N2	-5.67	115.93	119.90
36	5	277	G	O5'-P-OP1	-5.67	100.59	105.70
36	5	1076	C	N3-C4-C5	-5.67	119.63	121.90
36	5	1440	G	N9-C4-C5	5.67	107.67	105.40
36	5	1794	G	C4-C5-N7	-5.67	108.53	110.80
36	5	2366	C	N3-C4-C5	-5.67	119.63	121.90
36	5	570	A	N1-C6-N6	5.67	122.00	118.60
36	5	1300	G	C6-C5-N7	-5.67	127.00	130.40
36	1	2408	U	N3-C2-O2	-5.67	118.23	122.20
1	6	31	C	C6-N1-C2	-5.67	118.03	120.30
1	6	1001	A	N1-C6-N6	5.67	122.00	118.60
36	5	875	G	C5-C6-O6	5.67	132.00	128.60
36	5	1044	U	C5-C6-N1	-5.67	119.86	122.70
36	5	1149	G	N1-C6-O6	5.67	123.30	119.90
36	5	1868	G	C5-C6-O6	-5.67	125.20	128.60
38	8	63	G	N1-C6-O6	-5.67	116.50	119.90
36	5	47	C	C6-N1-C2	5.67	122.57	120.30
36	5	2944	U	N1-C2-O2	5.67	126.77	122.80
36	1	2878	G	N9-C4-C5	-5.67	103.13	105.40
36	5	639	G	O5'-P-OP1	5.67	117.50	110.70
36	5	970	A	C5-N7-C8	-5.67	101.07	103.90
36	5	2954	U	N1-C2-O2	5.67	126.77	122.80
36	1	2787	G	C5-C6-N1	5.67	114.33	111.50
1	6	1129	U	N3-C4-O4	-5.67	115.43	119.40
17	c5	36	LEU	CA-CB-CG	5.67	128.33	115.30
36	5	949	C	C2-N3-C4	-5.67	117.07	119.90
36	5	1561	G	O4'-C1'-N9	5.67	112.73	108.20
36	1	2138	A	C2-N3-C4	-5.67	107.77	110.60
54	M8	32	LEU	CA-CB-CG	5.66	128.32	115.30
36	5	518	G	C5-C6-O6	-5.66	125.20	128.60
36	5	2772	C	OP2-P-O3'	5.66	117.66	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	q3	50	GLY	N-CA-C	-5.66	98.94	113.10
36	1	1055	A	C8-N9-C4	5.66	108.06	105.80
36	1	1343	A	C4-C5-N7	5.66	113.53	110.70
1	6	386	G	OP2-P-O3'	5.66	117.66	105.20
36	5	1328	C	C6-N1-C2	-5.66	118.03	120.30
1	2	1462	G	C5-C6-O6	-5.66	125.20	128.60
36	1	221	A	O5'-P-OP2	-5.66	100.61	105.70
36	1	573	C	N3-C4-N4	-5.66	114.04	118.00
36	1	816	A	N1-C6-N6	-5.66	115.20	118.60
38	4	50	C	C6-N1-C2	-5.66	118.04	120.30
36	5	1927	G	N3-C2-N2	-5.66	115.94	119.90
36	5	2199	G	C4-C5-N7	5.66	113.06	110.80
36	5	2199	G	C5-N7-C8	-5.66	101.47	104.30
36	1	2664	C	C6-N1-C2	-5.66	118.04	120.30
1	6	542	A	C4-C5-N7	5.66	113.53	110.70
37	7	103	A	C5-C6-N6	-5.66	119.17	123.70
36	1	2339	C	OP1-P-O3'	5.66	117.64	105.20
1	6	987	G	N1-C6-O6	5.66	123.29	119.90
12	c0	97	PRO	N-CA-CB	5.66	110.09	103.30
36	5	1897	G	C5-N7-C8	-5.66	101.47	104.30
37	7	36	C	N3-C4-C5	5.66	124.16	121.90
1	2	145	A	C8-N9-C4	-5.65	103.54	105.80
1	2	1455	G	C5-C6-N1	-5.65	108.67	111.50
36	1	969	C	C2-N3-C4	-5.65	117.07	119.90
36	1	2728	G	O5'-P-OP2	-5.65	100.61	105.70
36	1	2893	C	C6-N1-C2	5.65	122.56	120.30
36	1	3057	U	N3-C4-O4	-5.65	115.44	119.40
1	6	1643	U	C5-C6-N1	-5.65	119.87	122.70
36	5	2820	A	O5'-P-OP1	5.65	117.48	110.70
36	5	3217	C	C2-N1-C1'	-5.65	112.58	118.80
36	5	3317	U	C5-C4-O4	5.65	129.29	125.90
40	l3	10	ARG	NE-CZ-NH1	5.65	123.13	120.30
36	1	2418	G	OP2-P-O3'	5.65	117.63	105.20
36	5	694	C	C6-N1-C2	-5.65	118.04	120.30
36	5	3218	A	C5-C6-N6	-5.65	119.18	123.70
36	1	639	G	C2-N3-C4	-5.65	109.08	111.90
1	6	767	U	C5-C4-O4	5.65	129.29	125.90
36	5	3005	A	N3-C4-C5	-5.65	122.85	126.80
36	1	754	G	C5-C6-N1	-5.65	108.68	111.50
36	1	1438	U	C4-C5-C6	5.65	123.09	119.70
36	5	558	U	N3-C2-O2	-5.65	118.25	122.20
36	5	770	G	O4'-C1'-N9	5.65	112.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	42	A	N1-C6-N6	5.65	121.99	118.60
41	L4	47	ARG	NE-CZ-NH2	5.65	123.12	120.30
36	5	2735	U	C6-N1-C2	-5.65	117.61	121.00
12	c0	83	PRO	N-CA-CB	5.64	110.07	103.30
36	5	1268	G	C8-N9-C4	-5.64	104.14	106.40
36	5	1496	C	OP1-P-OP2	-5.64	111.13	119.60
36	5	2659	G	C6-C5-N7	-5.64	127.01	130.40
36	5	3218	A	C2-N3-C4	-5.64	107.78	110.60
36	5	3376	A	N1-C6-N6	5.64	121.99	118.60
43	l6	77	ARG	NE-CZ-NH1	5.64	123.12	120.30
36	1	284	A	O4'-C1'-N9	5.64	112.72	108.20
36	5	2149	A	C8-N9-C4	5.64	108.06	105.80
1	6	1484	G	O5'-P-OP1	-5.64	100.62	105.70
36	5	3154	C	C5-C6-N1	5.64	123.82	121.00
1	2	730	G	C4-N9-C1'	5.64	133.83	126.50
36	1	2276	G	C8-N9-C4	-5.64	104.14	106.40
36	1	3229	G	N9-C4-C5	-5.64	103.14	105.40
1	6	75	U	N3-C2-O2	-5.64	118.25	122.20
1	6	970	A	O5'-P-OP2	-5.64	100.62	105.70
36	5	1201	C	C2-N3-C4	5.64	122.72	119.90
36	5	1592	G	N9-C4-C5	5.64	107.66	105.40
36	1	44	U	N3-C2-O2	5.64	126.15	122.20
1	6	1124	A	N9-C4-C5	-5.64	103.55	105.80
36	1	50	U	N1-C2-N3	5.64	118.28	114.90
36	1	2434	U	N3-C4-O4	-5.64	115.45	119.40
1	2	590	C	N1-C2-O2	5.63	122.28	118.90
36	1	1124	U	N3-C2-O2	-5.63	118.26	122.20
36	1	1379	G	N1-C2-N3	5.63	127.28	123.90
1	6	558	U	N3-C2-O2	-5.63	118.25	122.20
56	n0	155	ARG	CG-CD-NE	5.63	123.63	111.80
59	n3	45	ARG	NE-CZ-NH1	-5.63	117.48	120.30
36	1	374	A	O5'-P-OP2	-5.63	100.63	105.70
36	1	1342	C	N3-C4-C5	5.63	124.15	121.90
36	1	295	A	C8-N9-C4	-5.63	103.55	105.80
36	1	1180	A	C5-N7-C8	5.63	106.72	103.90
36	1	343	U	C4-C5-C6	5.63	123.08	119.70
36	1	1440	G	C8-N9-C4	5.63	108.65	106.40
1	2	619	A	OP2-P-O3'	5.63	117.58	105.20
36	5	1128	U	C5-C6-N1	-5.63	119.89	122.70
36	5	2606	G	O5'-P-OP1	-5.63	100.64	105.70
36	5	2702	A	C4-C5-C6	5.63	119.81	117.00
39	l2	216	HIS	N-CA-C	-5.63	95.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	901	G	O5'-P-OP1	-5.62	100.64	105.70
1	2	1426	C	N3-C2-O2	5.62	125.84	121.90
36	1	830	A	N9-C4-C5	-5.62	103.55	105.80
36	1	1432	C	C6-N1-C2	-5.62	118.05	120.30
36	1	1433	A	O4'-C1'-N9	-5.62	103.70	108.20
36	1	1447	G	N9-C4-C5	5.62	107.65	105.40
36	1	2899	C	O4'-C1'-N1	5.62	112.70	108.20
36	1	3214	U	C6-N1-C2	-5.62	117.63	121.00
36	5	796	U	N1-C2-N3	5.62	118.27	114.90
36	1	1376	C	N3-C4-N4	5.62	121.94	118.00
36	5	938	C	C5-C4-N4	-5.62	116.27	120.20
36	5	1321	G	C2-N3-C4	-5.62	109.09	111.90
36	5	2848	G	C4-C5-C6	5.62	122.17	118.80
36	1	1111	U	C6-N1-C2	5.62	124.37	121.00
36	1	2827	U	C2-N1-C1'	-5.62	110.96	117.70
36	5	2426	U	C6-N1-C2	-5.62	117.63	121.00
36	5	3091	A	C6-N1-C2	-5.62	115.23	118.60
36	5	3105	U	N1-C2-N3	5.62	118.27	114.90
1	6	163	G	C5-N7-C8	-5.62	101.49	104.30
36	1	2715	A	O5'-P-OP1	-5.62	100.65	105.70
36	1	2756	C	C4-C5-C6	5.62	120.21	117.40
36	5	128	G	N1-C6-O6	5.62	123.27	119.90
36	5	980	A	N1-C6-N6	-5.62	115.23	118.60
36	1	1159	A	O4'-C1'-N9	5.61	112.69	108.20
36	1	2952	G	C6-C5-N7	-5.61	127.03	130.40
36	1	3204	C	N3-C2-O2	-5.61	117.97	121.90
38	4	38	U	C2-N1-C1'	5.61	124.44	117.70
36	5	1206	G	N3-C4-C5	-5.61	125.79	128.60
36	5	1448	U	C6-N1-C2	5.61	124.37	121.00
1	6	815	G	C4-N9-C1'	5.61	133.80	126.50
36	5	2381	G	C8-N9-C4	-5.61	104.16	106.40
1	2	406	U	O5'-P-OP2	-5.61	100.65	105.70
1	2	1572	G	C4-C5-N7	5.61	113.04	110.80
36	1	2171	G	C2-N3-C4	5.61	114.70	111.90
36	1	2624	G	C4-C5-N7	5.61	113.04	110.80
36	5	998	A	OP2-P-O3'	5.61	117.54	105.20
36	1	2868	U	C6-N1-C1'	-5.61	113.35	121.20
1	6	359	A	C8-N9-C4	5.61	108.04	105.80
1	6	815	G	N7-C8-N9	5.61	115.90	113.10
36	5	1115	G	C8-N9-C1'	-5.61	119.71	127.00
36	1	233	C	C5-C6-N1	-5.61	118.20	121.00
36	1	659	G	C5-C6-N1	5.61	114.30	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1493	G	C5-C6-N1	5.61	114.30	111.50
36	1	2777	G	C5-C6-O6	5.61	131.97	128.60
1	6	815	G	C4-C5-N7	5.61	113.04	110.80
36	5	1331	U	N3-C4-C5	5.61	117.96	114.60
36	5	3382	U	N3-C2-O2	-5.61	118.27	122.20
37	7	98	C	C6-N1-C2	5.61	122.54	120.30
36	1	1000	C	C2-N1-C1'	5.61	124.97	118.80
36	1	2704	A	N1-C2-N3	5.61	132.10	129.30
1	6	1787	C	N3-C4-N4	5.61	121.92	118.00
36	5	1080	A	C8-N9-C4	5.61	108.04	105.80
36	5	1909	A	N7-C8-N9	-5.61	111.00	113.80
36	5	2814	G	C6-C5-N7	-5.61	127.04	130.40
38	8	125	U	C2-N1-C1'	5.61	124.43	117.70
51	m5	164	LEU	CA-CB-CG	-5.61	102.41	115.30
1	6	371	G	C4-C5-C6	5.60	122.16	118.80
36	1	906	A	C5-C6-N1	5.60	120.50	117.70
36	1	1320	C	N3-C4-C5	-5.60	119.66	121.90
36	5	278	U	N3-C4-O4	5.60	123.32	119.40
36	5	1931	U	C5-C6-N1	-5.60	119.90	122.70
36	5	2765	C	C5-C4-N4	-5.60	116.28	120.20
38	8	4	C	N3-C4-C5	5.60	124.14	121.90
38	8	96	A	N9-C4-C5	-5.60	103.56	105.80
36	1	595	G	C2-N3-C4	-5.60	109.10	111.90
36	1	894	G	OP1-P-O3'	5.60	117.52	105.20
36	1	3178	A	C6-C5-N7	-5.60	128.38	132.30
1	6	306	U	C2-N3-C4	-5.60	123.64	127.00
1	6	426	G	N3-C4-C5	-5.60	125.80	128.60
36	5	63	A	N9-C4-C5	-5.60	103.56	105.80
36	5	1449	A	N1-C2-N3	5.60	132.10	129.30
38	8	23	U	N1-C2-O2	-5.60	118.88	122.80
36	1	1115	G	N9-C4-C5	5.60	107.64	105.40
36	1	1180	A	C4-C5-N7	-5.60	107.90	110.70
36	1	1297	C	C4-C5-C6	5.60	120.20	117.40
36	1	2823	G	N9-C4-C5	5.60	107.64	105.40
1	6	321	C	N3-C2-O2	-5.60	117.98	121.90
1	6	1269	U	N3-C2-O2	-5.60	118.28	122.20
36	5	420	G	N9-C4-C5	5.60	107.64	105.40
36	5	739	G	N1-C6-O6	-5.60	116.54	119.90
36	1	1151	U	N1-C2-O2	-5.60	118.88	122.80
36	1	1312	C	N1-C2-O2	-5.60	115.54	118.90
36	5	2334	U	N3-C4-C5	5.60	117.96	114.60
36	5	3199	G	N1-C6-O6	-5.60	116.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2637	A	C8-N9-C4	-5.59	103.56	105.80
36	1	2802	A	OP2-P-O3'	5.59	117.51	105.20
1	6	1697	G	C2-N3-C4	5.59	114.70	111.90
36	5	437	G	N9-C4-C5	5.59	107.64	105.40
36	5	1403	C	N3-C4-C5	5.59	124.14	121.90
36	5	1834	U	C4-C5-C6	5.59	123.06	119.70
36	1	193	C	C6-N1-C2	-5.59	118.06	120.30
36	1	403	C	N3-C4-N4	-5.59	114.08	118.00
36	1	701	G	C5-C6-O6	-5.59	125.25	128.60
36	1	2885	C	C5-C6-N1	-5.59	118.20	121.00
36	1	3115	C	N3-C2-O2	5.59	125.81	121.90
36	5	2297	U	C2-N1-C1'	-5.59	110.99	117.70
36	5	2905	U	C2-N3-C4	-5.59	123.64	127.00
1	2	1636	C	C6-N1-C2	-5.59	118.06	120.30
36	1	317	A	C2-N3-C4	-5.59	107.81	110.60
36	5	530	G	N1-C6-O6	-5.59	116.55	119.90
1	2	553	G	C5-C6-N1	-5.59	108.71	111.50
36	1	663	C	C5-C4-N4	-5.59	116.29	120.20
36	5	339	C	C6-N1-C1'	5.59	127.51	120.80
36	5	2613	U	OP1-P-O3'	5.59	117.49	105.20
1	2	1432	U	C6-N1-C2	5.59	124.35	121.00
36	1	661	G	C4-N9-C1'	5.59	133.76	126.50
36	1	1440	G	N3-C4-C5	5.59	131.39	128.60
36	5	1107	C	N1-C2-O2	-5.59	115.55	118.90
36	5	1223	A	C8-N9-C4	5.59	108.03	105.80
36	5	1452	A	C8-N9-C4	5.59	108.03	105.80
36	5	1866	C	C6-N1-C1'	-5.59	114.10	120.80
36	1	1331	U	OP2-P-O3'	5.58	117.49	105.20
36	1	2969	A	N1-C6-N6	5.58	121.95	118.60
36	1	3092	C	O5'-P-OP1	-5.58	100.67	105.70
38	4	58	G	C4-C5-N7	5.58	113.03	110.80
1	6	1764	C	C6-N1-C2	5.58	122.53	120.30
36	5	365	A	N9-C4-C5	-5.58	103.57	105.80
36	5	2617	U	N3-C4-C5	-5.58	111.25	114.60
36	5	3374	U	N3-C4-O4	-5.58	115.49	119.40
36	1	651	G	C8-N9-C1'	-5.58	119.74	127.00
36	1	779	G	O5'-P-OP2	-5.58	100.67	105.70
1	6	1133	A	N1-C6-N6	5.58	121.95	118.60
36	5	1150	A	O5'-P-OP2	-5.58	100.67	105.70
36	5	2607	G	N7-C8-N9	5.58	115.89	113.10
36	5	2931	C	N3-C4-C5	5.58	124.13	121.90
36	1	2249	G	N3-C4-N9	5.58	129.35	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2971	A	N3-C4-C5	-5.58	122.89	126.80
37	7	87	G	C5-C6-N1	-5.58	108.71	111.50
36	1	2642	A	C5-C6-N1	-5.58	114.91	117.70
36	1	3005	A	N9-C4-C5	5.58	108.03	105.80
1	2	1328	G	C8-N9-C4	5.58	108.63	106.40
36	1	404	G	C5-C6-N1	-5.58	108.71	111.50
36	1	421	G	C5-C6-O6	-5.58	125.25	128.60
36	1	1115	G	C6-N1-C2	-5.58	121.75	125.10
36	1	2144	A	C5-N7-C8	5.58	106.69	103.90
36	1	3005	A	N1-C6-N6	-5.58	115.25	118.60
1	6	107	C	O5'-P-OP2	-5.58	100.68	105.70
36	5	2832	C	C5-C6-N1	-5.58	118.21	121.00
36	1	3375	A	C8-N9-C4	-5.58	103.57	105.80
1	6	1600	A	N9-C1'-C2'	5.58	121.25	114.00
36	1	1343	A	O5'-P-OP2	-5.58	100.68	105.70
36	1	1371	G	N7-C8-N9	-5.58	110.31	113.10
36	1	2144	A	C6-N1-C2	-5.58	115.25	118.60
36	5	48	A	N1-C6-N6	-5.58	115.25	118.60
36	5	680	G	O5'-P-OP2	-5.58	100.68	105.70
36	5	1348	U	O4'-C1'-N1	5.58	112.66	108.20
36	1	321	C	N3-C2-O2	-5.57	118.00	121.90
1	6	1346	A	O4'-C1'-N9	5.57	112.66	108.20
36	5	1534	A	N3-C4-N9	5.57	131.86	127.40
36	5	2820	A	N7-C8-N9	5.57	116.59	113.80
36	5	2981	U	N1-C2-O2	5.57	126.70	122.80
1	2	1458	G	C8-N9-C1'	-5.57	119.76	127.00
1	2	75	U	C2-N1-C1'	5.57	124.38	117.70
36	1	288	C	N3-C2-O2	5.57	125.80	121.90
36	1	1442	U	N3-C2-O2	5.57	126.10	122.20
36	5	1001	G	N1-C6-O6	-5.57	116.56	119.90
36	5	2384	A	N1-C6-N6	5.57	121.94	118.60
36	1	1929	G	C4-C5-N7	5.57	113.03	110.80
36	1	2403	G	N9-C4-C5	-5.57	103.17	105.40
38	8	4	C	N3-C2-O2	-5.57	118.00	121.90
1	2	1101	G	C5-C6-O6	-5.57	125.26	128.60
36	1	935	U	C2-N3-C4	-5.57	123.66	127.00
36	1	1452	A	N1-C6-N6	5.57	121.94	118.60
36	1	2610	G	C4-C5-N7	5.57	113.03	110.80
36	1	3079	U	N1-C2-O2	-5.57	118.90	122.80
36	5	343	U	N3-C2-O2	-5.57	118.30	122.20
36	5	2915	U	C2-N3-C4	-5.57	123.66	127.00
1	2	647	G	N9-C4-C5	5.57	107.63	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	658	G	N3-C4-C5	-5.57	125.82	128.60
36	1	1712	G	C5-C6-O6	-5.57	125.26	128.60
36	1	2203	U	N1-C2-N3	5.57	118.24	114.90
36	1	2808	A	C4-C5-C6	5.57	119.78	117.00
1	6	39	A	O4'-C1'-N9	5.57	112.65	108.20
36	5	41	G	OP2-P-O3'	5.57	117.44	105.20
1	2	402	C	N3-C2-O2	5.56	125.79	121.90
36	1	2197	C	C5-C4-N4	-5.56	116.31	120.20
36	1	2953	U	N3-C4-O4	5.56	123.29	119.40
1	6	1672	G	C4-N9-C1'	5.56	133.73	126.50
36	5	1191	U	C5-C6-N1	-5.56	119.92	122.70
36	5	1917	C	OP2-P-O3'	5.56	117.44	105.20
1	2	554	C	N1-C2-O2	5.56	122.24	118.90
36	1	3212	C	C6-N1-C2	5.56	122.53	120.30
1	2	720	G	P-O3'-C3'	5.56	126.37	119.70
1	2	1490	C	C6-N1-C2	-5.56	118.08	120.30
36	1	2381	G	N1-C6-O6	-5.56	116.56	119.90
36	1	3273	A	C2-N3-C4	-5.56	107.82	110.60
36	5	1525	G	O5'-P-OP2	-5.56	100.70	105.70
36	5	3093	C	C6-N1-C2	5.56	122.52	120.30
36	5	3209	A	C8-N9-C4	-5.56	103.58	105.80
38	8	95	G	C4-N9-C1'	-5.56	119.27	126.50
1	2	313	U	N1-C2-N3	5.56	118.23	114.90
36	5	340	C	C2-N3-C4	-5.56	117.12	119.90
36	1	340	C	C2-N3-C4	-5.56	117.12	119.90
36	5	2357	A	N9-C4-C5	-5.56	103.58	105.80
36	5	2417	U	O5'-P-OP2	5.56	117.37	110.70
36	5	3123	A	C8-N9-C4	5.56	108.02	105.80
36	1	155	G	C5-C6-N1	5.55	114.28	111.50
36	1	930	U	C2-N3-C4	-5.55	123.67	127.00
36	1	1336	U	OP2-P-O3'	5.55	117.42	105.20
36	1	2198	A	N7-C8-N9	-5.55	111.02	113.80
36	1	2616	C	C5-C4-N4	-5.55	116.31	120.20
36	1	2797	C	O5'-P-OP1	-5.55	100.70	105.70
36	1	3177	G	C5-C6-O6	-5.55	125.27	128.60
1	6	1749	A	N9-C4-C5	-5.55	103.58	105.80
36	5	1119	C	C2-N3-C4	-5.55	117.12	119.90
36	5	1409	G	N1-C6-O6	-5.55	116.57	119.90
36	5	2150	G	C4-C5-C6	5.55	122.13	118.80
36	5	2376	G	O5'-P-OP2	-5.55	100.70	105.70
36	1	337	G	OP2-P-O3'	5.55	117.41	105.20
36	1	908	G	N1-C6-O6	5.55	123.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1058	U	P-O3'-C3'	5.55	126.36	119.70
36	5	919	U	O5'-P-OP1	5.55	117.36	110.70
37	7	33	U	O5'-P-OP1	-5.55	100.70	105.70
38	8	65	A	C8-N9-C4	5.55	108.02	105.80
36	1	672	A	C5-C6-N1	-5.55	114.92	117.70
36	5	803	C	N3-C4-N4	5.55	121.89	118.00
1	2	1596	C	C2-N1-C1'	5.55	124.90	118.80
36	1	2400	G	N3-C4-N9	5.55	129.33	126.00
1	6	317	C	C2-N3-C4	-5.55	117.13	119.90
36	5	1117	G	N1-C6-O6	-5.55	116.57	119.90
1	6	1473	U	N3-C2-O2	-5.54	118.32	122.20
36	5	1372	C	C5-C6-N1	-5.54	118.23	121.00
36	1	1911	A	C6-C5-N7	-5.54	128.42	132.30
36	1	2877	G	N9-C4-C5	5.54	107.62	105.40
1	6	630	A	C2-N3-C4	-5.54	107.83	110.60
36	5	2110	G	N9-C4-C5	-5.54	103.18	105.40
36	5	2911	A	C6-C5-N7	-5.54	128.42	132.30
36	1	1365	G	C4-N9-C1'	5.54	133.71	126.50
36	1	3111	U	C6-N1-C2	5.54	124.33	121.00
38	4	94	C	N3-C4-C5	5.54	124.12	121.90
36	5	2968	G	N1-C6-O6	-5.54	116.58	119.90
36	1	1890	U	N3-C2-O2	5.54	126.08	122.20
36	5	103	G	C5-C6-O6	5.54	131.92	128.60
36	5	1297	C	N1-C2-O2	-5.54	115.58	118.90
36	5	690	A	C8-N9-C4	5.54	108.02	105.80
36	5	912	G	C5-N7-C8	5.54	107.07	104.30
36	5	1448	U	C5-C6-N1	-5.54	119.93	122.70
36	5	1528	G	N9-C4-C5	-5.54	103.19	105.40
36	1	715	A	N7-C8-N9	5.54	116.57	113.80
36	1	2122	G	C8-N9-C4	-5.54	104.19	106.40
36	1	3004	C	C5-C6-N1	-5.54	118.23	121.00
1	6	359	A	C4-N9-C1'	-5.54	116.33	126.30
36	5	2931	C	C6-N1-C2	5.54	122.52	120.30
38	8	127	U	N1-C2-O2	5.54	126.67	122.80
1	2	1503	A	N1-C6-N6	5.53	121.92	118.60
1	2	1749	A	N1-C6-N6	5.53	121.92	118.60
36	1	155	G	N3-C4-C5	-5.53	125.83	128.60
1	6	358	U	O5'-P-OP1	-5.53	100.72	105.70
1	6	1765	A	C8-N9-C4	5.53	108.01	105.80
36	5	1129	A	O5'-P-OP1	5.53	117.34	110.70
36	5	2524	A	N9-C1'-C2'	5.53	121.19	114.00
36	5	3004	C	N3-C2-O2	5.53	125.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1082	U	C6-N1-C2	-5.53	117.68	121.00
1	2	571	G	N9-C4-C5	5.53	107.61	105.40
36	1	2984	C	N3-C4-N4	-5.53	114.13	118.00
36	1	3058	U	C2-N1-C1'	5.53	124.34	117.70
38	4	18	U	C5-C4-O4	-5.53	122.58	125.90
1	6	1673	G	O5'-P-OP2	-5.53	100.72	105.70
36	5	221	A	C8-N9-C4	5.53	108.01	105.80
36	5	282	G	C5-C6-O6	5.53	131.92	128.60
36	5	2815	G	C5-N7-C8	5.53	107.07	104.30
38	8	32	C	C2-N1-C1'	-5.53	112.72	118.80
36	1	776	U	N3-C2-O2	-5.53	118.33	122.20
36	1	2643	A	N9-C4-C5	-5.53	103.59	105.80
38	4	140	G	N9-C4-C5	5.53	107.61	105.40
36	5	929	A	N7-C8-N9	-5.53	111.04	113.80
36	1	817	A	C4-C5-C6	5.53	119.76	117.00
36	1	1180	A	N7-C8-N9	-5.53	111.04	113.80
36	1	1483	G	O4'-C1'-N9	5.53	112.62	108.20
36	1	2352	A	O5'-P-OP2	-5.53	100.73	105.70
1	6	1793	G	C4-C5-N7	-5.53	108.59	110.80
36	5	1446	A	N7-C8-N9	-5.53	111.04	113.80
36	5	1604	G	C4-N9-C1'	5.53	133.69	126.50
36	5	2116	G	C8-N9-C1'	-5.53	119.81	127.00
36	5	3048	A	N1-C6-N6	5.53	121.92	118.60
36	5	3200	G	C5-C6-O6	-5.53	125.28	128.60
36	5	3368	U	C2-N1-C1'	-5.53	111.07	117.70
36	1	188	U	N1-C2-N3	5.53	118.22	114.90
36	1	213	A	C5-N7-C8	-5.53	101.14	103.90
36	1	1655	G	N3-C4-N9	5.53	129.32	126.00
36	1	1845	G	C8-N9-C4	-5.53	104.19	106.40
36	1	2200	U	N3-C4-O4	5.53	123.27	119.40
36	5	2813	A	C2-N3-C4	5.53	113.36	110.60
36	5	2889	C	N3-C2-O2	-5.53	118.03	121.90
36	5	3087	A	C8-N9-C4	-5.53	103.59	105.80
1	6	163	G	N1-C2-N2	5.52	121.17	116.20
36	5	1395	G	C5-C6-O6	-5.52	125.29	128.60
36	5	1520	G	N1-C6-O6	5.52	123.21	119.90
36	5	2324	A	N1-C6-N6	5.52	121.91	118.60
36	5	2708	C	C5-C4-N4	-5.52	116.33	120.20
36	1	432	G	C5-C6-N1	-5.52	108.74	111.50
36	1	874	U	O5'-P-OP1	-5.52	100.73	105.70
1	6	1150	G	C8-N9-C4	5.52	108.61	106.40
36	5	217	U	N3-C4-O4	-5.52	115.53	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	630	A	C8-N9-C4	5.52	108.01	105.80
36	5	1813	A	C8-N9-C4	-5.52	103.59	105.80
1	2	1363	U	C2-N1-C1'	5.52	124.32	117.70
1	6	1514	U	N3-C4-O4	-5.52	115.54	119.40
36	5	1662	G	C2-N3-C4	-5.52	109.14	111.90
36	5	3054	U	N3-C4-C5	-5.52	111.29	114.60
54	m8	66	ARG	NE-CZ-NH2	-5.52	117.54	120.30
36	1	2397	A	C6-C5-N7	-5.52	128.44	132.30
36	1	3362	A	C2-N3-C4	-5.52	107.84	110.60
36	5	102	C	C2-N1-C1'	5.52	124.87	118.80
36	5	420	G	C6-N1-C2	-5.52	121.79	125.10
38	8	95	G	C8-N9-C1'	5.52	134.17	127.00
1	2	610	G	C4-N9-C1'	5.52	133.67	126.50
36	5	1628	C	C6-N1-C2	-5.52	118.09	120.30
36	5	3319	U	C2-N1-C1'	5.52	124.32	117.70
1	2	73	U	OP1-P-O3'	5.51	117.33	105.20
36	1	830	A	C4-C5-N7	5.51	113.46	110.70
36	1	1054	A	O5'-P-OP2	-5.51	100.74	105.70
36	1	1379	G	N3-C4-N9	-5.51	122.69	126.00
36	1	2378	C	N1-C2-O2	-5.51	115.59	118.90
1	6	305	C	N1-C2-O2	-5.51	115.59	118.90
36	5	2897	A	C6-N1-C2	-5.51	115.29	118.60
36	1	1578	C	N1-C2-O2	5.51	122.21	118.90
36	1	2996	U	N1-C2-N3	-5.51	111.59	114.90
36	1	2996	U	C5-C4-O4	-5.51	122.59	125.90
36	1	3000	A	C8-N9-C4	5.51	108.00	105.80
36	5	649	A	C5-C6-N6	-5.51	119.29	123.70
36	5	2273	G	C4-C5-N7	-5.51	108.59	110.80
38	8	92	A	O5'-P-OP1	-5.51	100.74	105.70
36	1	233	C	C6-N1-C2	5.51	122.50	120.30
36	1	1741	A	N1-C2-N3	5.51	132.06	129.30
1	6	1025	A	C2-N3-C4	-5.51	107.84	110.60
36	5	43	A	C5-C6-N6	-5.51	119.29	123.70
36	5	278	U	N1-C2-O2	-5.51	118.94	122.80
36	5	2980	U	N3-C2-O2	-5.51	118.34	122.20
36	5	3181	C	O5'-P-OP2	-5.51	100.74	105.70
36	5	3204	C	N1-C2-O2	-5.51	115.59	118.90
1	6	767	U	N3-C2-O2	-5.51	118.34	122.20
1	2	1536	G	N3-C4-N9	5.51	129.30	126.00
36	1	57	A	OP2-P-O3'	5.51	117.31	105.20
36	1	404	G	C8-N9-C4	-5.51	104.20	106.40
1	6	438	A	N1-C6-N6	5.51	121.90	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1120	U	C5-C4-O4	5.51	129.20	125.90
36	5	326	U	N3-C2-O2	5.51	126.05	122.20
36	5	1770	G	C8-N9-C1'	-5.51	119.84	127.00
36	5	3217	C	C5-C6-N1	-5.51	118.25	121.00
52	M6	33	ILE	CG1-CB-CG2	-5.50	99.29	111.40
36	5	1799	A	C4-C5-N7	5.50	113.45	110.70
1	2	608	U	N3-C2-O2	-5.50	118.35	122.20
36	1	358	G	N3-C4-N9	5.50	129.30	126.00
36	1	635	G	C5-C6-O6	-5.50	125.30	128.60
38	4	10	A	C5-C6-N1	5.50	120.45	117.70
36	5	607	A	C5-C6-N6	5.50	128.10	123.70
36	5	2753	G	N3-C2-N2	-5.50	116.05	119.90
36	1	1061	A	C4-C5-C6	5.50	119.75	117.00
36	1	2371	G	OP2-P-O3'	5.50	117.30	105.20
36	1	200	C	N3-C4-C5	5.50	124.10	121.90
36	1	957	C	N1-C2-O2	-5.50	115.60	118.90
36	5	2126	A	N9-C4-C5	-5.50	103.60	105.80
36	5	2630	C	C2-N3-C4	-5.50	117.15	119.90
36	1	198	A	C8-N9-C4	-5.50	103.60	105.80
36	1	2636	A	C5-N7-C8	-5.50	101.15	103.90
38	4	116	G	C8-N9-C1'	-5.50	119.85	127.00
36	5	281	G	N3-C2-N2	-5.50	116.05	119.90
36	5	2658	G	N1-C2-N3	5.50	127.20	123.90
36	1	1377	G	C5-N7-C8	-5.50	101.55	104.30
36	1	2629	U	O5'-P-OP2	-5.50	100.75	105.70
1	6	536	C	C6-N1-C2	-5.50	118.10	120.30
1	2	1634	C	C6-N1-C2	5.49	122.50	120.30
36	1	2679	A	N1-C6-N6	5.49	121.90	118.60
36	5	831	G	C2-N3-C4	5.49	114.65	111.90
1	2	1748	G	O5'-P-OP2	-5.49	100.76	105.70
36	1	432	G	C6-C5-N7	-5.49	127.11	130.40
36	1	2689	A	N1-C6-N6	-5.49	115.31	118.60
36	1	297	G	O4'-C1'-N9	5.49	112.59	108.20
36	1	3310	A	N9-C4-C5	-5.49	103.60	105.80
43	16	173	MET	CB-CG-SD	-5.49	95.93	112.40
36	1	2899	C	C4-C5-C6	5.49	120.14	117.40
36	5	971	G	C5-N7-C8	5.49	107.05	104.30
36	5	2385	G	O5'-P-OP2	5.49	117.29	110.70
1	2	1761	U	C5-C4-O4	5.49	129.19	125.90
38	4	25	G	C2-N3-C4	-5.49	109.16	111.90
36	5	1865	A	N1-C6-N6	5.49	121.89	118.60
1	2	15	U	C5-C4-O4	5.49	129.19	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	640	U	N1-C2-N3	5.49	118.19	114.90
36	5	51	A	C5-C6-N1	-5.49	114.96	117.70
36	5	399	A	N9-C4-C5	-5.49	103.61	105.80
36	5	2116	G	C5-C6-O6	-5.49	125.31	128.60
36	5	2297	U	C6-N1-C1'	5.49	128.88	121.20
1	6	965	U	C2-N1-C1'	5.48	124.28	117.70
36	5	3049	A	C6-N1-C2	5.48	121.89	118.60
36	1	59	G	C5-C6-O6	-5.48	125.31	128.60
36	1	277	G	C2-N3-C4	5.48	114.64	111.90
36	1	913	A	C8-N9-C4	-5.48	103.61	105.80
36	1	2198	A	C6-N1-C2	-5.48	115.31	118.60
36	5	2180	G	C2-N3-C4	-5.48	109.16	111.90
36	5	2242	A	C8-N9-C4	-5.48	103.61	105.80
36	5	2607	G	C8-N9-C4	-5.48	104.21	106.40
36	5	2943	G	N1-C6-O6	5.48	123.19	119.90
36	5	3092	C	N3-C4-C5	5.48	124.09	121.90
36	5	3185	U	O5'-P-OP2	-5.48	100.77	105.70
36	1	633	C	C5-C6-N1	-5.48	118.26	121.00
36	1	1148	G	N9-C4-C5	-5.48	103.21	105.40
36	1	1535	A	N1-C6-N6	5.48	121.89	118.60
38	4	50	C	C2-N1-C1'	5.48	124.83	118.80
1	6	1458	G	C4-N9-C1'	5.48	133.62	126.50
36	5	813	G	OP2-P-O3'	5.48	117.26	105.20
36	5	1578	C	N1-C2-O2	5.48	122.19	118.90
36	5	2349	U	N3-C4-O4	-5.48	115.56	119.40
36	5	2981	U	C6-N1-C1'	-5.48	113.53	121.20
36	1	1298	C	O5'-P-OP1	-5.48	100.77	105.70
36	5	971	G	C4-C5-N7	-5.48	108.61	110.80
1	2	864	U	C5-C4-O4	5.48	129.19	125.90
36	1	96	G	C2-N3-C4	-5.48	109.16	111.90
36	1	1000	C	C5-C4-N4	-5.48	116.36	120.20
36	1	2651	G	OP2-P-O3'	5.48	117.25	105.20
36	1	2809	C	N1-C2-O2	5.48	122.19	118.90
36	5	348	A	C8-N9-C4	5.48	107.99	105.80
36	1	1467	A	C6-N1-C2	-5.48	115.31	118.60
36	1	2404	A	C5-C6-N1	5.48	120.44	117.70
36	5	3093	C	C2-N1-C1'	-5.48	112.78	118.80
36	1	2284	C	C2-N1-C1'	5.47	124.82	118.80
36	5	918	C	N1-C2-O2	-5.47	115.62	118.90
36	5	960	U	N3-C4-O4	-5.47	115.57	119.40
36	5	1057	A	C4-C5-N7	5.47	113.44	110.70
36	5	3018	C	O5'-P-OP1	5.47	117.27	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	496	C	O5'-P-OP2	5.47	117.27	110.70
36	1	681	U	N1-C2-N3	5.47	118.18	114.90
36	1	2122	G	O5'-P-OP2	-5.47	100.77	105.70
38	4	58	G	N9-C4-C5	-5.47	103.21	105.40
36	5	341	G	C5-C6-O6	-5.47	125.32	128.60
36	5	2414	G	C5-C6-N1	-5.47	108.76	111.50
36	5	2647	A	C6-N1-C2	-5.47	115.32	118.60
36	1	230	U	C5-C6-N1	-5.47	119.97	122.70
36	1	2427	U	C5-C6-N1	-5.47	119.96	122.70
36	1	2775	U	C5-C6-N1	-5.47	119.97	122.70
1	6	57	G	O5'-P-OP2	-5.47	100.78	105.70
21	C9	57	ARG	NE-CZ-NH1	5.47	123.03	120.30
36	1	1200	A	O4'-C1'-N9	5.47	112.58	108.20
36	1	2320	A	C2-N3-C4	-5.47	107.86	110.60
36	1	2617	U	C2-N3-C4	-5.47	123.72	127.00
16	c4	35	GLY	N-CA-C	5.47	126.77	113.10
36	1	865	U	N3-C4-O4	-5.47	115.57	119.40
1	2	390	G	N3-C2-N2	-5.47	116.07	119.90
36	1	1110	U	N3-C4-C5	5.47	117.88	114.60
36	1	1377	G	C5-C6-O6	-5.47	125.32	128.60
36	5	1465	A	C8-N9-C4	-5.47	103.61	105.80
43	l6	30	LEU	CA-CB-CG	5.47	127.87	115.30
36	1	47	C	N3-C4-N4	5.46	121.83	118.00
36	1	2282	U	C2-N3-C4	-5.46	123.72	127.00
1	6	1747	G	C8-N9-C4	5.46	108.59	106.40
36	5	658	G	C5-C6-O6	-5.46	125.32	128.60
36	5	3000	A	C5-C6-N6	-5.46	119.33	123.70
36	1	658	G	C4-C5-C6	5.46	122.08	118.80
1	6	173	A	N1-C6-N6	5.46	121.88	118.60
36	5	1446	A	C5-N7-C8	5.46	106.63	103.90
36	5	1515	A	C8-N9-C4	-5.46	103.61	105.80
1	2	1565	C	C6-N1-C2	-5.46	118.11	120.30
36	1	34	A	C5-N7-C8	-5.46	101.17	103.90
36	1	89	A	N1-C2-N3	5.46	132.03	129.30
36	1	1351	U	C2-N1-C1'	5.46	124.25	117.70
1	6	400	A	N1-C6-N6	5.46	121.88	118.60
36	5	1303	A	O5'-P-OP1	-5.46	100.78	105.70
36	5	2306	C	O5'-P-OP2	-5.46	100.79	105.70
36	5	2881	C	N3-C2-O2	5.46	125.72	121.90
36	1	579	G	OP2-P-O3'	5.46	117.21	105.20
1	6	387	A	C2-N3-C4	5.46	113.33	110.60
36	5	795	G	N7-C8-N9	-5.46	110.37	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1201	C	C5-C6-N1	5.46	123.73	121.00
36	5	1507	G	O4'-C1'-N9	-5.46	103.83	108.20
36	1	1101	G	O5'-P-OP2	-5.46	100.79	105.70
36	5	1365	G	N1-C6-O6	5.46	123.17	119.90
36	5	2953	U	C5-C4-O4	-5.46	122.62	125.90
37	7	76	A	C8-N9-C4	5.46	107.98	105.80
1	2	308	C	C5-C6-N1	-5.46	118.27	121.00
36	1	970	A	C5-N7-C8	-5.46	101.17	103.90
38	4	102	U	N1-C2-O2	-5.46	118.98	122.80
36	5	645	A	N9-C4-C5	5.46	107.98	105.80
1	2	610	G	C8-N9-C1'	-5.46	119.91	127.00
36	1	1189	C	N1-C2-O2	-5.46	115.63	118.90
36	1	2968	G	N7-C8-N9	5.46	115.83	113.10
36	5	277	G	C5-C6-O6	5.46	131.87	128.60
36	5	2646	C	C6-N1-C2	5.46	122.48	120.30
38	8	32	C	N1-C2-O2	-5.46	115.63	118.90
36	1	2541	U	P-O3'-C3'	5.45	126.24	119.70
36	5	661	G	C6-C5-N7	-5.45	127.13	130.40
36	5	1338	C	N1-C2-O2	-5.45	115.63	118.90
36	5	1585	C	C6-N1-C2	5.45	122.48	120.30
36	5	3214	U	N1-C2-N3	5.45	118.17	114.90
56	n0	144	LEU	CA-CB-CG	-5.45	102.76	115.30
36	1	102	C	N3-C4-N4	5.45	121.82	118.00
36	1	1902	G	N3-C4-N9	5.45	129.27	126.00
36	5	1124	U	N3-C4-C5	5.45	117.87	114.60
36	5	2584	G	C8-N9-C1'	-5.45	119.92	127.00
36	1	201	A	C2-N3-C4	-5.45	107.88	110.60
36	1	1507	G	C5-C6-O6	-5.45	125.33	128.60
36	1	2726	C	N1-C2-N3	5.45	123.01	119.20
36	5	437	G	N3-C2-N2	-5.45	116.09	119.90
36	5	816	A	N1-C6-N6	-5.45	115.33	118.60
36	1	1007	U	C5-C6-N1	-5.45	119.98	122.70
36	1	1155	C	C5-C6-N1	5.45	123.72	121.00
36	1	2857	C	C5-C4-N4	-5.45	116.39	120.20
36	1	214	G	N1-C6-O6	5.45	123.17	119.90
36	1	262	U	N1-C2-O2	-5.45	118.99	122.80
36	5	969	C	C4-C5-C6	5.45	120.12	117.40
36	5	1495	U	OP1-P-O3'	5.45	117.18	105.20
36	5	1866	C	O4'-C1'-N1	-5.45	103.84	108.20
36	1	2731	U	OP2-P-O3'	5.44	117.18	105.20
36	1	3023	U	O5'-P-OP1	-5.44	100.80	105.70
1	6	1145	U	N3-C4-O4	5.44	123.21	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2685	C	N3-C4-N4	5.44	121.81	118.00
36	1	3144	G	C8-N9-C4	5.44	108.58	106.40
1	6	543	C	C6-N1-C2	-5.44	118.12	120.30
36	5	349	A	OP2-P-O3'	5.44	117.17	105.20
36	5	1506	A	C8-N9-C4	-5.44	103.62	105.80
1	2	590	C	C6-N1-C2	-5.44	118.12	120.30
36	1	1886	A	N1-C6-N6	-5.44	115.33	118.60
36	5	882	A	N1-C2-N3	5.44	132.02	129.30
36	5	1065	A	O5'-P-OP1	-5.44	100.80	105.70
36	5	2387	A	C6-N1-C2	-5.44	115.33	118.60
36	1	633	C	N1-C2-O2	-5.44	115.64	118.90
36	5	864	G	OP2-P-O3'	5.44	117.17	105.20
1	2	831	U	N3-C2-O2	-5.44	118.39	122.20
36	1	332	C	C5-C6-N1	-5.44	118.28	121.00
36	1	1058	U	N3-C2-O2	-5.44	118.39	122.20
36	1	1585	C	C6-N1-C2	5.44	122.47	120.30
36	1	2836	C	N3-C4-N4	-5.44	114.19	118.00
36	1	3318	G	C8-N9-C4	-5.44	104.22	106.40
51	M5	188	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	6	89	G	N1-C6-O6	5.44	123.16	119.90
36	5	1897	G	C6-C5-N7	-5.44	127.14	130.40
36	5	2136	C	OP2-P-O3'	5.44	117.16	105.20
36	5	2385	G	N3-C2-N2	-5.44	116.09	119.90
36	1	325	A	C5-C6-N1	5.44	120.42	117.70
1	6	1075	C	N1-C2-O2	-5.44	115.64	118.90
1	2	1276	U	O5'-P-OP2	-5.43	100.81	105.70
36	1	369	A	C2-N3-C4	5.43	113.32	110.60
36	1	930	U	C2-N1-C1'	-5.43	111.18	117.70
36	1	2093	A	C2-N3-C4	5.43	113.32	110.60
36	1	2600	C	C6-N1-C2	-5.43	118.13	120.30
1	6	687	G	N3-C4-N9	-5.43	122.74	126.00
1	2	552	G	N3-C4-N9	-5.43	122.74	126.00
1	2	1134	C	C6-N1-C2	-5.43	118.13	120.30
64	N8	43	ILE	CG1-CB-CG2	-5.43	99.45	111.40
36	5	180	C	N1-C2-O2	5.43	122.16	118.90
36	5	857	G	N1-C6-O6	5.43	123.16	119.90
36	5	2996	U	O5'-P-OP2	-5.43	100.81	105.70
36	5	3214	U	C5-C4-O4	5.43	129.16	125.90
36	5	1853	U	C5-C4-O4	5.43	129.16	125.90
1	2	1756	A	C5-C6-N6	-5.43	119.36	123.70
36	1	1695	U	C5-C6-N1	-5.43	119.98	122.70
36	1	2116	G	C5-C6-O6	5.43	131.86	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2409	G	C4-C5-C6	5.43	122.06	118.80
36	5	2360	C	O5'-P-OP1	5.43	117.22	110.70
1	6	1549	C	N3-C4-C5	-5.43	119.73	121.90
36	1	819	U	C4-C5-C6	5.43	122.96	119.70
36	1	951	A	N1-C6-N6	5.43	121.86	118.60
1	6	976	G	C6-C5-N7	-5.43	127.14	130.40
36	5	3107	U	OP2-P-O3'	5.43	117.14	105.20
36	5	3153	U	C2-N1-C1'	5.43	124.21	117.70
36	1	1157	G	N1-C2-N3	5.42	127.15	123.90
36	1	1416	C	N3-C4-N4	-5.42	114.20	118.00
36	1	2396	G	C4-C5-C6	5.42	122.05	118.80
1	2	1596	C	N1-C2-O2	5.42	122.15	118.90
1	6	795	U	C2-N1-C1'	5.42	124.21	117.70
36	5	986	U	N3-C2-O2	-5.42	118.40	122.20
38	4	32	C	O5'-P-OP2	-5.42	100.82	105.70
1	6	461	G	C5-C6-O6	-5.42	125.35	128.60
36	5	961	C	N3-C4-N4	5.42	121.80	118.00
36	5	1902	G	C6-N1-C2	-5.42	121.85	125.10
36	1	1159	A	N1-C6-N6	-5.42	115.35	118.60
36	1	2600	C	N3-C2-O2	-5.42	118.11	121.90
36	5	2400	G	N7-C8-N9	-5.42	110.39	113.10
1	2	158	U	P-O3'-C3'	5.42	126.20	119.70
36	1	1492	G	N1-C6-O6	-5.42	116.65	119.90
36	1	1906	G	N1-C6-O6	5.42	123.15	119.90
36	5	1661	G	N1-C6-O6	5.42	123.15	119.90
36	5	2116	G	C4-C5-C6	5.42	122.05	118.80
36	5	2895	G	N3-C4-N9	5.42	129.25	126.00
36	5	3075	G	N3-C2-N2	-5.42	116.11	119.90
36	5	3362	A	C6-C5-N7	-5.42	128.51	132.30
1	2	1432	U	C5-C6-N1	-5.42	119.99	122.70
36	1	308	A	O5'-P-OP2	-5.42	100.83	105.70
36	1	2965	U	N1-C2-N3	5.42	118.15	114.90
36	5	2118	C	O5'-P-OP1	-5.42	100.83	105.70
1	2	1170	G	C4-N9-C1'	5.41	133.54	126.50
36	1	1733	G	N3-C4-C5	-5.41	125.89	128.60
36	1	2867	C	N3-C2-O2	-5.41	118.11	121.90
1	6	25	C	N1-C2-O2	-5.41	115.65	118.90
1	6	1097	U	OP2-P-O3'	5.41	117.11	105.20
36	5	2165	G	C6-C5-N7	-5.41	127.15	130.40
36	5	2365	C	N1-C2-O2	-5.41	115.65	118.90
38	8	39	G	N3-C4-C5	-5.41	125.89	128.60
36	1	2242	A	N1-C2-N3	5.41	132.01	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	46	U	O5'-P-OP2	-5.41	100.83	105.70
36	1	2527	G	N3-C4-N9	-5.41	122.75	126.00
1	6	933	A	N1-C6-N6	-5.41	115.35	118.60
1	6	1537	C	C2-N3-C4	5.41	122.61	119.90
1	6	1614	A	C5-N7-C8	-5.41	101.19	103.90
36	5	2920	U	C5-C6-N1	-5.41	120.00	122.70
36	1	806	A	O4'-C1'-N9	-5.41	103.87	108.20
36	1	2316	G	C8-N9-C4	5.41	108.56	106.40
36	1	2748	A	C8-N9-C4	5.41	107.96	105.80
36	5	180	C	C6-N1-C2	-5.41	118.14	120.30
36	5	1184	A	C5-C6-N1	5.41	120.41	117.70
36	1	701	G	OP2-P-O3'	5.41	117.10	105.20
36	1	2871	G	C5-C6-O6	-5.41	125.36	128.60
1	6	1	U	N3-C2-O2	-5.41	118.42	122.20
36	5	2753	G	N9-C4-C5	5.41	107.56	105.40
1	2	934	C	C2-N1-C1'	5.41	124.75	118.80
36	1	116	A	O4'-C1'-N9	5.41	112.52	108.20
1	6	957	G	C5-C6-N1	-5.41	108.80	111.50
36	5	1301	A	N7-C8-N9	5.41	116.50	113.80
36	5	1829	G	C5-C6-O6	5.41	131.84	128.60
36	5	2411	U	N3-C4-O4	-5.41	115.62	119.40
36	5	3377	G	C5-C6-O6	-5.41	125.36	128.60
38	8	111	A	N1-C6-N6	5.41	121.84	118.60
36	1	2665	U	O5'-P-OP1	-5.40	100.84	105.70
1	2	779	U	O4'-C1'-N1	5.40	112.52	108.20
36	1	227	G	C5-C6-O6	-5.40	125.36	128.60
36	5	881	C	C2-N3-C4	5.40	122.60	119.90
36	5	1155	C	C6-N1-C1'	-5.40	114.32	120.80
36	5	1840	U	N3-C2-O2	-5.40	118.42	122.20
36	5	2396	G	N1-C2-N2	5.40	121.06	116.20
1	2	1762	A	C8-N9-C4	5.40	107.96	105.80
36	1	802	C	C6-N1-C2	-5.40	118.14	120.30
36	1	1685	C	N1-C2-O2	5.40	122.14	118.90
36	1	2714	G	C4-C5-N7	5.40	112.96	110.80
36	1	3107	U	C5-C6-N1	-5.40	120.00	122.70
38	4	41	A	N1-C2-N3	5.40	132.00	129.30
38	4	103	G	N9-C4-C5	5.40	107.56	105.40
1	6	90	C	N3-C4-C5	5.40	124.06	121.90
36	5	314	U	N3-C4-O4	-5.40	115.62	119.40
36	5	430	U	C4-C5-C6	-5.40	116.46	119.70
36	5	1376	C	O5'-P-OP2	-5.40	100.84	105.70
36	5	2134	G	O5'-P-OP2	-5.40	100.84	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	o5	55	LEU	CA-CB-CG	-5.40	102.88	115.30
36	1	397	A	OP2-P-O3'	5.40	117.08	105.20
1	6	17	C	N1-C2-O2	5.40	122.14	118.90
36	5	672	A	C6-C5-N7	-5.40	128.52	132.30
36	5	2112	U	C2-N1-C1'	5.40	124.18	117.70
37	7	49	G	C4-C5-C6	5.40	122.04	118.80
1	2	728	U	N1-C2-O2	5.40	126.58	122.80
36	1	3242	G	C6-C5-N7	5.40	133.64	130.40
36	1	404	G	O5'-P-OP2	-5.39	100.85	105.70
36	1	2656	A	O5'-P-OP1	-5.39	100.84	105.70
1	6	1354	G	C4-N9-C1'	5.39	133.51	126.50
36	5	636	C	OP1-P-O3'	5.39	117.07	105.20
36	5	3021	A	C5-C6-N1	5.39	120.40	117.70
36	1	1934	G	N3-C4-N9	-5.39	122.76	126.00
36	1	2847	A	N1-C6-N6	5.39	121.83	118.60
36	5	2356	A	N1-C2-N3	5.39	132.00	129.30
38	8	42	G	C8-N9-C4	5.39	108.56	106.40
1	2	48	G	OP2-P-O3'	5.39	117.06	105.20
36	1	51	A	N1-C6-N6	5.39	121.83	118.60
36	1	685	G	N1-C6-O6	5.39	123.13	119.90
36	5	841	A	C6-N1-C2	-5.39	115.36	118.60
36	5	2093	A	C4-C5-N7	5.39	113.39	110.70
36	5	2346	C	N1-C2-O2	-5.39	115.67	118.90
36	5	2699	G	N9-C4-C5	-5.39	103.24	105.40
36	1	1313	G	C6-C5-N7	-5.39	127.17	130.40
36	1	2634	U	N3-C2-O2	-5.39	118.43	122.20
1	6	391	A	C8-N9-C4	5.39	107.96	105.80
36	5	208	C	N3-C4-C5	-5.39	119.74	121.90
36	5	1868	G	C4-C5-N7	5.39	112.96	110.80
36	1	2554	A	P-O3'-C3'	5.39	126.17	119.70
36	1	2808	A	C2-N3-C4	-5.39	107.91	110.60
53	M7	41	LEU	CA-CB-CG	5.39	127.69	115.30
1	6	1025	A	C6-C5-N7	-5.39	128.53	132.30
36	5	2932	U	N1-C2-N3	5.39	118.13	114.90
36	5	2987	A	O5'-P-OP2	5.39	117.17	110.70
1	2	1280	C	N3-C4-N4	5.39	121.77	118.00
36	1	2537	U	P-O3'-C3'	5.39	126.16	119.70
36	5	1305	U	C6-N1-C1'	-5.39	113.66	121.20
36	5	3093	C	C4-C5-C6	5.39	120.09	117.40
1	2	973	A	C2-N3-C4	-5.38	107.91	110.60
36	1	188	U	C4-C5-C6	5.38	122.93	119.70
36	1	218	G	O5'-P-OP1	-5.38	100.85	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	363	G	OP1-P-O3'	5.38	117.05	105.20
36	1	906	A	C5-C6-N6	-5.38	119.39	123.70
36	1	2393	G	N3-C4-C5	-5.38	125.91	128.60
52	M6	84	LEU	CB-CG-CD2	-5.38	101.84	111.00
36	5	655	C	OP2-P-O3'	5.38	117.05	105.20
36	5	922	U	N1-C2-O2	5.38	126.57	122.80
36	5	924	G	C2-N3-C4	-5.38	109.21	111.90
36	5	1000	C	N3-C2-O2	5.38	125.67	121.90
36	5	2345	A	N3-C4-N9	5.38	131.71	127.40
36	5	2824	G	N1-C6-O6	5.38	123.13	119.90
36	1	1918	C	C6-N1-C2	-5.38	118.15	120.30
36	1	2976	A	C5-C6-N1	5.38	120.39	117.70
1	6	1759	C	C6-N1-C2	5.38	122.45	120.30
36	5	121	A	N9-C4-C5	-5.38	103.65	105.80
36	5	2909	U	C2-N3-C4	-5.38	123.77	127.00
36	1	1041	U	C5-C6-N1	-5.38	120.01	122.70
36	1	2765	C	N3-C4-C5	-5.38	119.75	121.90
36	5	2893	C	N1-C2-O2	-5.38	115.67	118.90
38	8	102	U	N1-C2-O2	-5.38	119.03	122.80
36	1	1379	G	C2-N3-C4	-5.38	109.21	111.90
36	1	1484	U	C2-N1-C1'	5.38	124.16	117.70
36	1	2337	C	C6-N1-C2	-5.38	118.15	120.30
36	1	3183	A	C4-C5-N7	5.38	113.39	110.70
39	L2	227	ARG	NE-CZ-NH1	5.38	122.99	120.30
36	5	522	A	O5'-P-OP1	-5.38	100.86	105.70
36	5	1332	A	N1-C2-N3	5.38	131.99	129.30
36	5	1484	U	C6-N1-C2	5.38	124.23	121.00
36	5	3215	A	C5-C6-N1	-5.38	115.01	117.70
1	2	627	C	C5-C4-N4	-5.38	116.44	120.20
36	1	1329	U	N1-C1'-C2'	-5.38	106.08	112.00
36	1	1556	C	C2-N1-C1'	5.38	124.72	118.80
36	5	24	G	O5'-P-OP2	-5.38	100.86	105.70
36	5	1194	G	C4-C5-N7	-5.38	108.65	110.80
36	5	1855	U	O5'-P-OP2	-5.38	100.86	105.70
37	7	77	G	C8-N9-C4	5.38	108.55	106.40
1	2	992	A	N1-C2-N3	5.38	131.99	129.30
1	2	1206	U	N3-C4-O4	5.38	123.16	119.40
36	1	2179	C	N1-C2-O2	5.38	122.13	118.90
36	5	335	G	N1-C6-O6	-5.38	116.67	119.90
36	5	914	A	N1-C6-N6	5.38	121.83	118.60
36	5	1385	C	C5-C4-N4	-5.38	116.44	120.20
36	5	2616	C	N1-C2-N3	-5.38	115.44	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1922	A	C2-N3-C4	-5.38	107.91	110.60
36	5	2211	U	N3-C4-C5	-5.38	111.38	114.60
36	1	32	U	O5'-P-OP2	-5.37	100.86	105.70
36	1	74	G	N3-C4-N9	5.37	129.22	126.00
36	1	633	C	C6-N1-C2	5.37	122.45	120.30
36	1	878	G	C5-C6-O6	5.37	131.82	128.60
36	1	2323	G	N3-C4-C5	-5.37	125.91	128.60
36	1	2618	G	C2-N3-C4	5.37	114.59	111.90
1	6	259	U	OP2-P-O3'	5.37	117.02	105.20
36	5	3137	C	N3-C4-C5	5.37	124.05	121.90
36	1	2417	U	N1-C2-N3	5.37	118.12	114.90
36	1	3326	G	N7-C8-N9	-5.37	110.42	113.10
36	5	3185	U	C2-N3-C4	-5.37	123.78	127.00
37	7	45	A	O5'-P-OP2	-5.37	100.86	105.70
36	1	1154	A	N1-C2-N3	5.37	131.99	129.30
36	5	116	A	O4'-C1'-N9	5.37	112.49	108.20
36	5	342	A	C5-N7-C8	-5.37	101.22	103.90
36	5	1188	U	N3-C2-O2	-5.37	118.44	122.20
36	5	1789	G	N3-C4-N9	-5.37	122.78	126.00
36	5	2112	U	N3-C2-O2	-5.37	118.44	122.20
36	5	2616	C	C6-N1-C2	5.37	122.45	120.30
36	5	3374	U	N1-C2-O2	5.37	126.56	122.80
36	5	31	C	C6-N1-C2	5.37	122.45	120.30
36	5	1403	C	C6-N1-C2	5.37	122.45	120.30
1	2	144	U	N3-C2-O2	-5.37	118.44	122.20
1	2	554	C	C2-N1-C1'	5.37	124.70	118.80
36	1	1103	A	OP1-P-O3'	5.37	117.00	105.20
36	1	1658	G	N3-C4-N9	-5.37	122.78	126.00
36	1	2662	G	C6-C5-N7	-5.37	127.18	130.40
36	1	2888	U	N3-C2-O2	5.37	125.96	122.20
36	5	324	A	OP1-P-O3'	5.37	117.00	105.20
36	5	2183	A	N9-C4-C5	-5.37	103.65	105.80
36	1	873	C	N3-C4-C5	5.36	124.05	121.90
36	1	908	G	C5-C6-O6	-5.36	125.38	128.60
36	1	966	U	C2-N1-C1'	5.36	124.14	117.70
36	1	1329	U	C2-N1-C1'	5.36	124.14	117.70
36	1	1792	C	N3-C4-C5	-5.36	119.75	121.90
36	5	62	A	N1-C2-N3	5.36	131.98	129.30
36	5	112	U	O4'-C1'-N1	5.36	112.49	108.20
36	5	1324	U	C5-C6-N1	-5.36	120.02	122.70
36	5	1788	C	C6-N1-C2	-5.36	118.15	120.30
36	1	3122	A	C8-N9-C4	-5.36	103.66	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2354	C	N3-C4-N4	5.36	121.75	118.00
36	1	1452	A	C2-N3-C4	-5.36	107.92	110.60
1	6	350	U	C5-C6-N1	-5.36	120.02	122.70
36	5	75	G	C5-C6-O6	-5.36	125.38	128.60
36	5	3305	A	C5-C6-N6	-5.36	119.41	123.70
36	1	637	C	C2-N1-C1'	-5.36	112.91	118.80
1	6	886	U	C5-C6-N1	-5.36	120.02	122.70
36	5	2335	G	N1-C6-O6	-5.36	116.69	119.90
36	5	2950	G	C6-N1-C2	5.36	128.31	125.10
41	14	202	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	2	992	A	O4'-C1'-N9	5.36	112.48	108.20
36	1	53	G	N7-C8-N9	-5.36	110.42	113.10
36	1	1903	U	N3-C4-O4	5.36	123.15	119.40
36	1	2901	G	N3-C2-N2	-5.36	116.15	119.90
1	6	1735	U	O5'-P-OP2	-5.36	100.88	105.70
36	5	1520	G	C6-N1-C2	-5.35	121.89	125.10
36	5	2148	U	C6-N1-C1'	5.35	128.70	121.20
36	1	1148	G	N7-C8-N9	-5.35	110.42	113.10
36	1	2144	A	C8-N9-C4	5.35	107.94	105.80
36	5	2978	U	C2-N3-C4	-5.35	123.79	127.00
37	7	103	A	N9-C4-C5	-5.35	103.66	105.80
1	2	1457	C	C5-C6-N1	5.35	123.68	121.00
36	1	874	U	N1-C2-O2	-5.35	119.05	122.80
36	1	1132	C	N3-C4-N4	-5.35	114.25	118.00
36	5	349	A	N9-C4-C5	5.35	107.94	105.80
36	5	561	C	C6-N1-C2	-5.35	118.16	120.30
36	5	3206	C	N1-C2-O2	5.35	122.11	118.90
36	1	1316	C	C5-C6-N1	-5.35	118.33	121.00
36	1	1368	U	C2-N3-C4	-5.35	123.79	127.00
36	1	2814	G	O5'-P-OP2	5.35	117.12	110.70
36	1	2920	U	C2-N3-C4	-5.35	123.79	127.00
36	1	2995	A	N7-C8-N9	-5.35	111.13	113.80
36	5	693	A	O5'-P-OP2	5.35	117.12	110.70
36	5	2700	G	C4-C5-N7	5.35	112.94	110.80
36	5	2857	C	C5-C4-N4	-5.35	116.45	120.20
1	2	316	A	N9-C4-C5	-5.35	103.66	105.80
1	6	1478	G	C4-N9-C1'	5.35	133.45	126.50
36	5	646	A	C8-N9-C4	-5.35	103.66	105.80
36	5	1846	C	C5-C6-N1	-5.35	118.33	121.00
36	1	2407	C	N3-C4-N4	5.35	121.74	118.00
1	6	1000	C	C2-N3-C4	-5.35	117.23	119.90
36	5	2824	G	N3-C2-N2	-5.35	116.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2975	U	C5-C6-N1	5.35	125.37	122.70
49	m3	46	ILE	CG1-CB-CG2	-5.35	99.64	111.40
1	2	1426	C	C4-C5-C6	-5.34	114.73	117.40
36	1	1694	U	C5-C6-N1	-5.34	120.03	122.70
1	6	1583	A	C8-N9-C4	5.34	107.94	105.80
36	5	2632	G	OP1-P-O3'	5.34	116.96	105.20
36	5	984	G	C4-C5-C6	5.34	122.01	118.80
36	1	25	U	N1-C2-N3	5.34	118.10	114.90
36	1	2376	G	C5-N7-C8	-5.34	101.63	104.30
36	1	2376	G	C8-N9-C4	-5.34	104.26	106.40
36	1	2411	U	N3-C4-C5	5.34	117.81	114.60
36	1	3278	C	N3-C4-C5	-5.34	119.76	121.90
1	6	1737	G	C4-C5-N7	5.34	112.94	110.80
36	5	314	U	OP1-P-OP2	5.34	127.61	119.60
36	5	800	G	N1-C2-N3	5.34	127.11	123.90
36	5	902	G	N1-C6-O6	5.34	123.11	119.90
36	5	1337	A	C8-N9-C4	-5.34	103.66	105.80
1	2	158	U	C2-N1-C1'	5.34	124.11	117.70
36	1	24	G	C6-C5-N7	-5.34	127.20	130.40
36	1	382	U	N3-C2-O2	5.34	125.94	122.20
36	1	765	C	N1-C2-O2	5.34	122.10	118.90
36	1	2884	C	C4-C5-C6	-5.34	114.73	117.40
1	6	337	G	N7-C8-N9	5.34	115.77	113.10
36	5	2686	A	N1-C2-N3	5.34	131.97	129.30
36	5	2957	G	C6-N1-C2	-5.34	121.90	125.10
38	4	96	A	N1-C6-N6	5.34	121.80	118.60
1	6	514	G	C8-N9-C4	5.34	108.53	106.40
36	5	2383	C	N3-C4-N4	5.34	121.74	118.00
36	5	2988	C	O5'-P-OP2	-5.34	100.90	105.70
1	2	426	G	C8-N9-C1'	-5.34	120.06	127.00
36	1	2198	A	C8-N9-C4	5.34	107.93	105.80
36	5	3005	A	C2-N3-C4	5.34	113.27	110.60
37	7	82	G	C8-N9-C4	-5.34	104.27	106.40
36	5	2365	C	C2-N3-C4	-5.33	117.23	119.90
1	2	139	C	P-O3'-C3'	5.33	126.10	119.70
36	1	32	U	O5'-P-OP1	5.33	117.10	110.70
36	5	2116	G	C4-N9-C1'	5.33	133.43	126.50
36	5	2169	G	N3-C2-N2	-5.33	116.17	119.90
36	5	3310	A	N1-C2-N3	5.33	131.97	129.30
36	1	360	G	C5-C6-O6	-5.33	125.40	128.60
36	1	873	C	O5'-P-OP2	-5.33	100.90	105.70
36	1	1495	U	C2-N1-C1'	-5.33	111.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	308	C	N3-C4-N4	-5.33	114.27	118.00
36	5	1515	A	N9-C4-C5	5.33	107.93	105.80
38	8	4	C	N3-C4-N4	-5.33	114.27	118.00
36	5	1107	C	N3-C4-N4	5.33	121.73	118.00
36	1	109	A	C5-C6-N6	5.33	127.96	123.70
36	1	357	A	N1-C6-N6	5.33	121.80	118.60
36	1	2373	A	N7-C8-N9	5.33	116.46	113.80
36	1	3335	A	O5'-P-OP2	-5.33	100.91	105.70
1	6	1670	G	O5'-P-OP2	-5.33	100.90	105.70
36	1	2434	U	C5-C6-N1	-5.33	120.04	122.70
47	M0	57	LEU	CA-CB-CG	5.33	127.55	115.30
36	5	2145	A	C6-N1-C2	-5.33	115.40	118.60
36	5	3091	A	N1-C6-N6	-5.33	115.40	118.60
1	2	1399	C	C5-C6-N1	5.33	123.66	121.00
36	1	430	U	N3-C4-C5	5.33	117.80	114.60
38	4	44	A	C5-C6-N6	-5.33	119.44	123.70
36	5	1048	A	C2-N3-C4	-5.33	107.94	110.60
36	5	2619	G	N1-C6-O6	5.33	123.10	119.90
36	5	2704	A	O5'-P-OP2	-5.33	100.91	105.70
36	1	1421	G	O5'-P-OP2	-5.32	100.91	105.70
36	5	700	C	C6-N1-C2	5.32	122.43	120.30
36	5	1000	C	C6-N1-C2	5.32	122.43	120.30
36	5	1352	A	P-O3'-C3'	5.32	126.09	119.70
36	5	1841	A	N1-C6-N6	5.32	121.79	118.60
36	5	1869	C	C6-N1-C2	5.32	122.43	120.30
36	5	2659	G	C4-C5-N7	5.32	112.93	110.80
36	5	2865	U	C4-C5-C6	-5.32	116.51	119.70
1	2	1642	G	N3-C4-N9	5.32	129.19	126.00
36	1	1344	G	C5-C6-O6	-5.32	125.41	128.60
36	1	1381	A	C5-C6-N6	-5.32	119.44	123.70
36	1	1410	U	O5'-P-OP1	-5.32	100.91	105.70
36	1	1911	A	N9-C4-C5	-5.32	103.67	105.80
1	6	1032	G	C8-N9-C4	5.32	108.53	106.40
1	6	1641	C	N3-C2-O2	5.32	125.62	121.90
36	5	957	C	N3-C2-O2	-5.32	118.17	121.90
36	5	1548	C	N3-C2-O2	5.32	125.62	121.90
36	5	2854	U	N3-C4-O4	5.32	123.12	119.40
36	5	2993	G	C5-C6-O6	-5.32	125.41	128.60
36	5	3154	C	N3-C2-O2	-5.32	118.18	121.90
48	m1	152	HIS	N-CA-C	-5.32	96.63	111.00
36	1	1425	U	N3-C2-O2	-5.32	118.48	122.20
36	1	2603	G	N3-C2-N2	5.32	123.62	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1057	A	C5-N7-C8	-5.32	101.24	103.90
36	5	1324	U	O5'-P-OP2	-5.32	100.91	105.70
38	8	74	U	C5-C4-O4	-5.32	122.71	125.90
36	1	1295	G	N1-C6-O6	-5.32	116.71	119.90
36	1	2855	U	N3-C4-C5	5.32	117.79	114.60
36	1	2968	G	C8-N9-C4	-5.32	104.27	106.40
36	5	1168	U	N3-C4-C5	5.32	117.79	114.60
36	5	2951	G	OP1-P-O3'	5.32	116.90	105.20
38	8	90	U	C6-N1-C2	5.32	124.19	121.00
36	1	1846	C	N1-C2-O2	-5.32	115.71	118.90
36	5	368	G	N1-C6-O6	-5.32	116.71	119.90
36	5	3245	A	C8-N9-C4	-5.32	103.67	105.80
36	1	1127	G	N1-C2-N3	-5.31	120.71	123.90
1	2	1182	U	N3-C2-O2	-5.31	118.48	122.20
11	S9	93	LEU	CA-CB-CG	5.31	127.52	115.30
36	1	1160	C	C2-N3-C4	5.31	122.56	119.90
36	1	2400	G	C6-C5-N7	-5.31	127.21	130.40
36	1	2983	C	C5-C4-N4	5.31	123.92	120.20
36	5	112	U	N1-C1'-C2'	-5.31	106.16	112.00
36	5	195	U	C4-C5-C6	5.31	122.89	119.70
36	5	520	U	N1-C2-O2	-5.31	119.08	122.80
38	8	102	U	N3-C4-O4	5.31	123.12	119.40
36	1	1420	C	C6-N1-C1'	5.31	127.17	120.80
36	1	1911	A	C4-C5-N7	5.31	113.36	110.70
36	1	2308	C	N1-C2-O2	-5.31	115.71	118.90
1	6	583	C	C2-N1-C1'	5.31	124.64	118.80
1	6	1614	A	C4-C5-N7	5.31	113.36	110.70
36	5	128	G	N3-C4-N9	5.31	129.19	126.00
36	5	366	A	C5-N7-C8	-5.31	101.25	103.90
36	5	886	C	N3-C4-C5	-5.31	119.78	121.90
37	7	13	A	C5-C6-N6	-5.31	119.45	123.70
1	6	1100	G	N1-C6-O6	-5.31	116.72	119.90
36	5	2169	G	C6-C5-N7	5.31	133.59	130.40
36	5	2553	U	N3-C2-O2	-5.31	118.48	122.20
36	5	3182	G	C4-C5-N7	-5.31	108.68	110.80
36	5	3199	G	C5-C6-O6	5.31	131.78	128.60
36	1	66	A	O4'-C1'-N9	-5.31	103.95	108.20
36	1	2139	A	N1-C6-N6	-5.31	115.42	118.60
36	1	3368	U	O4'-C1'-N1	5.31	112.45	108.20
36	5	1585	C	O5'-P-OP1	-5.31	100.92	105.70
1	2	1573	A	OP2-P-O3'	5.31	116.87	105.20
36	1	1323	G	C8-N9-C4	5.31	108.52	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2931	C	OP1-P-OP2	5.31	127.56	119.60
36	1	961	C	C6-N1-C2	5.30	122.42	120.30
36	1	1551	C	OP1-P-O3'	5.30	116.87	105.20
36	1	1932	A	C2-N3-C4	5.30	113.25	110.60
36	1	3187	A	N1-C6-N6	-5.30	115.42	118.60
52	M6	78	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	6	416	A	N1-C6-N6	5.30	121.78	118.60
36	5	1449	A	C2-N3-C4	-5.30	107.95	110.60
36	5	2159	U	C2-N1-C1'	5.30	124.06	117.70
36	5	2316	G	N1-C2-N3	5.30	127.08	123.90
36	5	2323	G	N9-C4-C5	5.30	107.52	105.40
36	1	860	G	N1-C2-N2	5.30	120.97	116.20
36	1	2408	U	O5'-P-OP1	-5.30	100.93	105.70
36	5	877	C	C4-C5-C6	-5.30	114.75	117.40
36	5	2257	C	P-O3'-C3'	5.30	126.06	119.70
14	c2	58	LEU	CA-CB-CG	5.30	127.49	115.30
36	5	3049	A	C5-C6-N1	-5.30	115.05	117.70
36	5	3336	A	C2-N3-C4	-5.30	107.95	110.60
37	7	41	G	C5-C6-O6	-5.30	125.42	128.60
36	1	1408	G	N3-C4-N9	5.30	129.18	126.00
36	1	2659	G	C5-C6-O6	-5.30	125.42	128.60
1	6	72	A	C8-N9-C4	-5.30	103.68	105.80
36	5	34	A	OP2-P-O3'	5.30	116.86	105.20
36	5	934	G	C5-C6-O6	-5.30	125.42	128.60
36	5	2681	U	N1-C2-N3	5.30	118.08	114.90
36	1	1189	C	C4-C5-C6	5.30	120.05	117.40
38	4	125	U	N1-C2-O2	5.30	126.51	122.80
1	6	1773	C	C5-C6-N1	5.30	123.65	121.00
36	5	283	G	C5-C6-O6	-5.30	125.42	128.60
36	5	3172	A	OP1-P-OP2	5.30	127.55	119.60
36	1	59	G	C6-C5-N7	-5.30	127.22	130.40
36	1	1386	A	C5-C6-N6	-5.30	119.46	123.70
36	1	2950	G	O4'-C1'-N9	5.30	112.44	108.20
1	6	418	G	C6-C5-N7	-5.30	127.22	130.40
1	6	1361	U	C6-N1-C1'	-5.30	113.78	121.20
36	1	645	A	N9-C4-C5	5.29	107.92	105.80
36	1	1397	C	OP1-P-O3'	5.29	116.84	105.20
1	6	1300	A	O5'-P-OP1	-5.29	100.94	105.70
36	5	107	A	N1-C6-N6	-5.29	115.42	118.60
36	5	644	G	C4-C5-N7	-5.29	108.68	110.80
36	5	1143	A	C2-N3-C4	-5.29	107.95	110.60
36	5	1152	G	N9-C4-C5	5.29	107.52	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1219	C	N3-C4-C5	5.29	124.02	121.90
36	5	1465	A	C2-N3-C4	-5.29	107.95	110.60
36	5	2919	A	C4-C5-C6	5.29	119.65	117.00
36	5	2959	C	OP2-P-O3'	5.29	116.84	105.20
38	8	100	U	C2-N1-C1'	5.29	124.05	117.70
36	1	5	G	OP1-P-O3'	5.29	116.84	105.20
36	1	950	G	N3-C4-C5	5.29	131.25	128.60
36	1	2316	G	N1-C6-O6	5.29	123.08	119.90
36	1	2880	U	OP2-P-O3'	5.29	116.84	105.20
1	6	1631	A	C5-C6-N6	5.29	127.93	123.70
1	6	1672	G	C8-N9-C1'	-5.29	120.12	127.00
36	5	1863	G	C4-C5-N7	5.29	112.92	110.80
36	5	354	U	C2-N1-C1'	5.29	124.05	117.70
36	5	859	G	C5-C6-O6	-5.29	125.43	128.60
36	5	2114	C	OP1-P-OP2	5.29	127.54	119.60
1	2	219	A	O5'-P-OP2	-5.29	100.94	105.70
1	2	1629	G	C6-C5-N7	-5.29	127.23	130.40
36	1	3264	G	OP2-P-O3'	5.29	116.83	105.20
36	5	1008	U	C5-C6-N1	-5.29	120.06	122.70
36	5	2626	A	OP1-P-OP2	-5.29	111.67	119.60
36	5	934	G	C6-C5-N7	-5.29	127.23	130.40
36	1	936	A	C5-N7-C8	-5.29	101.26	103.90
36	1	2651	G	N3-C2-N2	-5.29	116.20	119.90
1	6	418	G	C5-N7-C8	-5.29	101.66	104.30
36	5	2700	G	N3-C4-N9	5.29	129.17	126.00
37	7	74	C	N1-C2-O2	-5.29	115.73	118.90
1	2	1041	G	C8-N9-C4	-5.28	104.29	106.40
1	2	1773	C	N3-C4-N4	5.28	121.70	118.00
36	1	612	U	C5-C6-N1	-5.28	120.06	122.70
36	5	2249	G	C3'-C2'-C1'	-5.28	97.27	101.50
36	1	1132	C	N3-C2-O2	-5.28	118.20	121.90
36	1	1421	G	C8-N9-C4	5.28	108.51	106.40
1	2	1573	A	P-O3'-C3'	5.28	126.04	119.70
36	1	1188	U	N3-C2-O2	-5.28	118.50	122.20
36	1	2585	G	C2-N3-C4	5.28	114.54	111.90
38	4	17	A	C4-C5-C6	5.28	119.64	117.00
1	6	965	U	C6-N1-C1'	-5.28	113.81	121.20
36	5	345	G	N1-C6-O6	5.28	123.07	119.90
69	o3	18	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	2	1354	G	C8-N9-C4	-5.28	104.29	106.40
36	1	2782	U	N1-C2-O2	-5.28	119.11	122.80
1	2	552	G	N3-C4-C5	5.28	131.24	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	214	G	N3-C2-N2	-5.28	116.21	119.90
36	1	3269	U	N3-C2-O2	-5.28	118.51	122.20
1	6	421	A	N9-C4-C5	-5.28	103.69	105.80
36	5	1116	G	C5-C6-N1	-5.28	108.86	111.50
36	5	1148	G	C5-C6-N1	5.28	114.14	111.50
36	5	2234	G	C4-C5-N7	5.28	112.91	110.80
36	5	2861	U	O5'-P-OP2	5.28	117.03	110.70
1	2	1370	U	P-O3'-C3'	5.28	126.03	119.70
36	5	1116	G	N1-C2-N3	5.28	127.06	123.90
41	14	94	CYS	CA-CB-SG	-5.28	104.50	114.00
36	1	577	C	N3-C4-C5	-5.27	119.79	121.90
40	13	10	ARG	NE-CZ-NH2	-5.27	117.66	120.30
36	1	24	G	N3-C4-N9	5.27	129.16	126.00
36	1	262	U	N3-C2-O2	5.27	125.89	122.20
1	6	489	C	C2-N1-C1'	5.27	124.60	118.80
36	1	3175	U	C5-C4-O4	5.27	129.06	125.90
1	6	310	C	N3-C2-O2	5.27	125.59	121.90
1	6	1549	C	C6-N1-C2	-5.27	118.19	120.30
36	5	2144	A	O5'-P-OP2	-5.27	100.96	105.70
38	8	32	C	C6-N1-C2	5.27	122.41	120.30
47	m0	7	ARG	NE-CZ-NH1	-5.27	117.67	120.30
36	1	100	A	N1-C2-N3	5.27	131.93	129.30
36	1	281	G	C6-N1-C2	-5.27	121.94	125.10
36	1	281	G	O5'-P-OP2	5.27	117.02	110.70
36	1	902	G	O5'-P-OP2	-5.27	100.96	105.70
36	1	2572	C	C6-N1-C2	-5.27	118.19	120.30
36	5	706	A	C8-N9-C4	5.27	107.91	105.80
36	5	1063	G	C5-C6-O6	5.27	131.76	128.60
36	5	1147	G	N1-C2-N2	5.27	120.94	116.20
36	5	2889	C	N3-C4-C5	5.27	124.01	121.90
1	2	554	C	C6-N1-C1'	-5.27	114.48	120.80
36	1	971	G	O5'-P-OP2	-5.27	100.96	105.70
1	6	1	U	N1-C2-O2	5.27	126.49	122.80
1	6	630	A	C8-N9-C4	5.27	107.91	105.80
38	4	74	U	O5'-P-OP1	-5.26	100.96	105.70
36	5	1060	U	C5-C4-O4	5.26	129.06	125.90
36	5	2792	A	C8-N9-C4	-5.26	103.69	105.80
36	1	51	A	C4-C5-N7	5.26	113.33	110.70
36	1	2316	G	C5-C6-O6	-5.26	125.44	128.60
36	1	3176	G	C8-N9-C4	-5.26	104.30	106.40
36	1	3219	G	N1-C6-O6	5.26	123.06	119.90
1	2	426	G	C4-N9-C1'	5.26	133.34	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	909	G	N7-C8-N9	-5.26	110.47	113.10
36	1	1878	G	O4'-C1'-N9	-5.26	103.99	108.20
36	1	2888	U	C2-N3-C4	-5.26	123.84	127.00
38	4	25	G	N1-C2-N3	5.26	127.06	123.90
1	6	387	A	N1-C6-N6	-5.26	115.44	118.60
1	6	590	C	O5'-P-OP1	-5.26	100.97	105.70
36	5	2150	G	C8-N9-C4	-5.26	104.30	106.40
1	2	1043	A	O5'-P-OP2	-5.26	100.97	105.70
1	2	1608	U	O5'-P-OP1	-5.26	100.97	105.70
1	6	393	C	N3-C4-C5	5.26	124.00	121.90
36	5	2857	C	N3-C4-C5	5.26	124.00	121.90
36	5	2978	U	O4'-C1'-N1	5.26	112.41	108.20
36	5	3107	U	C2-N3-C4	-5.26	123.84	127.00
59	n3	15	LEU	CA-CB-CG	-5.26	103.20	115.30
36	1	3083	G	C5-C6-N1	5.26	114.13	111.50
44	L7	163	LEU	CA-CB-CG	-5.26	103.21	115.30
36	5	297	G	N1-C6-O6	-5.26	116.75	119.90
36	5	437	G	N3-C4-C5	5.26	131.23	128.60
1	2	810	G	C4-C5-N7	5.26	112.90	110.80
24	D2	65	LEU	CA-CB-CG	5.26	127.39	115.30
36	1	835	G	C5-C6-O6	-5.26	125.45	128.60
36	1	1179	A	OP2-P-O3'	5.26	116.77	105.20
36	1	1510	G	N1-C2-N2	-5.26	111.47	116.20
36	1	1589	A	N9-C4-C5	-5.26	103.70	105.80
36	1	1845	G	C4-C5-N7	-5.26	108.70	110.80
1	6	1672	G	N3-C4-C5	-5.26	125.97	128.60
36	5	2937	G	C5-C6-O6	-5.26	125.45	128.60
36	5	2956	A	C8-N9-C4	-5.26	103.70	105.80
36	5	2983	C	N3-C4-N4	5.26	121.68	118.00
36	5	3319	U	C5-C6-N1	5.26	125.33	122.70
38	4	112	U	O5'-P-OP2	5.25	117.01	110.70
36	5	3091	A	N9-C4-C5	5.25	107.90	105.80
36	5	3335	A	C5-C6-N6	-5.25	119.50	123.70
36	1	2272	G	O5'-P-OP2	-5.25	100.97	105.70
36	1	2688	U	N1-C2-N3	-5.25	111.75	114.90
38	4	18	U	N3-C4-O4	5.25	123.08	119.40
36	5	216	G	C5-N7-C8	-5.25	101.67	104.30
36	5	1506	A	N7-C8-N9	5.25	116.43	113.80
1	2	312	A	C8-N9-C4	-5.25	103.70	105.80
1	2	1389	C	C2-N1-C1'	5.25	124.58	118.80
36	1	2608	G	C5-C6-N1	-5.25	108.87	111.50
1	6	1697	G	N3-C4-N9	5.25	129.15	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1750	A	C2-N3-C4	-5.25	107.97	110.60
36	5	340	C	C5-C6-N1	-5.25	118.38	121.00
36	5	1840	U	N1-C2-N3	5.25	118.05	114.90
36	5	2359	C	C6-N1-C2	5.25	122.40	120.30
36	5	2608	G	OP2-P-O3'	5.25	116.75	105.20
36	1	3212	C	C5-C6-N1	-5.25	118.38	121.00
1	6	967	A	N3-C4-C5	-5.25	123.12	126.80
36	5	1014	U	C2-N1-C1'	5.25	124.00	117.70
1	2	423	G	N1-C6-O6	-5.25	116.75	119.90
25	D3	111	GLY	N-CA-C	-5.25	99.98	113.10
36	1	1179	A	C2-N3-C4	-5.25	107.98	110.60
36	1	2826	U	OP2-P-O3'	5.25	116.75	105.20
36	1	1661	G	N3-C4-N9	5.25	129.15	126.00
1	6	1658	G	C5-C6-O6	5.25	131.75	128.60
36	5	1104	G	C6-C5-N7	-5.25	127.25	130.40
36	5	2297	U	N1-C2-O2	-5.25	119.13	122.80
36	1	2906	C	N1-C2-N3	5.25	122.87	119.20
38	8	132	G	C4-N9-C1'	-5.25	119.68	126.50
36	1	788	C	C6-N1-C2	5.24	122.40	120.30
36	1	1001	G	N9-C4-C5	-5.24	103.30	105.40
37	3	85	G	OP2-P-O3'	5.24	116.74	105.20
36	5	369	A	C8-N9-C4	-5.24	103.70	105.80
36	5	2971	A	N3-C4-N9	5.24	131.59	127.40
36	5	3107	U	N3-C4-C5	5.24	117.75	114.60
36	1	857	G	N1-C6-O6	5.24	123.05	119.90
36	1	1007	U	C6-N1-C2	5.24	124.14	121.00
36	5	75	G	C6-C5-N7	-5.24	127.25	130.40
36	5	197	G	C5-C6-O6	-5.24	125.45	128.60
36	5	424	G	N3-C4-N9	5.24	129.15	126.00
36	1	2387	A	N7-C8-N9	-5.24	111.18	113.80
36	1	2424	A	N1-C2-N3	-5.24	126.68	129.30
1	6	1614	A	O4'-C1'-N9	5.24	112.39	108.20
1	6	1793	G	C5-C6-O6	5.24	131.75	128.60
36	5	1169	A	OP2-P-O3'	5.24	116.73	105.20
36	5	2149	A	N1-C6-N6	5.24	121.74	118.60
27	D5	95	HIS	N-CA-C	5.24	125.15	111.00
36	1	510	G	N1-C2-N2	5.24	120.92	116.20
36	5	847	A	C8-N9-C4	5.24	107.89	105.80
36	5	933	A	N1-C2-N3	5.24	131.92	129.30
36	5	2290	C	C5-C4-N4	-5.24	116.53	120.20
36	5	2399	A	C8-N9-C4	5.24	107.89	105.80
36	1	648	C	O5'-P-OP1	-5.24	100.99	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	860	G	N3-C2-N2	-5.24	116.23	119.90
36	5	2136	C	N3-C2-O2	-5.24	118.23	121.90
1	2	1747	G	N1-C6-O6	5.24	123.04	119.90
36	1	907	G	N7-C8-N9	5.24	115.72	113.10
36	1	2150	G	C5-C6-N1	-5.24	108.88	111.50
36	1	2179	C	OP2-P-O3'	5.24	116.72	105.20
36	1	2369	G	C2-N3-C4	5.24	114.52	111.90
36	5	630	A	O5'-P-OP1	5.24	116.98	110.70
36	1	347	G	C5-N7-C8	-5.23	101.68	104.30
36	1	694	C	C2-N3-C4	-5.23	117.28	119.90
36	1	2817	A	OP2-P-O3'	5.23	116.71	105.20
36	1	3212	C	O5'-P-OP1	5.23	116.98	110.70
36	5	1780	G	N1-C6-O6	-5.23	116.76	119.90
36	5	2600	C	C5-C6-N1	5.23	123.62	121.00
36	5	2888	U	N3-C4-O4	5.23	123.06	119.40
36	5	2975	U	C4-C5-C6	-5.23	116.56	119.70
36	5	3091	A	N1-C2-N3	5.23	131.92	129.30
36	5	3181	C	O5'-P-OP1	5.23	116.98	110.70
36	5	3362	A	C8-N9-C4	-5.23	103.71	105.80
50	m4	55	ARG	NE-CZ-NH2	-5.23	117.68	120.30
36	1	754	G	N1-C6-O6	5.23	123.04	119.90
36	1	1043	C	N3-C4-C5	5.23	123.99	121.90
36	1	3328	G	C8-N9-C4	-5.23	104.31	106.40
36	5	942	U	C6-N1-C2	-5.23	117.86	121.00
36	5	2352	A	C4-C5-C6	5.23	119.61	117.00
36	5	3209	A	C5-N7-C8	-5.23	101.28	103.90
36	1	1472	U	C5-C6-N1	-5.23	120.09	122.70
52	M6	110	PRO	C-N-CD	-5.23	109.10	120.60
36	5	1154	A	C2-N3-C4	5.23	113.21	110.60
36	5	1607	U	C5-C4-O4	5.23	129.04	125.90
36	5	2808	A	O4'-C1'-N9	-5.23	104.02	108.20
36	5	2836	C	C5-C6-N1	-5.23	118.39	121.00
1	2	499	U	C2-N1-C1'	5.23	123.97	117.70
36	1	1320	C	C5-C6-N1	5.23	123.61	121.00
36	1	2527	G	N3-C4-C5	5.23	131.21	128.60
36	1	2624	G	C5-N7-C8	-5.23	101.69	104.30
36	1	2687	G	N1-C6-O6	-5.23	116.76	119.90
36	1	3101	G	C5-C6-N1	5.23	114.11	111.50
73	O7	67	LEU	CA-CB-CG	5.23	127.32	115.30
36	5	880	G	O5'-P-OP2	-5.23	101.00	105.70
1	6	1672	G	N3-C4-N9	5.23	129.13	126.00
12	c0	88	PRO	N-CA-CB	5.23	109.57	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	323	A	OP1-P-O3'	5.23	116.70	105.20
1	2	458	G	C5-C6-N1	-5.22	108.89	111.50
36	1	339	C	N3-C2-O2	-5.22	118.24	121.90
36	1	421	G	O5'-P-OP1	-5.22	101.00	105.70
36	1	893	C	C6-N1-C2	-5.22	118.21	120.30
36	1	1367	G	C6-C5-N7	-5.22	127.27	130.40
36	5	399	A	N1-C6-N6	5.22	121.73	118.60
36	5	938	C	OP1-P-O3'	5.22	116.70	105.20
36	5	950	G	C5-C6-O6	-5.22	125.47	128.60
36	5	1187	C	N1-C2-O2	5.22	122.03	118.90
36	5	2607	G	C5-N7-C8	-5.22	101.69	104.30
63	n7	5	LEU	CA-CB-CG	5.22	127.31	115.30
1	2	22	A	N1-C6-N6	5.22	121.73	118.60
36	1	1510	G	C4-C5-C6	5.22	121.93	118.80
38	4	150	G	N3-C4-N9	5.22	129.13	126.00
44	L7	110	ARG	NE-CZ-NH2	-5.22	117.69	120.30
36	5	1199	C	O5'-P-OP2	-5.22	101.00	105.70
36	5	2681	U	C2-N3-C4	-5.22	123.87	127.00
36	5	3105	U	N3-C4-O4	-5.22	115.74	119.40
1	2	1437	U	N3-C4-O4	5.22	123.06	119.40
36	1	109	A	OP1-P-O3'	5.22	116.69	105.20
36	5	1489	A	N1-C6-N6	5.22	121.73	118.60
36	5	2159	U	N3-C2-O2	-5.22	118.55	122.20
36	1	1185	C	N1-C2-O2	-5.22	115.77	118.90
36	1	1186	G	OP2-P-O3'	5.22	116.68	105.20
36	1	2382	G	C5-C6-O6	5.22	131.73	128.60
36	1	2719	U	C6-N1-C1'	5.22	128.51	121.20
37	3	15	C	C6-N1-C2	5.22	122.39	120.30
1	6	66	U	P-O3'-C3'	5.22	125.96	119.70
36	5	1200	A	N3-C4-C5	-5.22	123.15	126.80
36	5	2326	A	C8-N9-C4	5.22	107.89	105.80
36	5	3000	A	C4-C5-N7	5.22	113.31	110.70
1	2	1432	U	C2-N1-C1'	-5.22	111.44	117.70
36	1	299	G	C6-C5-N7	-5.22	127.27	130.40
36	1	2393	G	C5-C6-O6	-5.22	125.47	128.60
36	5	1137	C	N1-C2-O2	5.22	122.03	118.90
42	15	22	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	2	970	A	C5-N7-C8	-5.22	101.29	103.90
36	1	2355	G	C5-C6-O6	-5.22	125.47	128.60
1	6	1743	U	C5-C6-N1	-5.22	120.09	122.70
36	5	220	G	OP1-P-O3'	5.22	116.68	105.20
36	5	1107	C	OP2-P-O3'	5.22	116.68	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1512	U	N3-C4-C5	-5.22	111.47	114.60
36	1	146	U	C2-N1-C1'	-5.21	111.44	117.70
36	1	1313	G	N1-C6-O6	5.21	123.03	119.90
36	1	3178	A	C2-N3-C4	-5.21	107.99	110.60
1	6	1624	C	O5'-P-OP1	-5.21	101.01	105.70
36	5	1420	C	C6-N1-C1'	5.21	127.06	120.80
36	5	2727	A	C8-N9-C4	-5.21	103.72	105.80
36	5	2765	C	C6-N1-C2	-5.21	118.21	120.30
35	SM	134	ASP	CB-CG-OD2	5.21	122.99	118.30
36	1	2187	G	C4-C5-C6	5.21	121.93	118.80
37	7	36	C	C6-N1-C2	5.21	122.39	120.30
36	1	1049	C	O5'-P-OP2	-5.21	101.01	105.70
36	1	1097	G	P-O3'-C3'	5.21	125.95	119.70
36	1	1151	U	N3-C4-C5	-5.21	111.47	114.60
36	1	2273	G	N7-C8-N9	-5.21	110.50	113.10
36	1	2819	A	O5'-P-OP2	-5.21	101.01	105.70
36	1	2996	U	N1-C1'-C2'	5.21	120.78	114.00
36	1	3209	A	N9-C4-C5	-5.21	103.72	105.80
1	6	542	A	P-O3'-C3'	5.21	125.95	119.70
36	5	938	C	N3-C2-O2	5.21	125.55	121.90
36	5	991	G	N1-C6-O6	-5.21	116.77	119.90
36	5	3183	A	OP2-P-O3'	5.21	116.67	105.20
36	1	878	G	N3-C4-N9	-5.21	122.87	126.00
36	5	984	G	N3-C4-C5	-5.21	126.00	128.60
36	5	2710	C	N3-C2-O2	5.21	125.55	121.90
1	2	616	G	N1-C6-O6	-5.21	116.78	119.90
36	1	1404	G	N3-C2-N2	5.21	123.55	119.90
36	5	191	U	N3-C4-O4	-5.21	115.75	119.40
36	5	1187	C	N3-C2-O2	-5.21	118.25	121.90
36	5	1308	A	C8-N9-C4	5.21	107.88	105.80
36	5	1449	A	C6-C5-N7	-5.21	128.65	132.30
36	5	1604	G	C8-N9-C1'	-5.21	120.23	127.00
37	7	44	C	N1-C2-O2	-5.21	115.78	118.90
1	2	1756	A	C4-C5-N7	5.21	113.30	110.70
36	1	125	C	C2-N3-C4	-5.21	117.30	119.90
1	6	1100	G	C8-N9-C1'	-5.21	120.23	127.00
1	6	1499	G	C4-N9-C1'	5.21	133.27	126.50
1	6	1662	G	N1-C6-O6	-5.21	116.78	119.90
36	5	915	A	OP1-P-OP2	5.21	127.41	119.60
38	8	42	G	C4-N9-C1'	-5.21	119.73	126.50
1	2	1780	G	N1-C6-O6	5.21	123.02	119.90
36	5	644	G	N9-C4-C5	5.21	107.48	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	794	U	P-O3'-C3'	5.20	125.94	119.70
36	1	217	U	N1-C2-O2	-5.20	119.16	122.80
36	1	1151	U	O5'-P-OP2	5.20	116.94	110.70
36	1	1335	C	C5-C4-N4	5.20	123.84	120.20
36	1	1444	G	C4-C5-N7	5.20	112.88	110.80
36	1	2709	C	C6-N1-C2	5.20	122.38	120.30
61	N5	34	LEU	CA-CB-CG	5.20	127.27	115.30
1	6	1503	A	O4'-C1'-N9	5.20	112.36	108.20
36	5	2113	A	N7-C8-N9	-5.20	111.20	113.80
36	1	1177	G	N1-C6-O6	5.20	123.02	119.90
36	1	1364	C	OP2-P-O3'	5.20	116.64	105.20
37	7	30	G	N1-C2-N3	5.20	127.02	123.90
36	1	942	U	O5'-P-OP1	5.20	116.94	110.70
36	1	1202	A	C2-N3-C4	-5.20	108.00	110.60
36	1	1227	C	C5-C6-N1	5.20	123.60	121.00
36	5	924	G	N3-C4-C5	5.20	131.20	128.60
36	5	1420	C	N1-C2-O2	-5.20	115.78	118.90
36	5	3308	C	C2-N3-C4	-5.20	117.30	119.90
36	1	963	G	C6-N1-C2	-5.20	121.98	125.10
36	1	1211	U	N3-C4-O4	-5.20	115.76	119.40
1	6	426	G	N1-C6-O6	-5.20	116.78	119.90
36	5	88	A	C8-N9-C4	5.20	107.88	105.80
36	5	970	A	C4-C5-N7	5.20	113.30	110.70
36	5	2408	U	N1-C2-O2	-5.20	119.16	122.80
1	6	116	U	N1-C2-O2	-5.20	119.16	122.80
1	6	1361	U	C5-C6-N1	5.20	125.30	122.70
36	5	345	G	C6-C5-N7	-5.20	127.28	130.40
36	5	2976	A	OP2-P-O3'	5.20	116.63	105.20
36	1	348	A	N9-C4-C5	-5.20	103.72	105.80
36	1	922	U	C4-C5-C6	-5.20	116.58	119.70
36	1	1121	U	N1-C2-N3	5.20	118.02	114.90
36	1	1940	G	N1-C2-N2	-5.20	111.52	116.20
36	1	2699	G	C4-C5-N7	5.20	112.88	110.80
36	1	2787	G	C2-N3-C4	5.20	114.50	111.90
36	5	916	G	O5'-P-OP1	-5.20	101.02	105.70
36	5	1898	G	N1-C6-O6	5.20	123.02	119.90
36	5	2323	G	OP1-P-OP2	-5.20	111.81	119.60
36	5	2639	G	N1-C6-O6	5.20	123.02	119.90
36	5	3266	G	C5-C6-O6	5.20	131.72	128.60
1	2	321	C	OP2-P-O3'	5.19	116.63	105.20
36	1	628	A	O5'-P-OP1	5.19	116.93	110.70
36	5	703	G	O5'-P-OP1	-5.19	101.03	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1495	U	C6-N1-C1'	5.19	128.47	121.20
36	1	2121	G	C5-C6-O6	5.19	131.72	128.60
38	4	17	A	N1-C2-N3	5.19	131.90	129.30
1	6	1782	A	N7-C8-N9	5.19	116.40	113.80
36	5	61	A	N1-C2-N3	5.19	131.90	129.30
36	5	973	A	C5-C6-N6	-5.19	119.55	123.70
36	5	1198	C	O5'-P-OP1	-5.19	101.03	105.70
36	5	1795	U	C2-N1-C1'	5.19	123.93	117.70
36	5	526	C	N3-C4-C5	5.19	123.98	121.90
36	5	578	A	C5-C6-N6	-5.19	119.55	123.70
36	5	2816	G	N9-C4-C5	-5.19	103.32	105.40
1	6	622	A	O5'-P-OP1	-5.19	101.03	105.70
36	5	530	G	O4'-C1'-N9	5.19	112.35	108.20
36	1	171	G	N1-C6-O6	5.19	123.01	119.90
36	1	2407	C	C5-C6-N1	-5.19	118.41	121.00
36	1	2622	C	C6-N1-C2	-5.19	118.22	120.30
1	6	311	U	N1-C2-O2	5.19	126.43	122.80
1	6	542	A	C4-C5-C6	5.19	119.59	117.00
1	6	1124	A	N1-C6-N6	5.19	121.71	118.60
1	6	1773	C	N3-C2-O2	5.19	125.53	121.90
38	8	23	U	OP1-P-OP2	5.19	127.38	119.60
36	1	646	A	O5'-P-OP2	-5.19	101.03	105.70
36	1	2188	A	C5-C6-N6	5.19	127.85	123.70
36	1	2950	G	C8-N9-C4	-5.19	104.33	106.40
36	5	3058	U	C2-N1-C1'	5.19	123.92	117.70
37	3	87	G	N9-C4-C5	-5.18	103.33	105.40
36	5	2145	A	OP1-P-OP2	-5.18	111.82	119.60
36	5	3345	G	N3-C2-N2	-5.18	116.27	119.90
1	2	17	C	O5'-P-OP2	-5.18	101.04	105.70
36	1	1144	U	C2-N3-C4	-5.18	123.89	127.00
36	1	1297	C	O5'-P-OP1	-5.18	101.04	105.70
36	1	1578	C	C6-N1-C1'	-5.18	114.58	120.80
36	1	2653	C	C5-C6-N1	-5.18	118.41	121.00
36	1	2893	C	C2-N3-C4	-5.18	117.31	119.90
1	6	163	G	C8-N9-C1'	5.18	133.74	127.00
1	6	359	A	C4-C5-C6	-5.18	114.41	117.00
1	6	448	C	OP1-P-O3'	5.18	116.60	105.20
36	5	648	C	C2-N1-C1'	5.18	124.50	118.80
36	1	884	A	C8-N9-C4	5.18	107.87	105.80
36	1	2413	A	C4-C5-C6	-5.18	114.41	117.00
1	6	387	A	O5'-P-OP2	-5.18	101.04	105.70
1	2	1431	C	N1-C2-N3	-5.18	115.57	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1201	C	C6-N1-C2	-5.18	118.23	120.30
1	6	359	A	N1-C2-N3	-5.18	126.71	129.30
1	6	800	U	N1-C2-N3	5.18	118.01	114.90
1	6	959	U	O4'-C1'-N1	-5.18	104.06	108.20
36	5	2662	G	N3-C4-N9	5.18	129.11	126.00
1	2	103	A	P-O3'-C3'	5.18	125.91	119.70
1	2	1486	G	C8-N9-C4	-5.18	104.33	106.40
36	1	515	C	O5'-P-OP2	-5.18	101.04	105.70
36	1	1395	G	C5-C6-O6	-5.18	125.49	128.60
1	6	426	G	O5'-P-OP2	-5.18	101.04	105.70
36	5	2236	G	N1-C6-O6	5.18	123.01	119.90
36	1	932	U	C2-N3-C4	-5.18	123.89	127.00
36	1	2973	G	N1-C6-O6	5.18	123.01	119.90
1	6	1659	A	N3-C4-C5	5.18	130.42	126.80
36	5	1341	U	C6-N1-C2	-5.18	117.89	121.00
36	5	1389	G	C6-C5-N7	-5.18	127.30	130.40
36	5	2353	G	OP2-P-O3'	5.18	116.59	105.20
36	1	515	C	C5-C6-N1	5.17	123.59	121.00
36	1	1503	A	C2-N3-C4	-5.17	108.01	110.60
36	1	2728	G	C2-N3-C4	5.17	114.49	111.90
36	1	2956	A	OP1-P-OP2	-5.17	111.84	119.60
36	5	969	C	C5-C6-N1	-5.17	118.41	121.00
36	1	1305	U	C5-C6-N1	5.17	125.29	122.70
36	1	2304	C	C6-N1-C2	-5.17	118.23	120.30
1	6	941	A	N9-C4-C5	5.17	107.87	105.80
36	5	2732	G	N1-C6-O6	-5.17	116.80	119.90
36	1	100	A	C2-N3-C4	-5.17	108.02	110.60
1	6	1227	A	P-O3'-C3'	5.17	125.90	119.70
36	5	1476	G	OP2-P-O3'	5.17	116.57	105.20
36	5	2821	C	C6-N1-C1'	5.17	127.00	120.80
36	5	2996	U	O5'-P-OP1	5.17	116.90	110.70
1	2	1600	A	P-O3'-C3'	5.17	125.90	119.70
36	1	2799	A	C6-N1-C2	-5.17	115.50	118.60
36	1	2993	G	N9-C4-C5	-5.17	103.33	105.40
1	6	1666	U	N1-C2-N3	5.17	118.00	114.90
36	5	1589	A	C5-C6-N1	5.17	120.28	117.70
36	5	1937	U	C5-C6-N1	-5.17	120.12	122.70
36	5	2187	G	C6-C5-N7	-5.17	127.30	130.40
36	5	3242	G	C2-N3-C4	-5.17	109.32	111.90
36	1	1329	U	N1-C2-N3	5.17	118.00	114.90
38	4	24	G	C4-C5-N7	5.17	112.87	110.80
36	5	871	U	N3-C4-O4	-5.17	115.78	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1909	A	O5'-P-OP2	-5.17	101.05	105.70
36	5	2775	U	C5-C6-N1	-5.17	120.12	122.70
1	2	970	A	C6-C5-N7	-5.17	128.69	132.30
36	5	82	C	C4-C5-C6	5.17	119.98	117.40
1	2	15	U	C6-N1-C2	-5.16	117.90	121.00
36	1	1113	G	C5-C6-N1	-5.16	108.92	111.50
36	1	3207	U	N1-C2-O2	-5.16	119.19	122.80
36	1	3246	G	C2-N3-C4	-5.16	109.32	111.90
1	6	804	A	N9-C4-C5	-5.16	103.73	105.80
1	6	1537	C	N1-C2-O2	-5.16	115.80	118.90
36	5	964	G	C8-N9-C4	-5.16	104.33	106.40
36	1	2847	A	C4-C5-N7	5.16	113.28	110.70
49	M3	67	ARG	NE-CZ-NH1	-5.16	117.72	120.30
36	1	1556	C	OP1-P-O3'	5.16	116.55	105.20
36	1	1858	A	C8-N9-C1'	-5.16	118.41	127.70
36	1	2905	U	N1-C2-O2	-5.16	119.19	122.80
36	1	2939	G	C4-C5-N7	-5.16	108.74	110.80
37	3	98	C	N3-C2-O2	5.16	125.51	121.90
36	5	420	G	N3-C4-C5	-5.16	126.02	128.60
36	5	834	U	C6-N1-C2	5.16	124.10	121.00
36	5	1113	G	N1-C6-O6	5.16	123.00	119.90
36	5	1528	G	C5-C6-O6	-5.16	125.50	128.60
36	5	1547	G	N1-C6-O6	5.16	123.00	119.90
36	5	3006	A	N9-C4-C5	5.16	107.86	105.80
1	2	612	U	C2-N3-C4	-5.16	123.91	127.00
1	2	1595	U	C4-C5-C6	5.16	122.80	119.70
36	5	622	A	N1-C6-N6	5.16	121.69	118.60
36	5	947	G	N3-C4-C5	-5.16	126.02	128.60
36	5	1844	C	N1-C2-N3	5.16	122.81	119.20
36	5	1856	C	C6-N1-C2	-5.16	118.24	120.30
36	5	2214	A	O5'-P-OP2	-5.16	101.06	105.70
38	8	80	A	N3-C4-C5	-5.16	123.19	126.80
36	1	1929	G	C8-N9-C4	5.16	108.46	106.40
36	5	400	G	N3-C4-N9	-5.16	122.91	126.00
36	5	3372	A	N1-C6-N6	-5.16	115.51	118.60
1	2	694	U	C5-C6-N1	5.16	125.28	122.70
36	1	364	G	N3-C4-C5	5.16	131.18	128.60
36	1	1163	A	OP1-P-OP2	5.16	127.33	119.60
36	5	649	A	N1-C6-N6	5.16	121.69	118.60
36	5	949	C	C5-C4-N4	-5.15	116.59	120.20
36	5	3052	G	N3-C4-N9	-5.15	122.91	126.00
36	1	278	U	N1-C2-N3	5.15	117.99	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	716	A	O5'-P-OP1	-5.15	101.06	105.70
36	1	2914	G	OP1-P-OP2	5.15	127.33	119.60
36	1	2923	U	O5'-P-OP1	-5.15	101.06	105.70
37	3	91	G	C2-N3-C4	-5.15	109.32	111.90
36	5	213	A	N1-C2-N3	-5.15	126.72	129.30
36	5	1116	G	C4-C5-C6	5.15	121.89	118.80
36	5	1171	G	C2-N3-C4	-5.15	109.33	111.90
36	5	2707	C	N3-C4-C5	5.15	123.96	121.90
36	1	2917	G	C2-N3-C4	5.15	114.47	111.90
1	6	1499	G	N1-C2-N2	-5.15	111.57	116.20
36	5	1110	U	C4-C5-C6	-5.15	116.61	119.70
37	7	81	U	N3-C4-O4	-5.15	115.80	119.40
1	2	307	G	C8-N9-C4	5.15	108.46	106.40
36	1	403	C	C5-C4-N4	5.15	123.80	120.20
36	1	1110	U	C4-C5-C6	-5.15	116.61	119.70
36	1	1151	U	C5-C6-N1	5.15	125.27	122.70
36	1	2873	U	N1-C2-N3	5.15	117.99	114.90
1	6	29	U	N3-C4-O4	-5.15	115.80	119.40
1	6	30	G	C8-N9-C4	-5.15	104.34	106.40
1	6	1568	C	C2-N1-C1'	5.15	124.46	118.80
36	5	152	U	C4-C5-C6	5.15	122.79	119.70
36	5	2093	A	C5-N7-C8	-5.15	101.33	103.90
36	1	2257	C	C2-N1-C1'	5.15	124.46	118.80
36	5	960	U	C6-N1-C1'	-5.15	114.00	121.20
1	2	1479	A	N1-C6-N6	5.14	121.69	118.60
36	1	937	G	OP1-P-OP2	5.14	127.32	119.60
36	1	1308	A	C5-C6-N1	-5.14	115.13	117.70
36	1	1381	A	OP1-P-O3'	5.14	116.52	105.20
36	1	1615	C	N3-C2-O2	-5.14	118.30	121.90
36	1	1822	C	C6-N1-C2	-5.14	118.24	120.30
36	1	2788	C	N3-C2-O2	5.14	125.50	121.90
36	1	2801	A	C8-N9-C1'	5.14	136.96	127.70
18	c6	113	ASP	CB-CG-OD1	5.14	122.93	118.30
36	5	1481	A	C5-N7-C8	-5.14	101.33	103.90
36	5	1609	C	N3-C4-N4	5.14	121.60	118.00
36	1	901	G	C5-C6-O6	-5.14	125.52	128.60
36	1	2212	C	OP2-P-O3'	5.14	116.52	105.20
36	1	3179	U	N1-C2-N3	5.14	117.98	114.90
1	6	1104	U	OP2-P-O3'	5.14	116.51	105.20
36	5	974	G	C5-C6-N1	5.14	114.07	111.50
36	5	2362	C	C2-N1-C1'	5.14	124.46	118.80
36	5	2600	C	C6-N1-C2	-5.14	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3133	C	O5'-P-OP1	5.14	116.87	110.70
36	1	3045	G	C2-N3-C4	5.14	114.47	111.90
36	5	802	C	N3-C4-C5	-5.14	119.84	121.90
36	5	1789	G	C4-N9-C1'	-5.14	119.82	126.50
1	2	213	A	C8-N9-C4	5.14	107.86	105.80
36	1	908	G	N1-C2-N2	5.14	120.83	116.20
36	1	2847	A	C5-C6-N6	-5.14	119.59	123.70
57	N1	78	LYS	CD-CE-NZ	5.14	123.52	111.70
1	6	1269	U	C6-N1-C2	-5.14	117.92	121.00
36	5	56	G	C5-C6-N1	5.14	114.07	111.50
36	5	710	A	C5-C6-N1	5.14	120.27	117.70
36	5	2815	G	C4-C5-N7	-5.14	108.74	110.80
1	6	1619	C	C6-N1-C2	-5.14	118.25	120.30
1	6	1774	G	O5'-P-OP2	5.14	116.87	110.70
36	5	346	C	C2-N1-C1'	5.14	124.45	118.80
1	2	124	A	O5'-P-OP2	-5.14	101.08	105.70
36	1	357	A	C5-C6-N6	-5.14	119.59	123.70
36	1	676	G	C6-C5-N7	-5.14	127.32	130.40
36	1	948	C	C2-N3-C4	-5.14	117.33	119.90
36	1	2888	U	C5-C4-O4	-5.14	122.82	125.90
50	M4	135	LEU	CA-CB-CG	5.14	127.11	115.30
1	6	377	G	N3-C4-N9	-5.14	122.92	126.00
1	6	1629	G	N3-C4-C5	-5.14	126.03	128.60
36	5	705	A	C8-N9-C4	5.14	107.86	105.80
36	5	2426	U	N1-C2-O2	5.14	126.40	122.80
36	5	3195	U	C6-N1-C1'	-5.14	114.01	121.20
1	2	590	C	N3-C2-O2	-5.13	118.31	121.90
1	6	1396	U	C6-N1-C2	-5.13	117.92	121.00
36	5	2246	G	C2-N3-C4	5.13	114.47	111.90
36	5	2362	C	C6-N1-C2	-5.13	118.25	120.30
36	1	908	G	N3-C2-N2	-5.13	116.31	119.90
36	1	930	U	C6-N1-C2	5.13	124.08	121.00
36	1	950	G	C5-N7-C8	-5.13	101.73	104.30
36	1	1315	U	C5-C6-N1	-5.13	120.13	122.70
36	1	2888	U	N1-C2-O2	-5.13	119.21	122.80
1	6	1600	A	P-O3'-C3'	5.13	125.86	119.70
1	6	1700	C	C6-N1-C1'	-5.13	114.64	120.80
36	5	1200	A	N3-C4-N9	5.13	131.51	127.40
36	5	2606	G	C8-N9-C4	-5.13	104.35	106.40
36	1	1325	U	C5-C4-O4	5.13	128.98	125.90
36	1	2351	U	C6-N1-C2	-5.13	117.92	121.00
36	1	2633	U	C4-C5-C6	5.13	122.78	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2805	G	N1-C2-N2	-5.13	111.58	116.20
36	1	2986	U	N1-C2-N3	5.13	117.98	114.90
57	N1	128	LEU	CA-CB-CG	5.13	127.10	115.30
36	5	1004	U	N1-C2-O2	5.13	126.39	122.80
36	5	1194	G	C6-N1-C2	-5.13	122.02	125.10
36	5	1306	G	C4-C5-N7	5.13	112.85	110.80
36	5	3041	U	N3-C2-O2	5.13	125.79	122.20
37	7	80	G	C6-C5-N7	-5.13	127.32	130.40
37	7	94	C	N3-C4-C5	5.13	123.95	121.90
36	1	386	A	C6-C5-N7	-5.13	128.71	132.30
1	6	622	A	OP1-P-O3'	5.13	116.49	105.20
36	1	45	A	C8-N9-C4	5.13	107.85	105.80
36	1	859	G	N1-C6-O6	5.13	122.98	119.90
36	1	1129	A	C8-N9-C4	5.13	107.85	105.80
36	1	1133	A	C4-C5-N7	5.13	113.26	110.70
36	1	3306	U	N1-C2-O2	5.13	126.39	122.80
41	L4	190	GLY	N-CA-C	5.13	125.92	113.10
1	6	187	G	P-O3'-C3'	5.13	125.86	119.70
1	6	377	G	C4-C5-C6	-5.13	115.72	118.80
1	6	1651	A	N1-C6-N6	5.13	121.68	118.60
36	5	50	U	OP1-P-O3'	5.13	116.48	105.20
36	5	1910	A	OP2-P-O3'	5.13	116.48	105.20
1	2	465	G	O5'-P-OP1	-5.13	101.09	105.70
1	2	1274	C	N3-C4-N4	-5.13	114.41	118.00
36	1	935	U	OP2-P-O3'	5.13	116.48	105.20
36	1	1364	C	N3-C4-C5	5.13	123.95	121.90
36	1	2383	C	C5-C4-N4	-5.13	116.61	120.20
36	5	500	C	OP1-P-O3'	5.13	116.48	105.20
36	5	3207	U	N1-C2-O2	-5.13	119.21	122.80
36	1	645	A	C2-N3-C4	5.12	113.16	110.60
36	1	1530	U	C6-N1-C2	5.12	124.07	121.00
1	6	1552	U	N3-C2-O2	5.12	125.79	122.20
36	5	1878	G	C4-N9-C1'	5.12	133.16	126.50
38	8	5	U	C5-C4-O4	-5.12	122.83	125.90
36	1	3053	G	C5-C6-O6	5.12	131.67	128.60
1	6	351	C	C6-N1-C1'	-5.12	114.65	120.80
1	6	1135	U	O5'-P-OP2	-5.12	101.09	105.70
36	5	213	A	OP2-P-O3'	5.12	116.47	105.20
1	6	68	A	C6-C5-N7	-5.12	128.72	132.30
1	6	1327	C	OP2-P-O3'	5.12	116.47	105.20
36	5	2858	U	C2-N1-C1'	5.12	123.84	117.70
1	2	1756	A	C6-C5-N7	-5.12	128.72	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1380	G	C4-C5-N7	5.12	112.85	110.80
36	1	2685	C	N1-C2-O2	-5.12	115.83	118.90
36	5	872	U	C2-N3-C4	-5.12	123.93	127.00
36	5	2808	A	N1-C6-N6	5.12	121.67	118.60
1	2	251	A	O5'-P-OP1	-5.12	101.09	105.70
36	1	907	G	N3-C4-N9	5.12	129.07	126.00
36	1	1154	A	O4'-C1'-N9	5.12	112.29	108.20
36	1	1385	C	C5-C6-N1	-5.12	118.44	121.00
36	1	2374	C	C4-C5-C6	5.12	119.96	117.40
36	5	1371	G	N1-C6-O6	-5.12	116.83	119.90
36	5	2817	A	OP2-P-O3'	5.12	116.46	105.20
36	5	2829	U	O5'-P-OP1	5.12	116.84	110.70
39	12	169	ILE	CG1-CB-CG2	-5.12	100.14	111.40
36	1	711	A	C8-N9-C4	5.12	107.85	105.80
36	1	1859	A	O5'-P-OP2	-5.12	101.10	105.70
36	1	2606	G	C4-N9-C1'	5.12	133.15	126.50
36	5	804	C	N3-C4-C5	-5.12	119.85	121.90
36	5	2379	U	C2-N3-C4	-5.12	123.93	127.00
36	5	2726	C	C4-C5-C6	5.12	119.96	117.40
36	1	1111	U	C5-C4-O4	-5.11	122.83	125.90
36	1	1154	A	C6-C5-N7	-5.11	128.72	132.30
36	1	1269	U	C2-N1-C1'	5.11	123.84	117.70
36	1	1392	G	C5-C6-O6	-5.11	125.53	128.60
1	6	976	G	C5-C6-N1	-5.11	108.94	111.50
36	5	749	C	C6-N1-C2	-5.11	118.25	120.30
36	5	1116	G	N7-C8-N9	5.11	115.66	113.10
36	5	1788	C	O5'-P-OP2	-5.11	101.10	105.70
36	5	2199	G	N1-C6-O6	5.11	122.97	119.90
36	5	2665	U	O5'-P-OP2	-5.11	101.10	105.70
36	1	627	U	C6-N1-C2	5.11	124.07	121.00
1	6	408	C	C6-N1-C2	-5.11	118.25	120.30
36	1	3214	U	C5-C4-O4	5.11	128.97	125.90
36	5	40	A	C4-C5-N7	5.11	113.26	110.70
36	5	649	A	C4-C5-N7	5.11	113.25	110.70
36	5	1389	G	C4-C5-N7	5.11	112.84	110.80
36	5	2910	A	OP2-P-O3'	5.11	116.44	105.20
37	7	86	U	OP1-P-O3'	5.11	116.44	105.20
36	1	1949	G	O5'-P-OP1	-5.11	101.10	105.70
1	6	119	A	N1-C2-N3	5.11	131.85	129.30
36	5	694	C	C2-N1-C1'	5.11	124.42	118.80
1	2	1258	U	C2-N1-C1'	5.11	123.83	117.70
36	1	1420	C	C2-N1-C1'	-5.11	113.18	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2920	U	N3-C4-C5	5.11	117.67	114.60
1	6	1227	A	OP2-P-O3'	5.11	116.44	105.20
1	6	1535	U	N1-C2-O2	5.11	126.38	122.80
36	5	367	A	N7-C8-N9	-5.11	111.25	113.80
36	5	974	G	C2-N3-C4	5.11	114.45	111.90
36	1	1329	U	O4'-C1'-N1	5.11	112.28	108.20
36	1	2257	C	O4'-C1'-N1	5.11	112.28	108.20
36	1	2297	U	P-O3'-C3'	5.11	125.83	119.70
38	4	58	G	N3-C4-N9	5.11	129.06	126.00
1	6	418	G	N7-C8-N9	5.11	115.65	113.10
36	5	3174	A	C5-N7-C8	-5.11	101.35	103.90
36	1	1336	U	O5'-P-OP1	5.10	116.82	110.70
1	6	1137	A	N7-C8-N9	-5.10	111.25	113.80
36	1	64	G	N3-C4-N9	-5.10	122.94	126.00
36	1	955	U	C5-C6-N1	-5.10	120.15	122.70
36	1	3041	U	N1-C2-N3	5.10	117.96	114.90
36	5	2121	G	O5'-P-OP2	-5.10	101.11	105.70
36	5	2831	G	C5-C6-O6	-5.10	125.54	128.60
36	1	118	U	C5-C6-N1	-5.10	120.15	122.70
36	1	3318	G	C4-N9-C1'	5.10	133.13	126.50
1	6	136	C	C6-N1-C1'	-5.10	114.68	120.80
36	5	1292	C	O5'-P-OP1	-5.10	101.11	105.70
36	5	2392	C	C2-N1-C1'	-5.10	113.19	118.80
36	5	2700	G	N9-C4-C5	-5.10	103.36	105.40
36	5	2984	C	C2-N3-C4	-5.10	117.35	119.90
1	2	1274	C	C6-N1-C2	-5.10	118.26	120.30
36	1	984	G	C6-C5-N7	-5.10	127.34	130.40
36	1	1170	A	C8-N9-C4	5.10	107.84	105.80
1	6	1659	A	N3-C4-N9	-5.10	123.32	127.40
36	5	2208	A	O4'-C1'-N9	5.10	112.28	108.20
36	5	2326	A	OP2-P-O3'	5.10	116.42	105.20
36	5	2692	A	N1-C6-N6	-5.10	115.54	118.60
1	2	307	G	C8-N9-C1'	-5.10	120.37	127.00
36	1	654	C	C5-C6-N1	-5.10	118.45	121.00
36	1	2508	U	C5-C6-N1	5.10	125.25	122.70
36	1	2800	G	C6-N1-C2	-5.10	122.04	125.10
1	6	297	U	N3-C4-O4	5.10	122.97	119.40
1	6	650	U	N1-C2-O2	5.10	126.37	122.80
1	6	1539	G	O4'-C1'-N9	-5.10	104.12	108.20
36	5	1578	C	C6-N1-C2	-5.10	118.26	120.30
36	5	353	G	C8-N9-C4	5.10	108.44	106.40
1	2	1751	C	C6-N1-C2	-5.09	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C8	3	LEU	CA-CB-CG	5.09	127.02	115.30
36	1	53	G	C8-N9-C4	5.09	108.44	106.40
36	1	312	C	C5-C4-N4	-5.09	116.63	120.20
36	1	1121	U	N1-C2-O2	-5.09	119.23	122.80
36	1	3302	U	C6-N1-C2	5.09	124.06	121.00
33	e1	100	LEU	CA-CB-CG	5.09	127.02	115.30
36	5	826	G	N3-C2-N2	-5.09	116.33	119.90
36	5	2828	G	N1-C2-N3	5.09	126.96	123.90
38	8	34	U	N1-C2-N3	5.09	117.96	114.90
1	6	1537	C	C5-C4-N4	5.09	123.77	120.20
36	5	2234	G	N9-C4-C5	-5.09	103.36	105.40
1	2	256	A	C8-N9-C4	-5.09	103.76	105.80
36	1	503	C	N1-C2-O2	5.09	121.95	118.90
36	1	2203	U	N1-C2-O2	-5.09	119.24	122.80
36	1	3268	A	C6-C5-N7	-5.09	128.74	132.30
1	6	113	U	C5-C4-O4	5.09	128.96	125.90
1	6	1750	A	C8-N9-C4	5.09	107.84	105.80
36	5	128	G	C5-C6-O6	-5.09	125.55	128.60
36	5	1495	U	N3-C4-O4	5.09	122.97	119.40
36	5	1834	U	C6-N1-C1'	5.09	128.33	121.20
36	5	2893	C	C4-C5-C6	5.09	119.95	117.40
36	5	3209	A	C4-N9-C1'	5.09	135.47	126.30
36	1	1008	U	C2-N1-C1'	-5.09	111.59	117.70
38	4	44	A	C4-C5-N7	5.09	113.25	110.70
36	5	816	A	C5-C6-N6	5.09	127.77	123.70
36	5	948	C	C6-N1-C2	5.09	122.33	120.30
36	5	1124	U	OP1-P-OP2	5.09	127.23	119.60
36	5	3055	U	C5-C4-O4	-5.09	122.85	125.90
36	1	2146	C	N1-C2-O2	5.09	121.95	118.90
1	6	144	U	N1-C2-N3	5.09	117.95	114.90
36	5	1313	G	OP1-P-O3'	5.09	116.39	105.20
36	5	2360	C	N3-C4-N4	5.09	121.56	118.00
36	5	2397	A	C8-N9-C4	5.09	107.83	105.80
1	2	1761	U	N3-C2-O2	-5.09	118.64	122.20
36	1	3362	A	C4-C5-N7	5.09	113.24	110.70
38	4	44	A	C2-N3-C4	-5.09	108.06	110.60
71	O5	28	LEU	CA-CB-CG	5.09	127.00	115.30
36	5	984	G	N3-C4-N9	5.09	129.05	126.00
36	5	1369	A	N9-C4-C5	-5.09	103.77	105.80
36	5	2948	C	O5'-P-OP1	5.09	116.80	110.70
1	2	970	A	C5-C6-N6	-5.08	119.63	123.70
36	5	943	U	C2-N3-C4	-5.08	123.95	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1314	C	C2-N1-C1'	5.08	124.39	118.80
36	5	3121	U	C2-N1-C1'	-5.08	111.60	117.70
36	1	635	G	C6-N1-C2	-5.08	122.05	125.10
36	5	889	U	N3-C4-C5	5.08	117.65	114.60
36	5	2283	G	C5-N7-C8	-5.08	101.76	104.30
36	5	2406	C	N3-C2-O2	5.08	125.46	121.90
36	5	3028	G	N1-C2-N2	-5.08	111.63	116.20
38	8	111	A	C2-N3-C4	-5.08	108.06	110.60
1	2	553	G	N3-C2-N2	-5.08	116.34	119.90
36	1	788	C	N3-C4-N4	-5.08	114.44	118.00
36	1	1101	G	C4-C5-N7	-5.08	108.77	110.80
36	1	1151	U	C6-N1-C2	-5.08	117.95	121.00
36	1	1767	C	C6-N1-C2	-5.08	118.27	120.30
36	1	3378	C	C6-N1-C2	5.08	122.33	120.30
51	M5	83	LYS	CD-CE-NZ	5.08	123.39	111.70
1	6	1090	C	C6-N1-C2	5.08	122.33	120.30
1	6	1667	A	OP1-P-OP2	-5.08	111.98	119.60
36	5	227	G	N1-C6-O6	5.08	122.95	119.90
36	5	806	A	N9-C4-C5	-5.08	103.77	105.80
36	5	880	G	O4'-C1'-N9	5.08	112.27	108.20
36	5	2648	G	C5-C6-N1	5.08	114.04	111.50
36	5	2878	G	C5-C6-N1	5.08	114.04	111.50
1	2	1745	G	C6-C5-N7	-5.08	127.35	130.40
36	1	2298	U	N3-C4-O4	-5.08	115.84	119.40
51	M5	22	LEU	CA-CB-CG	5.08	126.98	115.30
36	5	98	G	C2-N3-C4	-5.08	109.36	111.90
36	5	2417	U	N1-C2-O2	-5.08	119.24	122.80
36	5	2870	C	O4'-C1'-N1	5.08	112.26	108.20
36	1	612	U	C2-N3-C4	-5.08	123.95	127.00
36	1	1352	A	P-O3'-C3'	5.08	125.79	119.70
36	1	1387	G	OP1-P-O3'	5.08	116.37	105.20
38	4	111	A	C6-C5-N7	-5.08	128.75	132.30
1	6	1031	U	C2-N3-C4	-5.08	123.95	127.00
36	5	412	G	N7-C8-N9	5.08	115.64	113.10
36	5	1332	A	C6-N1-C2	-5.08	115.55	118.60
36	5	2875	U	N3-C4-O4	5.08	122.95	119.40
36	5	3118	C	C2-N1-C1'	5.08	124.39	118.80
36	1	2283	G	N3-C2-N2	-5.08	116.35	119.90
36	5	2622	C	OP2-P-O3'	5.08	116.37	105.20
36	5	3215	A	C2-N3-C4	-5.08	108.06	110.60
1	2	1458	G	C5-C6-O6	-5.08	125.56	128.60
36	1	326	U	N3-C4-O4	5.08	122.95	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	417	A	N1-C6-N6	5.08	121.64	118.60
36	1	2712	U	C5-C4-O4	5.08	128.95	125.90
36	1	2827	U	C4-C5-C6	5.08	122.75	119.70
36	5	3092	C	O4'-C1'-N1	5.08	112.26	108.20
1	2	7	G	N1-C6-O6	-5.07	116.86	119.90
1	2	55	A	N1-C6-N6	-5.07	115.56	118.60
36	1	960	U	OP2-P-O3'	5.07	116.36	105.20
36	1	2942	C	C5-C4-N4	-5.07	116.65	120.20
1	6	1458	G	C8-N9-C1'	-5.07	120.40	127.00
36	5	25	U	N3-C4-C5	-5.07	111.56	114.60
36	5	337	G	N1-C6-O6	-5.07	116.86	119.90
36	5	941	G	C5-C6-N1	5.07	114.04	111.50
36	5	3317	U	N3-C2-O2	-5.07	118.65	122.20
1	2	1482	C	C6-N1-C2	5.07	122.33	120.30
1	6	337	G	C4-C5-C6	5.07	121.84	118.80
36	5	1389	G	N3-C4-N9	5.07	129.04	126.00
36	5	2698	G	N7-C8-N9	-5.07	110.56	113.10
36	5	3130	A	N1-C2-N3	5.07	131.84	129.30
36	1	821	U	C5-C6-N1	-5.07	120.17	122.70
36	1	944	C	OP2-P-O3'	5.07	116.35	105.20
36	5	3133	C	C4-C5-C6	5.07	119.93	117.40
36	1	1307	G	C2'-C3'-O3'	5.07	121.81	113.70
36	5	2180	G	N3-C4-C5	5.07	131.13	128.60
36	5	2763	U	OP1-P-O3'	5.07	116.35	105.20
36	1	1002	A	C4-C5-C6	-5.07	114.47	117.00
36	5	105	C	C6-N1-C2	5.07	122.33	120.30
36	1	206	G	C5-N7-C8	5.06	106.83	104.30
36	5	787	G	C2-N3-C4	-5.06	109.37	111.90
36	5	3225	C	N1-C2-O2	5.06	121.94	118.90
36	1	1874	A	C8-N9-C4	5.06	107.83	105.80
36	1	2323	G	O5'-P-OP2	5.06	116.78	110.70
36	1	2362	C	C5-C4-N4	5.06	123.74	120.20
36	1	2994	A	N1-C2-N3	5.06	131.83	129.30
36	5	412	G	C8-N9-C4	-5.06	104.38	106.40
36	5	1151	U	N3-C4-O4	5.06	122.94	119.40
36	5	1370	G	C6-N1-C2	-5.06	122.06	125.10
36	5	2148	U	N3-C2-O2	5.06	125.74	122.20
36	5	2295	A	C4-C5-N7	5.06	113.23	110.70
36	5	2719	U	C2-N1-C1'	-5.06	111.62	117.70
36	5	2819	A	C5-C6-N1	-5.06	115.17	117.70
78	Q2	70	LEU	CA-CB-CG	5.06	126.94	115.30
1	6	457	G	N1-C6-O6	5.06	122.94	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3068	U	C5-C6-N1	-5.06	120.17	122.70
36	1	1660	C	N3-C4-N4	5.06	121.54	118.00
36	1	1934	G	C8-N9-C4	-5.06	104.38	106.40
36	1	2675	C	C6-N1-C1'	-5.06	114.73	120.80
36	1	3375	A	N9-C4-C5	5.06	107.82	105.80
37	3	79	A	N1-C2-N3	5.06	131.83	129.30
1	6	1280	C	C6-N1-C2	-5.06	118.28	120.30
36	5	889	U	C6-N1-C2	5.06	124.03	121.00
36	5	943	U	OP1-P-OP2	5.06	127.19	119.60
36	5	2407	C	N3-C4-N4	5.06	121.54	118.00
36	5	2742	C	C6-N1-C2	5.06	122.32	120.30
36	1	1659	U	N3-C4-C5	-5.06	111.57	114.60
36	1	2295	A	C6-C5-N7	-5.06	128.76	132.30
36	1	2333	C	O5'-P-OP1	-5.06	101.15	105.70
1	6	173	A	C2-N3-C4	-5.06	108.07	110.60
36	5	1392	G	N3-C4-N9	5.06	129.03	126.00
36	1	2927	C	C2-N3-C4	-5.06	117.37	119.90
36	5	3244	A	O4'-C1'-N9	-5.06	104.16	108.20
36	1	1334	U	C6-N1-C2	-5.05	117.97	121.00
38	4	147	U	C2-N1-C1'	5.05	123.77	117.70
1	6	1031	U	C6-N1-C2	5.05	124.03	121.00
36	5	795	G	C4-C5-N7	-5.05	108.78	110.80
36	5	862	U	N1-C2-N3	5.05	117.93	114.90
36	5	912	G	N3-C4-C5	-5.05	126.07	128.60
36	5	2333	C	N3-C2-O2	5.05	125.44	121.90
23	D1	78	LEU	CA-CB-CG	5.05	126.92	115.30
36	1	919	U	N3-C4-C5	5.05	117.63	114.60
60	N4	10	GLY	N-CA-C	-5.05	100.47	113.10
36	1	99	A	C2-N3-C4	5.05	113.12	110.60
36	1	1144	U	N1-C2-O2	-5.05	119.27	122.80
36	1	2130	G	N1-C2-N2	-5.05	111.66	116.20
36	1	2658	G	C8-N9-C4	5.05	108.42	106.40
37	3	49	G	C5-N7-C8	5.05	106.82	104.30
1	6	771	A	N1-C6-N6	5.05	121.63	118.60
36	5	1195	A	N3-C4-N9	-5.05	123.36	127.40
36	5	1301	A	C5-N7-C8	-5.05	101.38	103.90
36	5	1912	U	C6-N1-C2	5.05	124.03	121.00
36	5	2358	A	C4-C5-C6	-5.05	114.47	117.00
36	1	1859	A	N1-C6-N6	5.05	121.63	118.60
36	1	2289	U	N1-C2-N3	5.05	117.93	114.90
1	2	7	G	N3-C4-C5	-5.05	126.08	128.60
36	1	97	U	OP1-P-O3'	-5.05	94.10	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2623	G	N1-C2-N2	-5.05	111.66	116.20
36	5	341	G	N1-C6-O6	5.05	122.93	119.90
36	1	587	U	N1-C2-N3	5.04	117.93	114.90
36	1	2809	C	N3-C2-O2	-5.04	118.37	121.90
36	5	3129	A	C8-N9-C4	5.04	107.82	105.80
36	5	3248	C	N3-C4-N4	5.04	121.53	118.00
38	4	47	C	C2-N3-C4	-5.04	117.38	119.90
54	M8	99	THR	N-CA-C	5.04	124.62	111.00
1	6	339	C	N3-C2-O2	5.04	125.43	121.90
1	6	558	U	N1-C2-O2	5.04	126.33	122.80
36	5	811	U	C5-C4-O4	-5.04	122.87	125.90
36	5	2357	A	C5-C6-N6	-5.04	119.67	123.70
1	2	120	U	C2-N1-C1'	5.04	123.75	117.70
36	1	353	G	N3-C2-N2	5.04	123.43	119.90
36	1	371	G	C4-C5-N7	5.04	112.82	110.80
36	1	936	A	O5'-P-OP2	-5.04	101.16	105.70
36	1	2814	G	O5'-P-OP1	-5.04	101.16	105.70
1	6	1098	U	O5'-P-OP1	-5.04	101.16	105.70
1	6	1747	G	N7-C8-N9	-5.04	110.58	113.10
36	5	1876	U	C5-C6-N1	-5.04	120.18	122.70
36	5	2167	A	O5'-P-OP1	-5.04	101.16	105.70
36	5	2278	C	N1-C2-O2	5.04	121.92	118.90
36	5	2296	A	C5-C6-N6	-5.04	119.67	123.70
36	5	2818	U	C5'-C4'-O4'	-5.04	103.05	109.10
36	1	1176	C	O5'-P-OP2	5.04	116.75	110.70
1	6	421	A	C8-N9-C4	5.04	107.82	105.80
1	2	1108	G	C8-N9-C4	-5.04	104.38	106.40
1	2	1457	C	C6-N1-C2	-5.04	118.28	120.30
36	1	44	U	C2-N1-C1'	-5.04	111.65	117.70
36	1	2883	U	C4-C5-C6	-5.04	116.68	119.70
1	6	57	G	N3-C4-N9	5.04	129.02	126.00
1	6	599	A	N9-C4-C5	5.04	107.81	105.80
1	6	1027	A	N1-C6-N6	5.04	121.62	118.60
1	6	1757	G	C8-N9-C4	5.04	108.42	106.40
36	5	799	G	O5'-P-OP1	-5.04	101.17	105.70
36	5	951	A	C2-N3-C4	-5.04	108.08	110.60
36	5	1488	G	OP1-P-O3'	5.04	116.28	105.20
36	5	1872	C	C2-N3-C4	-5.04	117.38	119.90
36	5	2610	G	C2-N3-C4	-5.04	109.38	111.90
36	5	2917	G	C6-C5-N7	-5.04	127.38	130.40
1	2	1600	A	C6-C5-N7	-5.04	128.78	132.30
36	1	818	C	OP1-P-OP2	-5.04	112.05	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	929	A	OP1-P-O3'	5.04	116.28	105.20
36	1	1438	U	N1-C2-N3	5.04	117.92	114.90
36	1	1846	C	C4-C5-C6	5.04	119.92	117.40
38	4	81	U	C2-N1-C1'	5.04	123.74	117.70
1	6	295	A	C8-N9-C4	5.04	107.81	105.80
1	6	1773	C	C2-N3-C4	5.04	122.42	119.90
36	5	607	A	N9-C4-C5	5.04	107.81	105.80
36	5	856	G	C5-C6-O6	-5.04	125.58	128.60
36	5	2887	A	C4-C5-C6	5.04	119.52	117.00
36	5	3140	G	N9-C4-C5	-5.04	103.39	105.40
36	1	1193	A	C4-C5-N7	5.03	113.22	110.70
1	6	1037	C	C6-N1-C2	5.03	122.31	120.30
36	5	859	G	N3-C4-N9	5.03	129.02	126.00
36	5	1667	A	N9-C4-C5	-5.03	103.79	105.80
36	5	2405	C	N3-C2-O2	-5.03	118.38	121.90
36	1	125	C	C5-C6-N1	-5.03	118.48	121.00
36	1	954	U	C5-C4-O4	-5.03	122.88	125.90
36	1	2705	A	C2-N3-C4	5.03	113.12	110.60
36	5	61	A	C8-N9-C4	-5.03	103.79	105.80
36	5	1075	A	N7-C8-N9	-5.03	111.28	113.80
36	5	1381	A	O5'-P-OP2	5.03	116.74	110.70
36	1	810	A	N9-C4-C5	5.03	107.81	105.80
36	1	1307	G	C8-N9-C1'	5.03	133.54	127.00
36	1	2610	G	C2-N3-C4	-5.03	109.39	111.90
38	4	39	G	O5'-P-OP2	-5.03	101.17	105.70
1	6	633	U	OP2-P-O3'	5.03	116.27	105.20
1	6	1117	U	N1-C2-O2	-5.03	119.28	122.80
36	5	908	G	C4-N9-C1'	5.03	133.04	126.50
36	5	2335	G	N7-C8-N9	-5.03	110.58	113.10
36	5	3212	C	C2-N1-C1'	-5.03	113.27	118.80
36	5	49	A	C5-C6-N6	-5.03	119.68	123.70
36	5	874	U	N1-C2-O2	-5.03	119.28	122.80
36	5	1352	A	OP1-P-O3'	5.03	116.26	105.20
36	1	125	C	N3-C4-N4	-5.03	114.48	118.00
36	1	2112	U	P-O3'-C3'	5.03	125.73	119.70
1	6	65	A	N1-C6-N6	5.03	121.62	118.60
36	5	907	G	N3-C4-N9	5.03	129.02	126.00
36	5	1208	U	N3-C2-O2	-5.03	118.68	122.20
36	5	1516	C	N1-C2-O2	5.03	121.92	118.90
54	m8	151	ARG	NE-CZ-NH1	-5.03	117.79	120.30
36	1	611	A	O5'-P-OP2	-5.03	101.18	105.70
36	1	1899	G	C4-C5-N7	5.03	112.81	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2799	A	C5-C6-N6	-5.03	119.68	123.70
38	4	53	A	N1-C6-N6	-5.03	115.58	118.60
1	6	343	C	N1-C2-O2	-5.03	115.89	118.90
36	5	635	G	C4-C5-N7	5.03	112.81	110.80
36	1	2372	A	OP1-P-O3'	5.02	116.25	105.20
41	L4	313	LEU	CA-CB-CG	5.02	126.86	115.30
36	5	382	U	O5'-P-OP2	-5.02	101.18	105.70
36	5	1200	A	P-O3'-C3'	5.02	125.73	119.70
36	5	1868	G	C8-N9-C4	5.02	108.41	106.40
38	8	108	C	N1-C2-O2	-5.02	115.89	118.90
36	1	573	C	C5-C6-N1	-5.02	118.49	121.00
36	1	577	C	N1-C2-O2	-5.02	115.89	118.90
36	1	932	U	C5-C4-O4	-5.02	122.89	125.90
36	5	339	C	N3-C4-N4	-5.02	114.48	118.00
36	5	1049	C	N3-C4-C5	5.02	123.91	121.90
36	5	2896	A	C5'-C4'-O4'	-5.02	103.07	109.10
36	5	3309	G	C4-N9-C1'	5.02	133.03	126.50
38	8	10	A	C8-N9-C4	-5.02	103.79	105.80
36	1	2950	G	C5-C6-O6	5.02	131.61	128.60
1	6	474	A	C8-N9-C4	5.02	107.81	105.80
36	5	1496	C	N3-C4-C5	5.02	123.91	121.90
36	5	2810	C	C4-C5-C6	5.02	119.91	117.40
36	1	1329	U	N3-C2-O2	-5.02	118.69	122.20
36	1	2762	A	N1-C6-N6	-5.02	115.59	118.60
38	4	142	C	C6-N1-C2	-5.02	118.29	120.30
1	6	557	G	N3-C4-C5	-5.02	126.09	128.60
25	d3	33	LEU	CB-CG-CD1	-5.02	102.47	111.00
36	5	2163	C	N1-C2-N3	5.02	122.71	119.20
36	5	3053	G	N1-C2-N3	-5.02	120.89	123.90
36	5	3092	C	C2-N3-C4	-5.02	117.39	119.90
38	8	92	A	N1-C6-N6	5.02	121.61	118.60
36	1	650	C	N1-C2-O2	-5.02	115.89	118.90
36	1	1162	U	C5-C6-N1	5.02	125.21	122.70
36	1	2808	A	C5-C6-N6	-5.02	119.69	123.70
36	5	1077	U	N3-C2-O2	5.02	125.71	122.20
36	5	2105	G	N1-C6-O6	5.02	122.91	119.90
36	5	2292	U	N3-C2-O2	-5.02	118.69	122.20
36	5	2945	G	OP1-P-OP2	-5.02	112.07	119.60
36	1	1131	G	N9-C4-C5	-5.02	103.39	105.40
36	5	1140	G	OP1-P-O3'	5.02	116.23	105.20
1	2	1495	C	O5'-P-OP1	-5.01	101.19	105.70
36	1	619	A	N9-C4-C5	-5.01	103.79	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	58	G	O5'-P-OP2	-5.01	101.19	105.70
1	6	1743	U	C4-C5-C6	5.01	122.71	119.70
36	5	530	G	C8-N9-C1'	5.01	133.52	127.00
36	1	1384	U	OP2-P-O3'	5.01	116.23	105.20
36	1	1617	G	C8-N9-C4	5.01	108.41	106.40
36	1	1851	G	C8-N9-C4	-5.01	104.39	106.40
36	1	2871	G	O5'-P-OP2	-5.01	101.19	105.70
1	6	1060	U	C6-N1-C2	-5.01	117.99	121.00
36	5	2199	G	C5-C6-O6	-5.01	125.59	128.60
36	5	3250	U	O4'-C1'-N1	5.01	112.21	108.20
63	n7	134	LEU	CA-CB-CG	5.01	126.83	115.30
1	6	53	G	N3-C4-N9	5.01	129.01	126.00
36	5	506	U	OP2-P-O3'	5.01	116.23	105.20
36	5	1398	U	OP2-P-O3'	5.01	116.22	105.20
36	5	2640	A	N1-C2-N3	5.01	131.81	129.30
47	m0	60	LEU	CA-CB-CG	5.01	126.83	115.30
36	1	339	C	N1-C2-N3	5.01	122.71	119.20
36	1	1189	C	C5-C6-N1	-5.01	118.50	121.00
36	1	1513	G	N1-C2-N3	5.01	126.91	123.90
36	1	2212	C	C5-C6-N1	-5.01	118.50	121.00
36	1	3022	G	C4-N9-C1'	-5.01	119.99	126.50
36	1	3121	U	N1-C2-O2	-5.01	119.29	122.80
37	3	95	A	C5-N7-C8	-5.01	101.40	103.90
36	5	1195	A	C2-N3-C4	-5.01	108.09	110.60
37	7	79	A	N1-C6-N6	5.01	121.61	118.60
36	1	51	A	C5-C6-N6	-5.01	119.69	123.70
36	1	221	A	N1-C2-N3	5.01	131.80	129.30
36	1	663	C	N3-C4-N4	5.01	121.51	118.00
36	1	2282	U	O5'-P-OP1	5.01	116.71	110.70
1	2	59	C	N1-C2-O2	5.01	121.90	118.90
36	1	24	G	N1-C2-N3	5.01	126.90	123.90
36	1	2878	G	OP1-P-O3'	5.01	116.22	105.20
44	L7	160	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	6	1127	G	N1-C2-N3	5.01	126.90	123.90
36	5	19	U	N3-C4-O4	5.01	122.91	119.40
36	5	146	U	N3-C4-O4	-5.01	115.90	119.40
39	12	237	LEU	CA-CB-CG	-5.01	103.78	115.30
1	2	1104	U	O5'-P-OP2	-5.00	101.19	105.70
36	1	2990	G	OP1-P-O3'	5.00	116.21	105.20
54	M8	178	ARG	NE-CZ-NH1	-5.00	117.80	120.30
25	d3	45	GLY	N-CA-C	-5.00	100.59	113.10
36	5	2158	A	C5-C6-N1	5.00	120.20	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3136	G	N1-C2-N3	5.00	126.90	123.90
37	7	90	U	C5-C4-O4	-5.00	122.90	125.90
1	2	44	U	N1-C2-O2	-5.00	119.30	122.80
36	1	18	G	OP2-P-O3'	5.00	116.21	105.20
36	1	54	C	C2-N3-C4	-5.00	117.40	119.90
36	1	410	U	N3-C4-O4	5.00	122.90	119.40
36	1	410	U	N3-C4-C5	-5.00	111.60	114.60
36	1	2751	G	C5-C6-O6	-5.00	125.60	128.60
36	5	928	C	O5'-P-OP1	5.00	116.70	110.70
36	5	1119	C	OP2-P-O3'	5.00	116.21	105.20
36	5	1309	U	C2-N1-C1'	-5.00	111.69	117.70
36	5	2375	G	O4'-C1'-N9	5.00	112.20	108.20
36	5	2395	G	C5-N7-C8	-5.00	101.80	104.30
36	5	2739	A	N1-C2-N3	5.00	131.80	129.30
36	5	2942	C	C5-C4-N4	-5.00	116.70	120.20
36	5	3130	A	C4-C5-C6	5.00	119.50	117.00
38	8	96	A	C5-C6-N6	-5.00	119.70	123.70
36	1	1402	C	N3-C4-N4	-5.00	114.50	118.00
36	1	3039	C	C6-N1-C2	-5.00	118.30	120.30
38	4	81	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	C6	113	ASP	Peptide
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
25	D3	78	LYS	Peptide
27	D5	94	LYS	Peptide
27	D5	96	SER	Peptide
33	E1	137	ASP	Peptide
39	L2	19	HIS	Peptide
39	L2	48	ILE	Peptide
41	L4	318	LEU	Peptide
43	L6	51	ARG	Peptide
48	M1	8	PRO	Peptide
49	M3	164	GLU	Peptide
50	M4	112	LEU	Peptide
52	M6	110	PRO	Peptide
52	M6	111	PRO	Peptide
53	M7	120	ASN	Peptide

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Mol	Chain	Res	Type	Group
57	N1	16	GLN	Peptide
63	N7	3	LYS	Peptide
64	N8	30	GLY	Peptide
65	N9	20	GLY	Peptide
67	O1	5	LYS	Peptide
9	S7	131	PHE	Peptide
12	c0	33	GLU	Peptide
16	c4	123	SER	Peptide
17	c5	52	LYS	Peptide
18	c6	40	GLU	Peptide
19	c7	87	GLU	Peptide
22	d0	70	THR	Peptide
26	d4	59	GLY	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
45	l8	221	ASN	Peptide
52	m6	110	PRO	Peptide
56	n0	133	ALA	Peptide
56	n0	170	THR	Peptide
64	n8	18	GLY	Peptide
64	n8	26	ARG	Peptide
64	n8	66	ALA	Peptide
2	s0	165	ARG	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide
9	s7	130	VAL	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	142 (70%)	40 (20%)	22 (11%)	0	2
2	s0	204/251 (81%)	155 (76%)	28 (14%)	21 (10%)	0	3
3	S1	212/254 (84%)	144 (68%)	35 (16%)	33 (16%)	0	0
3	s1	214/254 (84%)	174 (81%)	27 (13%)	13 (6%)	1	9
4	S2	215/253 (85%)	182 (85%)	22 (10%)	11 (5%)	2	13
4	s2	215/253 (85%)	178 (83%)	22 (10%)	15 (7%)	1	7
5	S3	221/239 (92%)	177 (80%)	25 (11%)	19 (9%)	1	4
5	s3	221/239 (92%)	179 (81%)	28 (13%)	14 (6%)	1	8
6	S4	258/260 (99%)	205 (80%)	36 (14%)	17 (7%)	1	7
6	s4	258/260 (99%)	212 (82%)	29 (11%)	17 (7%)	1	7
7	S5	204/224 (91%)	155 (76%)	33 (16%)	16 (8%)	1	5
7	s5	204/224 (91%)	160 (78%)	23 (11%)	21 (10%)	0	3
8	S6	224/236 (95%)	195 (87%)	17 (8%)	12 (5%)	2	12
8	s6	216/236 (92%)	181 (84%)	22 (10%)	13 (6%)	1	9
9	S7	182/189 (96%)	128 (70%)	28 (15%)	26 (14%)	0	1
9	s7	184/189 (97%)	148 (80%)	26 (14%)	10 (5%)	2	12
10	S8	184/200 (92%)	152 (83%)	21 (11%)	11 (6%)	1	9
10	s8	184/200 (92%)	155 (84%)	17 (9%)	12 (6%)	1	8
11	S9	183/196 (93%)	149 (81%)	24 (13%)	10 (6%)	2	11
11	s9	183/196 (93%)	152 (83%)	22 (12%)	9 (5%)	2	14
12	C0	94/105 (90%)	77 (82%)	10 (11%)	7 (7%)	1	6
12	c0	92/105 (88%)	58 (63%)	19 (21%)	15 (16%)	0	0
13	C1	153/155 (99%)	121 (79%)	23 (15%)	9 (6%)	1	10
13	c1	144/155 (93%)	122 (85%)	15 (10%)	7 (5%)	2	14
14	C2	122/142 (86%)	66 (54%)	30 (25%)	26 (21%)	0	0
14	c2	122/142 (86%)	62 (51%)	37 (30%)	23 (19%)	0	0
15	C3	148/150 (99%)	124 (84%)	19 (13%)	5 (3%)	3	21
15	c3	148/150 (99%)	116 (78%)	22 (15%)	10 (7%)	1	7
16	C4	125/136 (92%)	90 (72%)	25 (20%)	10 (8%)	1	5
16	c4	126/136 (93%)	100 (79%)	16 (13%)	10 (8%)	1	5
17	C5	122/141 (86%)	85 (70%)	26 (21%)	11 (9%)	1	4
17	c5	133/141 (94%)	93 (70%)	23 (17%)	17 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C6	139/142 (98%)	114 (82%)	19 (14%)	6 (4%)	2	16
18	c6	140/142 (99%)	120 (86%)	13 (9%)	7 (5%)	2	13
19	C7	116/136 (85%)	86 (74%)	18 (16%)	12 (10%)	0	3
19	c7	113/136 (83%)	89 (79%)	17 (15%)	7 (6%)	1	9
20	C8	143/145 (99%)	106 (74%)	25 (18%)	12 (8%)	1	5
20	c8	143/145 (99%)	116 (81%)	16 (11%)	11 (8%)	1	5
21	C9	141/143 (99%)	116 (82%)	18 (13%)	7 (5%)	2	13
21	c9	141/143 (99%)	119 (84%)	18 (13%)	4 (3%)	5	25
22	D0	105/120 (88%)	84 (80%)	16 (15%)	5 (5%)	2	14
22	d0	108/120 (90%)	82 (76%)	16 (15%)	10 (9%)	0	3
23	D1	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	1	10
23	d1	85/87 (98%)	70 (82%)	9 (11%)	6 (7%)	1	6
24	D2	127/129 (98%)	102 (80%)	19 (15%)	6 (5%)	2	14
24	d2	127/129 (98%)	114 (90%)	10 (8%)	3 (2%)	6	27
25	D3	142/144 (99%)	114 (80%)	22 (16%)	6 (4%)	3	16
25	d3	142/144 (99%)	125 (88%)	13 (9%)	4 (3%)	5	25
26	D4	132/134 (98%)	104 (79%)	17 (13%)	11 (8%)	1	5
26	d4	132/134 (98%)	111 (84%)	15 (11%)	6 (4%)	2	15
27	D5	68/107 (64%)	48 (71%)	12 (18%)	8 (12%)	0	1
27	d5	67/107 (63%)	51 (76%)	10 (15%)	6 (9%)	1	4
28	D6	95/97 (98%)	59 (62%)	18 (19%)	18 (19%)	0	0
28	d6	95/97 (98%)	74 (78%)	10 (10%)	11 (12%)	0	2
29	D7	79/81 (98%)	65 (82%)	8 (10%)	6 (8%)	1	5
29	d7	79/81 (98%)	59 (75%)	14 (18%)	6 (8%)	1	5
30	D8	61/66 (92%)	49 (80%)	6 (10%)	6 (10%)	0	3
30	d8	61/66 (92%)	42 (69%)	14 (23%)	5 (8%)	1	5
31	D9	51/55 (93%)	40 (78%)	9 (18%)	2 (4%)	3	18
31	d9	51/55 (93%)	40 (78%)	6 (12%)	5 (10%)	0	3
32	E0	58/60 (97%)	43 (74%)	12 (21%)	3 (5%)	2	12
33	E1	69/76 (91%)	36 (52%)	14 (20%)	19 (28%)	0	0
33	e1	74/76 (97%)	35 (47%)	20 (27%)	19 (26%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	SR	316/318 (99%)	242 (77%)	50 (16%)	24 (8%)	1	5
34	sR	316/318 (99%)	253 (80%)	48 (15%)	15 (5%)	2	14
35	SM	155/273 (57%)	103 (66%)	30 (19%)	22 (14%)	0	1
35	sM	98/273 (36%)	65 (66%)	18 (18%)	15 (15%)	0	0
39	L2	250/253 (99%)	224 (90%)	20 (8%)	6 (2%)	6	27
39	l2	250/253 (99%)	215 (86%)	24 (10%)	11 (4%)	2	15
40	L3	384/386 (100%)	328 (85%)	38 (10%)	18 (5%)	2	14
40	l3	384/386 (100%)	338 (88%)	35 (9%)	11 (3%)	4	24
41	L4	359/361 (99%)	299 (83%)	36 (10%)	24 (7%)	1	7
41	l4	359/361 (99%)	287 (80%)	51 (14%)	21 (6%)	1	10
42	L5	294/296 (99%)	241 (82%)	37 (13%)	16 (5%)	2	12
42	l5	292/296 (99%)	247 (85%)	37 (13%)	8 (3%)	5	25
43	L6	152/175 (87%)	128 (84%)	21 (14%)	3 (2%)	7	31
43	l6	153/175 (87%)	131 (86%)	17 (11%)	5 (3%)	4	21
44	L7	220/243 (90%)	186 (84%)	23 (10%)	11 (5%)	2	13
44	l7	221/243 (91%)	194 (88%)	23 (10%)	4 (2%)	8	34
45	L8	231/255 (91%)	190 (82%)	32 (14%)	9 (4%)	3	18
45	l8	229/255 (90%)	177 (77%)	30 (13%)	22 (10%)	0	3
46	L9	189/191 (99%)	164 (87%)	21 (11%)	4 (2%)	7	30
46	l9	189/191 (99%)	172 (91%)	14 (7%)	3 (2%)	9	37
47	M0	207/220 (94%)	172 (83%)	24 (12%)	11 (5%)	2	12
47	m0	209/220 (95%)	168 (80%)	28 (13%)	13 (6%)	1	9
48	M1	167/173 (96%)	126 (75%)	28 (17%)	13 (8%)	1	5
48	m1	167/173 (96%)	137 (82%)	16 (10%)	14 (8%)	1	5
49	M3	191/198 (96%)	161 (84%)	22 (12%)	8 (4%)	3	16
49	m3	192/198 (97%)	162 (84%)	21 (11%)	9 (5%)	2	14
50	M4	134/137 (98%)	113 (84%)	11 (8%)	10 (8%)	1	6
50	m4	135/137 (98%)	119 (88%)	13 (10%)	3 (2%)	6	29
51	M5	201/203 (99%)	182 (90%)	15 (8%)	4 (2%)	7	31
51	m5	201/203 (99%)	179 (89%)	17 (8%)	5 (2%)	5	27
52	M6	195/198 (98%)	173 (89%)	14 (7%)	8 (4%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	m6	195/198 (98%)	178 (91%)	11 (6%)	6 (3%)	4	23
53	M7	181/183 (99%)	146 (81%)	30 (17%)	5 (3%)	5	25
53	m7	153/183 (84%)	138 (90%)	11 (7%)	4 (3%)	5	26
54	M8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	4	21
54	m8	183/185 (99%)	154 (84%)	19 (10%)	10 (6%)	2	11
55	M9	186/188 (99%)	164 (88%)	18 (10%)	4 (2%)	6	29
55	m9	186/188 (99%)	162 (87%)	18 (10%)	6 (3%)	4	22
56	N0	170/172 (99%)	149 (88%)	16 (9%)	5 (3%)	4	24
56	n0	170/172 (99%)	156 (92%)	13 (8%)	1 (1%)	25	59
57	N1	157/159 (99%)	134 (85%)	16 (10%)	7 (4%)	2	15
57	n1	157/159 (99%)	143 (91%)	12 (8%)	2 (1%)	12	42
58	N2	98/120 (82%)	77 (79%)	15 (15%)	6 (6%)	1	9
58	n2	96/120 (80%)	76 (79%)	14 (15%)	6 (6%)	1	8
59	N3	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	10	39
59	n3	134/136 (98%)	125 (93%)	6 (4%)	3 (2%)	6	29
60	N4	96/155 (62%)	65 (68%)	20 (21%)	11 (12%)	0	2
60	n4	133/155 (86%)	108 (81%)	17 (13%)	8 (6%)	1	9
61	N5	119/141 (84%)	103 (87%)	15 (13%)	1 (1%)	19	54
61	n5	118/141 (84%)	99 (84%)	10 (8%)	9 (8%)	1	5
62	N6	124/126 (98%)	113 (91%)	6 (5%)	5 (4%)	3	17
62	n6	124/126 (98%)	110 (89%)	11 (9%)	3 (2%)	6	27
63	N7	133/135 (98%)	114 (86%)	12 (9%)	7 (5%)	2	12
63	n7	133/135 (98%)	109 (82%)	13 (10%)	11 (8%)	1	5
64	N8	146/148 (99%)	125 (86%)	16 (11%)	5 (3%)	3	21
64	n8	146/148 (99%)	121 (83%)	19 (13%)	6 (4%)	3	16
65	N9	56/58 (97%)	48 (86%)	7 (12%)	1 (2%)	8	34
65	n9	56/58 (97%)	41 (73%)	10 (18%)	5 (9%)	1	4
66	O0	95/104 (91%)	82 (86%)	12 (13%)	1 (1%)	14	46
66	o0	98/104 (94%)	81 (83%)	14 (14%)	3 (3%)	4	23
67	O1	107/112 (96%)	96 (90%)	5 (5%)	6 (6%)	2	11
67	o1	107/112 (96%)	88 (82%)	12 (11%)	7 (6%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	O2	125/129 (97%)	114 (91%)	10 (8%)	1 (1%)	19	54
68	o2	125/129 (97%)	101 (81%)	18 (14%)	6 (5%)	2	14
69	O3	104/106 (98%)	93 (89%)	9 (9%)	2 (2%)	8	33
69	o3	104/106 (98%)	94 (90%)	9 (9%)	1 (1%)	15	49
70	O4	110/119 (92%)	91 (83%)	16 (14%)	3 (3%)	5	25
70	o4	110/119 (92%)	92 (84%)	15 (14%)	3 (3%)	5	25
71	O5	117/119 (98%)	96 (82%)	17 (14%)	4 (3%)	3	21
71	o5	117/119 (98%)	96 (82%)	14 (12%)	7 (6%)	1	9
72	O6	97/99 (98%)	77 (79%)	12 (12%)	8 (8%)	1	5
72	o6	97/99 (98%)	77 (79%)	14 (14%)	6 (6%)	1	9
73	O7	85/87 (98%)	76 (89%)	7 (8%)	2 (2%)	6	27
73	o7	85/87 (98%)	73 (86%)	9 (11%)	3 (4%)	3	20
74	O8	75/77 (97%)	63 (84%)	10 (13%)	2 (3%)	5	25
74	o8	75/77 (97%)	62 (83%)	11 (15%)	2 (3%)	5	25
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	7	30
75	o9	48/50 (96%)	39 (81%)	7 (15%)	2 (4%)	3	16
76	Q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3	17
76	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	7	31
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	19 (83%)	3 (13%)	1 (4%)	2	16
78	Q2	103/105 (98%)	82 (80%)	15 (15%)	6 (6%)	1	10
78	q2	103/105 (98%)	92 (89%)	7 (7%)	4 (4%)	3	18
79	Q3	89/91 (98%)	73 (82%)	15 (17%)	1 (1%)	14	46
79	q3	89/91 (98%)	78 (88%)	10 (11%)	1 (1%)	14	46
80	e0	60/62 (97%)	46 (77%)	9 (15%)	5 (8%)	1	5
82	p0	139/311 (45%)	109 (78%)	20 (14%)	10 (7%)	1	6
All	All	22333/24141 (92%)	18272 (82%)	2751 (12%)	1310 (6%)	1	10

All (1310) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
2	S0	66	ALA
2	S0	158	VAL
2	S0	191	ARG
2	S0	194	PRO
3	S1	49	ASN
3	S1	51	SER
3	S1	81	PHE
3	S1	132	ASP
3	S1	181	LEU
3	S1	182	ALA
3	S1	206	PRO
3	S1	223	PHE
4	S2	107	SER
4	S2	182	PRO
5	S3	62	ASN
5	S3	64	ARG
5	S3	65	ARG
5	S3	93	ASP
5	S3	211	PRO
5	S3	220	PRO
6	S4	26	CYS
6	S4	96	ASN
6	S4	104	ASP
6	S4	223	ASN
6	S4	245	LYS
7	S5	39	GLU
7	S5	43	PHE
7	S5	81	ARG
7	S5	101	GLY
8	S6	54	GLY
8	S6	122	GLU
8	S6	173	PRO
9	S7	5	GLN
9	S7	31	SER
9	S7	32	PRO
9	S7	47	ARG
9	S7	49	ILE
9	S7	64	VAL
9	S7	85	PHE
9	S7	111	LYS
9	S7	112	ARG
9	S7	129	LEU

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Mol	Chain	Res	Type
9	S7	131	PHE
9	S7	186	PRO
10	S8	81	VAL
10	S8	82	VAL
10	S8	105	ASP
11	S9	98	ALA
11	S9	134	ILE
11	S9	164	PHE
11	S9	169	PRO
12	C0	60	SER
12	C0	81	ASN
12	C0	88	PRO
12	C0	94	GLU
13	C1	7	VAL
13	C1	132	SER
13	C1	145	ALA
14	C2	91	VAL
14	C2	101	ALA
14	C2	126	TRP
15	C3	22	ALA
16	C4	50	ALA
16	C4	124	ASP
16	C4	126	THR
17	C5	11	VAL
17	C5	39	ALA
17	C5	80	MET
17	C5	125	PRO
17	C5	126	VAL
18	C6	116	LEU
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	118	PRO
19	C7	124	VAL
20	C8	14	ILE
20	C8	25	ASN
20	C8	60	GLU
20	C8	61	LEU
20	C8	82	PRO
20	C8	91	ASP
20	C8	92	ILE
21	C9	31	PRO

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Mol	Chain	Res	Type
21	C9	53	TRP
23	D1	4	ASP
23	D1	11	LEU
24	D2	6	VAL
24	D2	83	ILE
25	D3	11	SER
25	D3	53	VAL
25	D3	54	LEU
27	D5	43	ASP
27	D5	86	GLU
27	D5	97	LYS
28	D6	18	VAL
28	D6	36	ILE
28	D6	45	VAL
28	D6	47	ALA
28	D6	65	PRO
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
29	D7	38	PRO
29	D7	62	ILE
31	D9	25	SER
32	E0	47	VAL
33	E1	85	TYR
33	E1	103	LEU
33	E1	144	CYS
34	SR	22	SER
34	SR	72	THR
34	SR	161	LYS
34	SR	188	ILE
34	SR	201	THR
34	SR	231	MET
35	SM	52	PRO
35	SM	83	LYS
35	SM	89	ARG
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
35	SM	173	GLU
39	L2	20	THR
39	L2	130	SER
39	L2	144	ASN

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Mol	Chain	Res	Type
39	L2	246	LEU
40	L3	3	HIS
40	L3	140	ASP
40	L3	173	GLN
40	L3	347	SER
40	L3	386	ASP
41	L4	4	PRO
41	L4	15	ALA
41	L4	130	ALA
41	L4	131	VAL
41	L4	270	SER
41	L4	311	HIS
41	L4	338	LYS
42	L5	7	ALA
42	L5	58	LYS
42	L5	233	ALA
42	L5	234	ASP
42	L5	258	LYS
42	L5	259	LYS
43	L6	6	ALA
43	L6	98	VAL
44	L7	26	VAL
44	L7	91	GLY
44	L7	211	SER
45	L8	25	PRO
45	L8	36	ILE
46	L9	190	ASP
47	M0	219	ALA
47	M0	220	GLN
48	M1	9	MET
48	M1	11	ASP
48	M1	151	SER
48	M1	165	GLN
49	M3	47	ALA
49	M3	129	ASN
50	M4	8	LYS
50	M4	9	ALA
50	M4	135	LEU
50	M4	136	ALA
51	M5	74	PRO
51	M5	184	LYS
52	M6	110	PRO

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Mol	Chain	Res	Type
52	M6	111	PRO
52	M6	128	ARG
53	M7	157	VAL
54	M8	99	THR
55	M9	53	LYS
57	N1	124	VAL
58	N2	31	ALA
58	N2	52	ASN
58	N2	59	ASP
58	N2	60	GLY
60	N4	4	GLU
60	N4	76	VAL
60	N4	81	PRO
60	N4	97	LYS
62	N6	126	LEU
63	N7	3	LYS
63	N7	33	SER
64	N8	76	ASP
67	O1	6	ASP
70	O4	74	ARG
71	O5	118	ILE
72	O6	33	ALA
74	O8	33	LYS
76	Q0	78	ILE
78	Q2	30	ALA
78	Q2	100	LYS
2	s0	4	PRO
2	s0	29	VAL
2	s0	164	ASN
2	s0	186	GLY
2	s0	206	ASP
3	s1	206	PRO
4	s2	92	ALA
5	s3	179	GLN
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	12	LEU
6	s4	95	THR
6	s4	104	ASP
6	s4	118	GLU

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Mol	Chain	Res	Type
6	s4	163	ASP
6	s4	195	ILE
6	s4	196	VAL
7	s5	28	PRO
7	s5	36	ALA
7	s5	55	ASP
7	s5	184	PHE
8	s6	25	ARG
8	s6	70	PRO
8	s6	122	GLU
8	s6	153	VAL
8	s6	154	ARG
8	s6	156	PHE
8	s6	173	PRO
8	s6	174	LYS
9	s7	13	PRO
9	s7	64	VAL
9	s7	131	PHE
9	s7	185	ILE
10	s8	36	THR
10	s8	62	THR
10	s8	101	ILE
10	s8	149	SER
11	s9	134	ILE
11	s9	150	LEU
12	c0	2	LEU
12	c0	32	HIS
12	c0	82	LEU
12	c0	83	PRO
12	c0	88	PRO
12	c0	97	PRO
13	c1	144	ALA
14	c2	22	VAL
14	c2	131	ASP
15	c3	19	SER
15	c3	29	SER
15	c3	66	ILE
15	c3	87	ASP
15	c3	137	PRO
15	c3	139	TRP
15	c3	140	LYS
16	c4	96	PRO

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Mol	Chain	Res	Type
16	c4	124	ASP
16	c4	132	ARG
17	c5	50	THR
17	c5	51	SER
17	c5	52	LYS
17	c5	117	GLY
17	c5	125	PRO
17	c5	126	VAL
17	c5	127	ARG
18	c6	42	GLU
18	c6	115	THR
18	c6	116	LEU
19	c7	63	LYS
19	c7	88	VAL
19	c7	99	VAL
20	c8	18	LEU
20	c8	91	ASP
20	c8	145	ARG
21	c9	29	GLU
22	d0	15	GLN
22	d0	51	VAL
22	d0	118	VAL
23	d1	4	ASP
24	d2	68	ARG
26	d4	33	ALA
26	d4	78	SER
27	d5	85	LYS
27	d5	104	ALA
28	d6	61	GLU
29	d7	3	LEU
29	d7	57	GLU
29	d7	59	CYS
29	d7	62	ILE
30	d8	57	MET
31	d9	6	VAL
31	d9	7	TRP
31	d9	16	LYS
80	e0	45	VAL
80	e0	51	ASN
33	e1	83	LYS
33	e1	84	VAL
33	e1	87	THR

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Mol	Chain	Res	Type
33	e1	92	LYS
33	e1	98	VAL
33	e1	103	LEU
33	e1	106	TYR
34	sR	4	ASN
34	sR	163	ASP
34	sR	165	ASP
34	sR	250	TYR
34	sR	306	THR
35	sM	172	VAL
39	l2	24	GLN
39	l2	194	ASN
39	l2	213	GLY
40	l3	129	ALA
40	l3	140	ASP
40	l3	142	ALA
40	l3	187	SER
40	l3	347	SER
40	l3	386	ASP
41	l4	14	GLU
41	l4	56	ALA
41	l4	90	PHE
41	l4	142	VAL
41	l4	302	ALA
41	l4	342	LYS
42	l5	5	LYS
42	l5	258	LYS
42	l5	260	PHE
42	l5	269	SER
43	l6	81	ALA
43	l6	98	VAL
45	l8	25	PRO
45	l8	26	LEU
45	l8	118	GLU
45	l8	121	SER
45	l8	122	LYS
45	l8	203	VAL
45	l8	222	PHE
46	l9	144	ILE
47	m0	3	ARG
47	m0	220	GLN
48	m1	8	PRO

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Mol	Chain	Res	Type
48	m1	9	MET
48	m1	10	ARG
48	m1	28	ASP
48	m1	95	ASN
48	m1	108	GLU
48	m1	173	ASP
49	m3	47	ALA
49	m3	76	THR
49	m3	93	ILE
49	m3	134	GLU
50	m4	136	ALA
51	m5	183	THR
52	m6	110	PRO
52	m6	111	PRO
54	m8	99	THR
55	m9	112	ALA
55	m9	128	LYS
55	m9	155	LEU
57	n1	122	GLN
60	n4	26	SER
60	n4	63	ILE
60	n4	76	VAL
61	n5	24	LEU
61	n5	40	LEU
61	n5	44	PRO
62	n6	125	LYS
63	n7	5	LEU
63	n7	125	GLY
64	n8	28	HIS
65	n9	21	ILE
65	n9	23	LYS
65	n9	39	PHE
67	o1	7	VAL
67	o1	45	GLY
67	o1	91	SER
68	o2	4	LEU
68	o2	27	ARG
68	o2	89	THR
70	o4	79	SER
71	o5	82	ALA
71	o5	119	LYS
72	o6	33	ALA

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Mol	Chain	Res	Type
72	o6	98	ARG
73	o7	84	SER
73	o7	85	LYS
74	o8	19	ASP
78	q2	17	CYS
78	q2	77	CYS
82	p0	93	LEU
82	p0	198	PRO
2	S0	5	ALA
2	S0	49	ASN
2	S0	94	GLY
2	S0	139	VAL
2	S0	185	ARG
2	S0	188	LEU
2	S0	190	ASP
2	S0	196	SER
3	S1	58	SER
3	S1	63	GLY
3	S1	64	ARG
3	S1	82	ARG
3	S1	93	GLY
3	S1	131	ASP
3	S1	147	ALA
3	S1	148	ASN
3	S1	209	ASN
4	S2	91	ARG
4	S2	134	LEU
4	S2	148	LEU
4	S2	207	LEU
4	S2	236	PRO
5	S3	38	GLU
5	S3	40	ARG
5	S3	216	PRO
6	S4	12	LEU
6	S4	86	PHE
6	S4	142	HIS
6	S4	164	LEU
6	S4	242	LYS
7	S5	26	ALA
7	S5	58	LEU
7	S5	63	GLN
7	S5	152	GLY

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Mol	Chain	Res	Type
7	S5	156	ARG
8	S6	70	PRO
8	S6	152	ASP
8	S6	165	GLY
9	S7	159	VAL
10	S8	106	ALA
10	S8	149	SER
11	S9	100	LYS
11	S9	117	GLY
11	S9	163	PRO
11	S9	170	GLY
12	C0	54	TYR
13	C1	3	THR
13	C1	4	GLU
13	C1	55	ASP
13	C1	72	THR
14	C2	21	GLU
14	C2	42	ALA
14	C2	83	GLU
14	C2	93	ASP
14	C2	115	VAL
14	C2	127	GLY
14	C2	130	THR
15	C3	68	GLY
16	C4	42	VAL
16	C4	125	SER
17	C5	54	ALA
18	C6	114	ARG
18	C6	138	PHE
19	C7	111	LYS
19	C7	113	LEU
19	C7	115	LEU
20	C8	83	ALA
20	C8	125	ILE
20	C8	144	ARG
21	C9	130	ARG
22	D0	49	ASN
24	D2	66	ASN
26	D4	4	ALA
26	D4	11	LYS
27	D5	39	ALA
27	D5	44	GLN

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Mol	Chain	Res	Type
28	D6	46	GLU
28	D6	63	ALA
28	D6	86	VAL
29	D7	51	GLN
29	D7	63	LEU
30	D8	14	LYS
30	D8	36	THR
33	E1	84	VAL
33	E1	98	VAL
33	E1	102	VAL
33	E1	111	GLU
33	E1	127	GLY
33	E1	128	ALA
34	SR	189	GLU
34	SR	203	THR
34	SR	230	ALA
35	SM	64	LYS
35	SM	72	ARG
35	SM	87	THR
35	SM	153	ASP
35	SM	165	LYS
39	L2	47	GLN
40	L3	4	ARG
40	L3	5	LYS
40	L3	185	GLY
40	L3	188	ILE
40	L3	351	LEU
41	L4	190	GLY
41	L4	220	ARG
41	L4	232	SER
41	L4	268	ALA
41	L4	317	PRO
41	L4	319	LYS
41	L4	320	ASN
42	L5	178	ASN
42	L5	188	GLU
44	L7	24	GLU
45	L8	37	GLY
45	L8	39	ALA
45	L8	156	ASP
47	M0	7	ARG
47	M0	117	GLY

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Mol	Chain	Res	Type
47	M0	189	GLU
47	M0	207	GLU
48	M1	8	PRO
48	M1	94	ARG
48	M1	114	ILE
48	M1	140	ARG
48	M1	167	TYR
50	M4	28	SER
50	M4	113	THR
51	M5	75	VAL
52	M6	127	LEU
52	M6	196	ALA
53	M7	164	LYS
54	M8	112	ALA
55	M9	133	LYS
56	N0	2	ALA
56	N0	155	ARG
57	N1	16	GLN
57	N1	122	GLN
57	N1	159	PHE
58	N2	11	ILE
58	N2	107	PHE
60	N4	64	THR
60	N4	96	LEU
62	N6	53	ASP
62	N6	84	LYS
63	N7	52	LYS
63	N7	102	GLU
63	N7	125	GLY
64	N8	66	ALA
67	O1	83	GLU
70	O4	3	GLN
70	O4	77	GLY
71	O5	97	ALA
72	O6	3	VAL
72	O6	34	SER
72	O6	98	ARG
78	Q2	8	ARG
79	Q3	58	SER
2	s0	10	THR
2	s0	14	ALA
2	s0	44	GLY

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Mol	Chain	Res	Type
2	s0	49	ASN
2	s0	95	ALA
2	s0	189	VAL
2	s0	196	SER
3	s1	93	GLY
3	s1	209	ASN
3	s1	223	PHE
4	s2	93	GLY
4	s2	121	VAL
4	s2	163	GLY
5	s3	61	GLU
5	s3	195	SER
6	s4	164	LEU
6	s4	245	LYS
7	s5	35	GLN
7	s5	43	PHE
7	s5	54	LYS
7	s5	58	LEU
7	s5	100	ASN
7	s5	204	GLY
7	s5	206	SER
8	s6	68	LEU
9	s7	30	SER
9	s7	116	ARG
9	s7	155	ASP
10	s8	199	LYS
11	s9	118	LEU
12	c0	23	ALA
12	c0	73	VAL
12	c0	92	ILE
12	c0	94	GLU
13	c1	82	ARG
14	c2	45	LEU
14	c2	101	ALA
14	c2	119	SER
15	c3	43	LYS
16	c4	35	GLY
17	c5	11	VAL
17	c5	132	GLY
18	c6	39	VAL
20	c8	92	ILE
21	c9	33	TYR

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Mol	Chain	Res	Type
22	d0	39	SER
22	d0	52	LYS
23	d1	44	ARG
26	d4	4	ALA
26	d4	35	VAL
27	d5	87	GLY
28	d6	5	ARG
28	d6	13	LYS
28	d6	34	LYS
28	d6	62	TYR
28	d6	63	ALA
30	d8	33	LEU
30	d8	58	GLU
33	e1	102	VAL
33	e1	127	GLY
34	sR	149	ASP
34	sR	318	ALA
35	sM	42	ALA
35	sM	67	GLY
39	l2	96	LEU
39	l2	215	ASN
39	l2	249	SER
40	l3	22	ALA
41	l4	15	ALA
41	l4	146	PRO
41	l4	311	HIS
44	l7	27	ALA
44	l7	129	LEU
44	l7	178	ILE
45	l8	39	ALA
45	l8	117	ALA
45	l8	133	LYS
45	l8	223	ALA
45	l8	239	GLY
45	l8	240	ASN
47	m0	7	ARG
47	m0	45	GLU
47	m0	101	LYS
47	m0	117	GLY
47	m0	196	PHE
48	m1	94	ARG
48	m1	114	ILE

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Mol	Chain	Res	Type
49	m3	129	ASN
50	m4	135	LEU
51	m5	81	TYR
51	m5	182	ASN
51	m5	184	LYS
52	m6	183	ALA
54	m8	21	SER
55	m9	156	ASN
58	n2	49	ASN
58	n2	52	ASN
59	n3	42	SER
60	n4	77	LYS
61	n5	25	LYS
61	n5	38	LEU
61	n5	55	ASN
62	n6	126	LEU
63	n7	7	ALA
63	n7	16	GLY
63	n7	56	LYS
63	n7	134	LEU
67	o1	47	ASP
68	o2	5	PRO
68	o2	124	GLY
72	o6	64	SER
75	o9	44	TRP
76	q0	78	ILE
2	S0	30	GLN
2	S0	36	TYR
2	S0	95	ALA
2	S0	192	THR
2	S0	195	TRP
3	S1	35	PRO
3	S1	54	LEU
3	S1	59	ASP
3	S1	105	PHE
3	S1	224	ASP
4	S2	150	GLN
5	S3	139	SER
5	S3	212	LYS
5	S3	217	ILE
5	S3	218	LEU
6	S4	17	HIS

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Mol	Chain	Res	Type
6	S4	38	LEU
6	S4	195	ILE
6	S4	222	LEU
7	S5	51	VAL
7	S5	127	GLN
7	S5	154	ALA
9	S7	73	VAL
9	S7	98	ILE
9	S7	155	ASP
10	S8	59	ARG
10	S8	120	THR
10	S8	153	GLU
11	S9	150	LEU
14	C2	68	GLU
14	C2	89	ILE
14	C2	106	ILE
14	C2	108	ARG
14	C2	112	ALA
14	C2	119	SER
15	C3	12	SER
16	C4	18	ARG
17	C5	38	PRO
17	C5	51	SER
19	C7	87	GLU
20	C8	7	GLU
20	C8	8	GLN
21	C9	50	ALA
23	D1	10	GLU
23	D1	82	VAL
24	D2	57	ARG
24	D2	98	GLN
25	D3	112	LYS
25	D3	115	GLY
26	D4	5	VAL
26	D4	32	ARG
26	D4	34	ASN
28	D6	15	ARG
30	D8	16	LEU
30	D8	37	SER
32	E0	51	ASN
33	E1	87	THR
34	SR	4	ASN

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Mol	Chain	Res	Type
34	SR	51	ASP
34	SR	153	GLN
34	SR	155	ARG
34	SR	244	ALA
35	SM	97	THR
35	SM	101	ASP
35	SM	139	GLU
35	SM	174	LEU
39	L2	201	GLY
40	L3	348	ARG
41	L4	291	ASN
41	L4	292	SER
42	L5	137	ASP
42	L5	253	PHE
44	L7	32	ALA
44	L7	163	LEU
45	L8	80	TYR
46	L9	120	ASP
47	M0	145	LYS
48	M1	115	LYS
48	M1	173	ASP
49	M3	130	GLY
49	M3	136	GLU
50	M4	10	SER
51	M5	91	GLU
52	M6	195	ALA
53	M7	161	ALA
54	M8	98	LYS
57	N1	114	ALA
62	N6	52	ARG
63	N7	128	GLN
64	N8	47	LYS
66	O0	99	ASP
67	O1	5	LYS
67	O1	82	GLU
68	O2	127	ALA
72	O6	97	SER
72	O6	99	ARG
73	O7	86	ALA
74	O8	37	PRO
78	Q2	15	LYS
2	s0	8	ASP

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Mol	Chain	Res	Type
2	s0	152	PRO
2	s0	167	LYS
3	s1	22	ASP
3	s1	59	ASP
3	s1	94	LYS
3	s1	232	HIS
4	s2	91	ARG
4	s2	107	SER
5	s3	43	PRO
5	s3	90	ARG
6	s4	90	ILE
7	s5	127	GLN
9	s7	74	GLN
10	s8	100	ALA
10	s8	122	GLY
10	s8	147	ALA
11	s9	147	MET
11	s9	167	ALA
11	s9	183	ALA
12	c0	30	ALA
12	c0	31	LYS
13	c1	7	VAL
13	c1	55	ASP
14	c2	26	ASP
14	c2	39	ASP
14	c2	42	ALA
14	c2	108	ARG
14	c2	136	ILE
16	c4	33	LEU
16	c4	58	TYR
17	c5	17	TYR
17	c5	136	SER
19	c7	62	GLN
20	c8	61	LEU
22	d0	17	GLN
22	d0	49	ASN
22	d0	96	PRO
23	d1	21	ASN
23	d1	64	GLU
23	d1	81	ASN
24	d2	56	HIS
25	d3	70	LYS

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Mol	Chain	Res	Type
25	d3	131	SER
26	d4	58	PHE
27	d5	38	HIS
28	d6	8	ASN
28	d6	35	ALA
28	d6	60	PRO
29	d7	38	PRO
29	d7	63	LEU
30	d8	61	ARG
31	d9	11	PRO
31	d9	17	GLY
80	e0	54	ARG
80	e0	60	PRO
33	e1	85	TYR
33	e1	111	GLU
33	e1	128	ALA
33	e1	136	LYS
34	sR	141	LEU
34	sR	161	LYS
34	sR	164	ASP
34	sR	226	ALA
35	sM	120	GLU
35	sM	166	VAL
39	l2	56	ALA
40	l3	297	SER
40	l3	378	ALA
41	l4	5	GLN
41	l4	145	ILE
41	l4	231	ALA
41	l4	301	PRO
41	l4	338	LYS
42	l5	115	LEU
42	l5	178	ASN
43	l6	10	TYR
43	l6	93	VAL
45	l8	116	VAL
45	l8	188	THR
45	l8	196	ALA
45	l8	202	GLU
45	l8	209	ALA
45	l8	237	ILE
47	m0	25	ALA

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Mol	Chain	Res	Type
47	m0	193	ASP
47	m0	207	GLU
48	m1	39	GLN
48	m1	117	ASP
48	m1	167	TYR
49	m3	130	GLY
49	m3	135	ALA
53	m7	66	SER
54	m8	41	ASP
54	m8	91	ALA
54	m8	98	LYS
54	m8	155	MET
55	m9	36	ASN
56	n0	2	ALA
58	n2	44	GLU
58	n2	48	GLY
59	n3	16	GLY
61	n5	39	LYS
61	n5	45	LYS
61	n5	47	ALA
63	n7	34	LYS
64	n8	12	ARG
67	o1	82	GLU
72	o6	12	ASN
72	o6	34	SER
73	o7	55	ARG
74	o8	60	GLY
75	o9	3	ALA
79	q3	51	ALA
82	p0	33	VAL
82	p0	72	ASP
82	p0	102	SER
82	p0	220	ILE
2	S0	28	ASN
2	S0	103	THR
2	S0	152	PRO
3	S1	55	LYS
3	S1	158	SER
3	S1	177	GLN
3	S1	213	ARG
3	S1	217	LEU
3	S1	221	PRO

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Mol	Chain	Res	Type
5	S3	31	GLU
5	S3	72	LEU
6	S4	153	ASN
6	S4	205	PHE
7	S5	21	THR
7	S5	64	VAL
8	S6	69	LEU
8	S6	138	ALA
8	S6	174	LYS
9	S7	36	ALA
9	S7	84	LYS
9	S7	116	ARG
9	S7	134	GLU
10	S8	52	ASN
10	S8	152	ILE
13	C1	6	THR
14	C2	107	ASP
14	C2	125	ASN
14	C2	141	SER
15	C3	19	SER
16	C4	40	ALA
18	C6	142	TYR
19	C7	23	LYS
19	C7	123	ASN
21	C9	39	THR
21	C9	116	ILE
23	D1	8	LEU
25	D3	41	SER
27	D5	93	SER
28	D6	61	GLU
28	D6	64	LEU
29	D7	75	GLU
30	D8	22	ARG
32	E0	13	LYS
33	E1	90	LYS
33	E1	93	HIS
33	E1	145	HIS
34	SR	112	SER
34	SR	146	GLY
34	SR	242	SER
35	SM	17	VAL
35	SM	53	ARG

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Mol	Chain	Res	Type
35	SM	86	ASN
40	L3	142	ALA
40	L3	155	ALA
40	L3	221	THR
41	L4	90	PHE
41	L4	182	LEU
41	L4	294	GLU
42	L5	6	ASP
42	L5	91	GLY
42	L5	252	ALA
42	L5	260	PHE
44	L7	159	GLN
45	L8	122	LYS
46	L9	2	LYS
46	L9	108	GLY
47	M0	172	GLY
47	M0	188	GLY
49	M3	25	HIS
50	M4	29	ALA
50	M4	36	VAL
52	M6	16	VAL
53	M7	160	ALA
53	M7	162	GLU
54	M8	91	ALA
54	M8	162	ALA
54	M8	183	GLY
55	M9	20	ARG
56	N0	24	LEU
56	N0	167	ARG
57	N1	115	LYS
59	N3	44	SER
60	N4	69	LYS
61	N5	105	VAL
63	N7	103	GLN
64	N8	78	LEU
67	O1	7	VAL
67	O1	33	VAL
72	O6	27	SER
73	O7	12	HIS
75	O9	3	ALA
76	Q0	79	GLU
78	Q2	17	CYS

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Mol	Chain	Res	Type
2	s0	111	ILE
2	s0	185	ARG
2	s0	203	PHE
3	s1	177	GLN
3	s1	207	LEU
3	s1	218	LEU
4	s2	85	PRO
4	s2	106	ASP
4	s2	150	GLN
4	s2	234	PRO
4	s2	235	LEU
4	s2	238	SER
5	s3	45	LYS
5	s3	144	ALA
6	s4	78	THR
6	s4	80	THR
6	s4	117	GLU
6	s4	168	LYS
6	s4	171	ASP
7	s5	29	ILE
7	s5	45	LYS
7	s5	169	ASN
8	s6	18	ILE
10	s8	136	SER
11	s9	168	ARG
12	c0	3	MET
12	c0	9	ASN
14	c2	89	ILE
14	c2	90	LYS
14	c2	103	LEU
14	c2	106	ILE
16	c4	79	VAL
16	c4	90	ARG
17	c5	8	LYS
17	c5	14	THR
17	c5	75	PRO
17	c5	131	ALA
18	c6	57	LEU
18	c6	97	VAL
19	c7	120	SER
20	c8	14	ILE
20	c8	55	HIS

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Mol	Chain	Res	Type
20	c8	60	GLU
25	d3	13	ARG
25	d3	138	GLU
28	d6	59	TYR
33	e1	131	PHE
33	e1	146	SER
35	sM	43	ASP
35	sM	47	ALA
39	l2	130	SER
39	l2	180	LEU
39	l2	247	ARG
40	l3	235	THR
41	l4	24	ALA
41	l4	339	LEU
42	l5	220	SER
43	l6	173	MET
44	l7	191	VAL
45	l8	120	LYS
46	l9	2	LYS
47	m0	145	LYS
47	m0	176	LEU
49	m3	60	ALA
52	m6	16	VAL
52	m6	177	LYS
53	m7	3	ARG
53	m7	75	GLU
58	n2	45	GLY
58	n2	50	LEU
60	n4	25	ASP
60	n4	83	THR
62	n6	83	ASP
63	n7	17	ARG
63	n7	103	GLN
63	n7	127	ASN
64	n8	129	PHE
65	n9	5	LYS
67	o1	83	GLU
67	o1	99	ALA
70	o4	82	ALA
71	o5	40	SER
71	o5	83	LYS
72	o6	4	LYS

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Mol	Chain	Res	Type
77	q1	23	ARG
78	q2	33	ALA
82	p0	206	ASP
3	S1	179	SER
4	S2	235	LEU
5	S3	36	GLY
5	S3	70	THR
5	S3	81	PRO
6	S4	77	ARG
8	S6	146	GLY
9	S7	14	THR
9	S7	29	ASN
9	S7	132	PRO
10	S8	22	ARG
11	S9	147	MET
12	C0	34	GLU
13	C1	30	ARG
14	C2	36	LEU
14	C2	87	PRO
14	C2	113	ARG
15	C3	27	LYS
16	C4	51	ASP
16	C4	135	ARG
17	C5	52	LYS
17	C5	53	PRO
17	C5	69	GLU
18	C6	33	GLY
22	D0	16	GLN
22	D0	17	GLN
24	D2	30	SER
26	D4	6	THR
26	D4	53	ASP
26	D4	58	PHE
26	D4	60	PHE
27	D5	41	ILE
27	D5	88	ILE
28	D6	62	TYR
29	D7	3	LEU
31	D9	11	PRO
33	E1	99	LYS
33	E1	100	LEU
33	E1	138	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	SR	70	ASP
34	SR	98	GLU
34	SR	247	PRO
35	SM	102	THR
40	L3	289	ASP
40	L3	317	ILE
40	L3	385	LYS
41	L4	5	GLN
41	L4	258	LEU
41	L4	318	LEU
41	L4	349	THR
42	L5	125	VAL
43	L6	87	THR
44	L7	25	GLN
44	L7	158	LYS
45	L8	157	VAL
47	M0	143	SER
48	M1	117	ASP
49	M3	13	HIS
50	M4	6	ILE
52	M6	184	THR
55	M9	3	ASN
60	N4	46	PRO
60	N4	77	LYS
69	O3	94	PHE
71	O5	10	ARG
72	O6	21	THR
78	Q2	34	SER
2	s0	103	THR
2	s0	139	VAL
2	s0	194	PRO
6	s4	30	ARG
7	s5	21	THR
7	s5	26	ALA
8	s6	152	ASP
9	s7	112	ARG
10	s8	52	ASN
10	s8	78	ILE
10	s8	105	ASP
11	s9	67	PRO
13	c1	61	THR
14	c2	21	GLU

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Mol	Chain	Res	Type
14	c2	87	PRO
16	c4	131	GLY
17	c5	128	HIS
21	c9	62	ALA
22	d0	45	ALA
23	d1	10	GLU
26	d4	68	LYS
27	d5	83	LEU
30	d8	6	PRO
33	e1	81	LYS
33	e1	100	LEU
33	e1	124	PRO
33	e1	148	TYR
34	sR	160	GLU
34	sR	186	PHE
34	sR	285	ALA
35	sM	46	LYS
35	sM	65	THR
35	sM	72	ARG
35	sM	84	LYS
35	sM	168	GLU
41	l4	233	LEU
41	l4	270	SER
41	l4	304	GLN
41	l4	321	LYS
45	l8	69	LEU
46	l9	167	VAL
48	m1	12	LEU
49	m3	152	THR
50	m4	3	THR
52	m6	13	GLY
54	m8	112	ALA
54	m8	171	LYS
55	m9	154	ALA
57	n1	16	GLN
64	n8	48	TYR
65	n9	24	PRO
66	o0	9	SER
66	o0	41	LEU
66	o0	46	ALA
71	o5	84	LYS
78	q2	78	LYS

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Mol	Chain	Res	Type
3	S1	201	THR
3	S1	210	ILE
5	S3	71	LEU
7	S5	65	ARG
8	S6	148	SER
9	S7	35	LYS
14	C2	37	VAL
14	C2	40	GLY
21	C9	29	GLU
22	D0	20	ILE
26	D4	52	LYS
33	E1	110	ALA
33	E1	124	PRO
34	SR	194	GLY
34	SR	237	GLN
35	SM	12	VAL
42	L5	295	GLY
44	L7	178	ILE
48	M1	108	GLU
49	M3	166	ALA
49	M3	192	GLU
57	N1	18	ASP
59	N3	66	LYS
60	N4	86	SER
64	N8	96	LYS
65	N9	21	ILE
69	O3	59	VAL
71	O5	119	LYS
3	s1	114	VAL
3	s1	129	THR
4	s2	119	LYS
5	s3	93	ASP
6	s4	260	GLY
7	s5	60	ASP
7	s5	151	GLY
7	s5	173	ALA
8	s6	123	GLY
12	c0	35	ILE
13	c1	28	SER
14	c2	40	GLY
14	c2	118	ALA
16	c4	125	SER

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Mol	Chain	Res	Type
17	c5	133	ALA
18	c6	4	VAL
20	c8	7	GLU
20	c8	90	ASN
20	c8	139	LYS
22	d0	97	VAL
80	e0	47	VAL
35	sM	49	LYS
35	sM	171	LYS
40	l3	333	LYS
41	l4	144	LYS
42	l5	125	VAL
45	l8	216	SER
48	m1	7	ASN
54	m8	42	ALA
54	m8	113	LYS
60	n4	98	PRO
63	n7	36	HIS
64	n8	47	LYS
68	o2	6	HIS
71	o5	3	GLY
71	o5	43	LYS
82	p0	71	PRO
3	S1	176	VAL
3	S1	226	GLY
4	S2	36	VAL
9	S7	13	PRO
9	S7	125	ILE
14	C2	22	VAL
26	D4	100	VAL
28	D6	59	TYR
30	D8	20	GLY
33	E1	112	GLY
35	SM	67	GLY
47	M0	16	PRO
5	s3	163	PRO
7	s5	152	GLY
11	s9	162	SER
14	c2	63	VAL
19	c7	86	PRO
21	c9	118	PRO
24	d2	6	VAL

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Mol	Chain	Res	Type
35	sM	52	PRO
51	m5	74	PRO
53	m7	84	PRO
60	n4	132	GLY
82	p0	47	GLY
82	p0	197	PHE
4	S2	145	GLY
14	C2	81	ASP
22	D0	19	ILE
34	SR	15	GLY
41	L4	97	GLY
44	L7	191	VAL
45	L8	135	GLY
60	N4	10	GLY
4	s2	83	ILE
5	s3	203	PRO
9	s7	73	VAL
14	c2	66	VAL
14	c2	91	VAL
14	c2	115	VAL
27	d5	50	ILE
34	sR	28	GLY
47	m0	204	GLY
64	n8	56	VAL
12	C0	92	ILE
19	C7	110	VAL
34	SR	113	VAL
40	L3	33	PRO
15	c3	22	ALA
39	l2	13	GLY
59	n3	134	GLY
7	S5	151	GLY
8	S6	162	VAL
18	C6	40	GLU
28	D6	60	PRO
28	D6	75	VAL
4	s2	149	GLY
14	c2	82	PRO
15	c3	98	VAL
16	C4	79	VAL
56	N0	22	PRO
62	N6	92	GLY

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Mol	Chain	Res	Type
8	s6	69	LEU
13	c1	129	ARG
19	c7	117	LEU
28	d6	16	GLY
69	o3	59	VAL
70	o4	78	GLY

### 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%)	136 (83%)	28 (17%)	2	9
2	s0	165/209 (79%)	130 (79%)	35 (21%)	1	5
3	S1	191/223 (86%)	150 (78%)	41 (22%)	1	4
3	s1	192/223 (86%)	151 (79%)	41 (21%)	1	4
4	S2	176/204 (86%)	137 (78%)	39 (22%)	1	4
4	s2	176/204 (86%)	133 (76%)	43 (24%)	0	2
5	S3	182/194 (94%)	138 (76%)	44 (24%)	0	2
5	s3	182/194 (94%)	144 (79%)	38 (21%)	1	5
6	S4	221/221 (100%)	175 (79%)	46 (21%)	1	5
6	s4	221/221 (100%)	183 (83%)	38 (17%)	2	9
7	S5	173/190 (91%)	137 (79%)	36 (21%)	1	5
7	s5	173/190 (91%)	140 (81%)	33 (19%)	1	6
8	S6	188/201 (94%)	152 (81%)	36 (19%)	1	6
8	s6	187/201 (93%)	152 (81%)	35 (19%)	1	7
9	S7	165/169 (98%)	140 (85%)	25 (15%)	3	12
9	s7	165/169 (98%)	135 (82%)	30 (18%)	1	7
10	S8	150/161 (93%)	128 (85%)	22 (15%)	3	13
10	s8	150/161 (93%)	119 (79%)	31 (21%)	1	5
11	S9	158/165 (96%)	126 (80%)	32 (20%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	s9	158/165 (96%)	124 (78%)	34 (22%)	1	4
12	C0	77/98 (79%)	64 (83%)	13 (17%)	2	9
12	c0	73/98 (74%)	61 (84%)	12 (16%)	2	10
13	C1	129/136 (95%)	115 (89%)	14 (11%)	6	25
13	c1	129/136 (95%)	109 (84%)	20 (16%)	2	11
14	C2	88/118 (75%)	62 (70%)	26 (30%)	0	1
14	c2	88/118 (75%)	64 (73%)	24 (27%)	0	1
15	C3	127/127 (100%)	102 (80%)	25 (20%)	1	6
15	c3	127/127 (100%)	104 (82%)	23 (18%)	1	7
16	C4	81/104 (78%)	57 (70%)	24 (30%)	0	1
16	c4	97/104 (93%)	70 (72%)	27 (28%)	0	1
17	C5	101/117 (86%)	82 (81%)	19 (19%)	1	6
17	c5	103/117 (88%)	83 (81%)	20 (19%)	1	6
18	C6	117/118 (99%)	90 (77%)	27 (23%)	1	3
18	c6	118/118 (100%)	96 (81%)	22 (19%)	1	7
19	C7	94/124 (76%)	74 (79%)	20 (21%)	1	4
19	c7	92/124 (74%)	72 (78%)	20 (22%)	1	4
20	C8	128/128 (100%)	107 (84%)	21 (16%)	2	10
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	3
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	5
21	c9	115/115 (100%)	94 (82%)	21 (18%)	1	7
22	D0	100/113 (88%)	72 (72%)	28 (28%)	0	1
22	d0	103/113 (91%)	77 (75%)	26 (25%)	0	1
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	8
23	d1	74/74 (100%)	62 (84%)	12 (16%)	2	10
24	D2	110/110 (100%)	91 (83%)	19 (17%)	2	9
24	d2	110/110 (100%)	94 (86%)	16 (14%)	3	13
25	D3	119/119 (100%)	97 (82%)	22 (18%)	1	7
25	d3	119/119 (100%)	98 (82%)	21 (18%)	2	8
26	D4	112/112 (100%)	98 (88%)	14 (12%)	4	18
26	d4	112/112 (100%)	93 (83%)	19 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	D5	61/88 (69%)	43 (70%)	18 (30%)	0	1
27	d5	61/88 (69%)	51 (84%)	10 (16%)	2	10
28	D6	83/83 (100%)	63 (76%)	20 (24%)	0	2
28	d6	83/83 (100%)	66 (80%)	17 (20%)	1	5
29	D7	70/70 (100%)	59 (84%)	11 (16%)	2	11
29	d7	70/70 (100%)	60 (86%)	10 (14%)	3	14
30	D8	56/59 (95%)	43 (77%)	13 (23%)	1	3
30	d8	56/59 (95%)	46 (82%)	10 (18%)	2	8
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	9
31	d9	47/48 (98%)	38 (81%)	9 (19%)	1	6
32	E0	51/51 (100%)	39 (76%)	12 (24%)	1	3
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0	1
33	e1	66/66 (100%)	50 (76%)	16 (24%)	0	2
34	SR	260/261 (100%)	211 (81%)	49 (19%)	1	6
34	sR	260/261 (100%)	231 (89%)	29 (11%)	6	24
35	SM	97/228 (42%)	80 (82%)	17 (18%)	2	8
35	sM	54/228 (24%)	41 (76%)	13 (24%)	0	2
39	L2	193/195 (99%)	157 (81%)	36 (19%)	1	7
39	l2	192/195 (98%)	158 (82%)	34 (18%)	2	8
40	L3	320/322 (99%)	252 (79%)	68 (21%)	1	4
40	l3	321/322 (100%)	252 (78%)	69 (22%)	1	4
41	L4	288/288 (100%)	230 (80%)	58 (20%)	1	5
41	l4	288/288 (100%)	231 (80%)	57 (20%)	1	5
42	L5	244/244 (100%)	206 (84%)	38 (16%)	2	11
42	l5	243/244 (100%)	191 (79%)	52 (21%)	1	4
43	L6	134/152 (88%)	114 (85%)	20 (15%)	3	13
43	l6	135/152 (89%)	114 (84%)	21 (16%)	2	11
44	L7	186/204 (91%)	160 (86%)	26 (14%)	3	15
44	l7	187/204 (92%)	157 (84%)	30 (16%)	2	11
45	L8	187/207 (90%)	157 (84%)	30 (16%)	2	11
45	l8	177/207 (86%)	138 (78%)	39 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	L9	171/171 (100%)	128 (75%)	43 (25%)	0	1
46	l9	171/171 (100%)	136 (80%)	35 (20%)	1	5
47	M0	177/186 (95%)	139 (78%)	38 (22%)	1	4
47	m0	179/186 (96%)	149 (83%)	30 (17%)	2	9
48	M1	147/150 (98%)	109 (74%)	38 (26%)	0	1
48	m1	147/150 (98%)	117 (80%)	30 (20%)	1	5
49	M3	154/158 (98%)	124 (80%)	30 (20%)	1	6
49	m3	154/158 (98%)	125 (81%)	29 (19%)	1	6
50	M4	107/108 (99%)	87 (81%)	20 (19%)	1	7
50	m4	108/108 (100%)	91 (84%)	17 (16%)	2	11
51	M5	175/175 (100%)	139 (79%)	36 (21%)	1	5
51	m5	175/175 (100%)	146 (83%)	29 (17%)	2	9
52	M6	160/161 (99%)	132 (82%)	28 (18%)	2	8
52	m6	160/161 (99%)	134 (84%)	26 (16%)	2	10
53	M7	140/145 (97%)	106 (76%)	34 (24%)	0	2
53	m7	125/145 (86%)	101 (81%)	24 (19%)	1	6
54	M8	150/150 (100%)	121 (81%)	29 (19%)	1	6
54	m8	150/150 (100%)	121 (81%)	29 (19%)	1	6
55	M9	153/153 (100%)	131 (86%)	22 (14%)	3	14
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	4
56	N0	156/156 (100%)	127 (81%)	29 (19%)	1	7
56	n0	156/156 (100%)	123 (79%)	33 (21%)	1	5
57	N1	136/136 (100%)	111 (82%)	25 (18%)	1	7
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	4
58	N2	87/106 (82%)	72 (83%)	15 (17%)	2	9
58	n2	85/106 (80%)	65 (76%)	20 (24%)	1	3
59	N3	104/104 (100%)	84 (81%)	20 (19%)	1	6
59	n3	104/104 (100%)	91 (88%)	13 (12%)	4	18
60	N4	57/129 (44%)	50 (88%)	7 (12%)	4	19
60	n4	100/129 (78%)	84 (84%)	16 (16%)	2	11
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	n5	104/117 (89%)	86 (83%)	18 (17%)	2	9
62	N6	109/109 (100%)	88 (81%)	21 (19%)	1	6
62	n6	109/109 (100%)	86 (79%)	23 (21%)	1	5
63	N7	115/115 (100%)	92 (80%)	23 (20%)	1	5
63	n7	115/115 (100%)	90 (78%)	25 (22%)	1	4
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	8
64	n8	118/118 (100%)	103 (87%)	15 (13%)	4	18
65	N9	46/46 (100%)	38 (83%)	8 (17%)	2	9
65	n9	46/46 (100%)	32 (70%)	14 (30%)	0	0
66	O0	81/87 (93%)	63 (78%)	18 (22%)	1	4
66	o0	84/87 (97%)	63 (75%)	21 (25%)	0	2
67	O1	92/96 (96%)	76 (83%)	16 (17%)	2	9
67	o1	94/96 (98%)	68 (72%)	26 (28%)	0	1
68	O2	109/110 (99%)	87 (80%)	22 (20%)	1	5
68	o2	109/110 (99%)	87 (80%)	22 (20%)	1	5
69	O3	90/90 (100%)	80 (89%)	10 (11%)	6	24
69	o3	90/90 (100%)	72 (80%)	18 (20%)	1	5
70	O4	95/101 (94%)	77 (81%)	18 (19%)	1	6
70	o4	95/101 (94%)	76 (80%)	19 (20%)	1	5
71	O5	104/104 (100%)	78 (75%)	26 (25%)	0	2
71	o5	103/104 (99%)	84 (82%)	19 (18%)	1	7
72	O6	81/81 (100%)	61 (75%)	20 (25%)	0	2
72	o6	80/81 (99%)	54 (68%)	26 (32%)	0	0
73	O7	70/70 (100%)	52 (74%)	18 (26%)	0	1
73	o7	70/70 (100%)	56 (80%)	14 (20%)	1	5
74	O8	68/68 (100%)	49 (72%)	19 (28%)	0	1
74	o8	67/68 (98%)	51 (76%)	16 (24%)	0	2
75	O9	45/45 (100%)	37 (82%)	8 (18%)	2	8
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	8
76	Q0	47/47 (100%)	41 (87%)	6 (13%)	4	18
76	q0	47/47 (100%)	40 (85%)	7 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	Q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	0
78	Q2	90/90 (100%)	74 (82%)	16 (18%)	2	8
78	q2	90/90 (100%)	67 (74%)	23 (26%)	0	1
79	Q3	71/71 (100%)	55 (78%)	16 (22%)	1	3
79	q3	71/71 (100%)	57 (80%)	14 (20%)	1	6
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1	3
82	p0	105/253 (42%)	87 (83%)	18 (17%)	2	9
All	All	18729/20239 (92%)	15053 (80%)	3676 (20%)	1	6

All (3676) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	6	THR
2	S0	7	PHE
2	S0	28	ASN
2	S0	37	VAL
2	S0	50	VAL
2	S0	57	LEU
2	S0	59	LEU
2	S0	84	ARG
2	S0	86	VAL
2	S0	96	THR
2	S0	101	ARG
2	S0	103	THR
2	S0	119	ARG
2	S0	120	LEU
2	S0	122	ILE
2	S0	131	GLN
2	S0	135	GLU
2	S0	156	VAL
2	S0	157	ASP
2	S0	165	ARG
2	S0	168	HIS
2	S0	172	LEU
2	S0	185	ARG
2	S0	188	LEU
2	S0	189	VAL
2	S0	196	SER

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Mol	Chain	Res	Type
2	S0	198	MET
2	S0	200	ASP
3	S1	20	VAL
3	S1	21	VAL
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	42	ASN
3	S1	46	THR
3	S1	47	LEU
3	S1	61	LEU
3	S1	64	ARG
3	S1	65	VAL
3	S1	70	LEU
3	S1	77	GLU
3	S1	78	ASP
3	S1	81	PHE
3	S1	85	LYS
3	S1	89	ASP
3	S1	97	LEU
3	S1	104	ASP
3	S1	105	PHE
3	S1	108	ASP
3	S1	111	ARG
3	S1	117	TRP
3	S1	125	VAL
3	S1	126	THR
3	S1	137	ILE
3	S1	144	ARG
3	S1	145	LYS
3	S1	148	ASN
3	S1	154	SER
3	S1	169	SER
3	S1	181	LEU
3	S1	193	ILE
3	S1	202	LYS
3	S1	204	ILE
3	S1	206	PRO
3	S1	214	LYS
3	S1	217	LEU
3	S1	218	LEU
3	S1	219	LYS

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Mol	Chain	Res	Type
3	S1	223	PHE
4	S2	41	LEU
4	S2	53	ILE
4	S2	54	GLU
4	S2	69	ILE
4	S2	70	ASP
4	S2	76	LEU
4	S2	77	GLN
4	S2	83	ILE
4	S2	87	GLN
4	S2	89	GLN
4	S2	94	GLN
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	111	VAL
4	S2	113	LEU
4	S2	117	THR
4	S2	119	LYS
4	S2	130	ILE
4	S2	134	LEU
4	S2	137	ILE
4	S2	139	ILE
4	S2	140	ARG
4	S2	141	ARG
4	S2	146	THR
4	S2	148	LEU
4	S2	153	SER
4	S2	154	LEU
4	S2	166	THR
4	S2	187	LEU
4	S2	201	ASN
4	S2	208	GLU
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	235	LEU
4	S2	245	ASP
4	S2	246	GLU
4	S2	250	GLN
5	S3	4	LEU
5	S3	7	LYS

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Mol	Chain	Res	Type
5	S3	9	ARG
5	S3	21	LEU
5	S3	23	GLU
5	S3	37	VAL
5	S3	45	LYS
5	S3	65	ARG
5	S3	70	THR
5	S3	74	GLN
5	S3	76	ARG
5	S3	89	GLU
5	S3	90	ARG
5	S3	91	VAL
5	S3	92	GLN
5	S3	93	ASP
5	S3	103	GLU
5	S3	104	SER
5	S3	105	MET
5	S3	111	ASN
5	S3	113	LEU
5	S3	122	VAL
5	S3	124	ARG
5	S3	134	CYS
5	S3	141	LYS
5	S3	142	LEU
5	S3	143	ARG
5	S3	146	ARG
5	S3	151	LYS
5	S3	158	ILE
5	S3	172	THR
5	S3	175	VAL
5	S3	176	LEU
5	S3	178	ARG
5	S3	179	GLN
5	S3	181	VAL
5	S3	182	LEU
5	S3	196	ARG
5	S3	200	LYS
5	S3	207	THR
5	S3	212	LYS
5	S3	217	ILE
5	S3	222	VAL
5	S3	224	ASP

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Mol	Chain	Res	Type
6	S4	9	LEU
6	S4	12	LEU
6	S4	38	LEU
6	S4	41	SER
6	S4	42	LEU
6	S4	49	ARG
6	S4	56	LEU
6	S4	62	LYS
6	S4	65	LEU
6	S4	67	GLN
6	S4	68	ARG
6	S4	77	ARG
6	S4	78	THR
6	S4	93	ASP
6	S4	95	THR
6	S4	108	ARG
6	S4	116	ASP
6	S4	117	GLU
6	S4	123	LEU
6	S4	126	VAL
6	S4	128	LYS
6	S4	131	LEU
6	S4	133	LYS
6	S4	145	ARG
6	S4	151	ASP
6	S4	166	SER
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	198	LYS
6	S4	206	ASP
6	S4	210	ILE
6	S4	215	ASP
6	S4	220	THR
6	S4	221	ARG
6	S4	226	PHE
6	S4	227	VAL
6	S4	231	GLN
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU
6	S4	247	SER

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Mol	Chain	Res	Type
6	S4	248	ILE
6	S4	256	ARG
6	S4	259	GLN
6	S4	261	LEU
7	S5	25	LEU
7	S5	32	GLU
7	S5	38	THR
7	S5	41	LYS
7	S5	43	PHE
7	S5	45	LYS
7	S5	46	TRP
7	S5	50	GLU
7	S5	59	VAL
7	S5	65	ARG
7	S5	66	GLN
7	S5	76	ARG
7	S5	79	ASN
7	S5	89	ILE
7	S5	92	ARG
7	S5	93	LEU
7	S5	94	THR
7	S5	97	LEU
7	S5	99	MET
7	S5	122	ASN
7	S5	126	ASP
7	S5	146	THR
7	S5	147	THR
7	S5	149	VAL
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	162	VAL
7	S5	166	ARG
7	S5	172	ILE
7	S5	186	ASN
7	S5	187	ILE
7	S5	190	ILE
7	S5	194	LEU
7	S5	223	SER
7	S5	225	ARG
8	S6	6	SER
8	S6	13	GLN

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Mol	Chain	Res	Type
8	S6	25	ARG
8	S6	43	ASP
8	S6	44	GLU
8	S6	45	PHE
8	S6	49	VAL
8	S6	58	LYS
8	S6	67	VAL
8	S6	69	LEU
8	S6	76	LEU
8	S6	79	LYS
8	S6	81	VAL
8	S6	82	SER
8	S6	89	ASP
8	S6	98	ARG
8	S6	109	LEU
8	S6	113	ILE
8	S6	120	GLU
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	129	VAL
8	S6	132	ARG
8	S6	133	LEU
8	S6	141	ILE
8	S6	154	ARG
8	S6	162	VAL
8	S6	169	TYR
8	S6	170	THR
8	S6	175	ILE
8	S6	176	GLN
8	S6	177	ARG
8	S6	211	LEU
8	S6	212	LEU
8	S6	223	LYS
9	S7	24	PHE
9	S7	28	GLU
9	S7	37	GLU
9	S7	38	LEU
9	S7	42	GLN
9	S7	44	LYS
9	S7	46	ILE
9	S7	51	VAL

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Mol	Chain	Res	Type
9	S7	60	ILE
9	S7	67	LEU
9	S7	79	ARG
9	S7	85	PHE
9	S7	87	ASP
9	S7	97	ARG
9	S7	107	ARG
9	S7	114	ARG
9	S7	118	LEU
9	S7	126	LEU
9	S7	130	VAL
9	S7	147	ASN
9	S7	149	ILE
9	S7	174	ASN
9	S7	181	ILE
9	S7	182	VAL
9	S7	185	ILE
10	S8	4	SER
10	S8	7	SER
10	S8	8	ARG
10	S8	21	PHE
10	S8	22	ARG
10	S8	26	LYS
10	S8	29	LEU
10	S8	36	THR
10	S8	37	LYS
10	S8	46	VAL
10	S8	56	ARG
10	S8	58	LEU
10	S8	66	SER
10	S8	74	LYS
10	S8	97	THR
10	S8	123	LYS
10	S8	138	ASN
10	S8	151	LYS
10	S8	152	ILE
10	S8	155	SER
10	S8	164	ARG
10	S8	195	ARG
11	S9	3	ARG
11	S9	6	ARG
11	S9	7	THR

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Mol	Chain	Res	Type
11	S9	14	THR
11	S9	21	SER
11	S9	28	LEU
11	S9	40	LYS
11	S9	50	SER
11	S9	61	THR
11	S9	63	ASP
11	S9	66	ASP
11	S9	78	ARG
11	S9	79	ARG
11	S9	81	VAL
11	S9	82	ARG
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	94	ASP
11	S9	99	LEU
11	S9	100	LYS
11	S9	105	LEU
11	S9	110	GLN
11	S9	118	LEU
11	S9	130	THR
11	S9	134	ILE
11	S9	138	LYS
11	S9	149	ARG
11	S9	161	THR
11	S9	162	SER
11	S9	171	ARG
11	S9	172	VAL
12	C0	8	ARG
12	C0	20	VAL
12	C0	26	ASP
12	C0	28	ASN
12	C0	32	HIS
12	C0	40	LEU
12	C0	55	VAL
12	C0	56	LYS
12	C0	60	SER
12	C0	71	GLU
12	C0	76	LEU
12	C0	81	ASN
12	C0	82	LEU

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Mol	Chain	Res	Type
13	C1	7	VAL
13	C1	8	GLN
13	C1	21	ASN
13	C1	29	LYS
13	C1	40	LEU
13	C1	44	THR
13	C1	67	ARG
13	C1	69	LYS
13	C1	80	MET
13	C1	105	LYS
13	C1	107	VAL
13	C1	109	VAL
13	C1	131	ILE
13	C1	143	SER
14	C2	33	ARG
14	C2	36	LEU
14	C2	37	VAL
14	C2	39	ASP
14	C2	41	LEU
14	C2	43	ARG
14	C2	46	ARG
14	C2	50	LYS
14	C2	52	LEU
14	C2	53	THR
14	C2	54	ARG
14	C2	62	LEU
14	C2	63	VAL
14	C2	66	VAL
14	C2	71	ILE
14	C2	74	LEU
14	C2	85	LYS
14	C2	89	ILE
14	C2	103	LEU
14	C2	121	VAL
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	139	HIS
14	C2	140	PHE
14	C2	143	GLN
15	C3	3	ARG
15	C3	9	LYS

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Mol	Chain	Res	Type
15	C3	16	ILE
15	C3	27	LYS
15	C3	30	SER
15	C3	33	VAL
15	C3	39	LYS
15	C3	43	LYS
15	C3	45	LEU
15	C3	46	THR
15	C3	56	ASP
15	C3	62	GLN
15	C3	64	ARG
15	C3	66	ILE
15	C3	76	LYS
15	C3	80	LEU
15	C3	83	GLU
15	C3	88	LEU
15	C3	102	LEU
15	C3	114	ARG
15	C3	115	LEU
15	C3	125	LEU
15	C3	131	THR
15	C3	134	VAL
15	C3	149	LEU
16	C4	16	VAL
16	C4	29	HIS
16	C4	30	VAL
16	C4	31	THR
16	C4	38	THR
16	C4	42	VAL
16	C4	43	THR
16	C4	48	VAL
16	C4	49	LYS
16	C4	51	ASP
16	C4	53	ASP
16	C4	55	SER
16	C4	81	VAL
16	C4	92	LYS
16	C4	93	THR
16	C4	102	LEU
16	C4	103	ARG
16	C4	114	ARG
16	C4	119	THR

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Mol	Chain	Res	Type
16	C4	123	SER
16	C4	126	THR
16	C4	135	ARG
16	C4	136	ARG
16	C4	137	LEU
17	C5	11	VAL
17	C5	20	VAL
17	C5	22	LEU
17	C5	28	MET
17	C5	31	GLU
17	C5	34	VAL
17	C5	44	ARG
17	C5	47	ARG
17	C5	52	LYS
17	C5	69	GLU
17	C5	70	ASN
17	C5	84	ILE
17	C5	86	VAL
17	C5	98	ASN
17	C5	100	LYS
17	C5	110	GLU
17	C5	121	ILE
17	C5	124	THR
17	C5	125	PRO
18	C6	4	VAL
18	C6	8	GLN
18	C6	14	LYS
18	C6	26	LYS
18	C6	28	LEU
18	C6	43	ILE
18	C6	47	LYS
18	C6	53	LEU
18	C6	54	LEU
18	C6	68	ARG
18	C6	69	VAL
18	C6	82	ARG
18	C6	98	ASP
18	C6	101	SER
18	C6	104	GLU
18	C6	106	LYS
18	C6	114	ARG
18	C6	118	ILE

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Mol	Chain	Res	Type
18	C6	121	SER
18	C6	123	ARG
18	C6	127	LYS
18	C6	136	SER
18	C6	137	ARG
18	C6	138	PHE
18	C6	139	GLN
18	C6	141	SER
18	C6	143	ARG
19	C7	3	ARG
19	C7	5	ARG
19	C7	6	THR
19	C7	10	LYS
19	C7	25	THR
19	C7	30	THR
19	C7	34	LEU
19	C7	40	THR
19	C7	45	ARG
19	C7	58	MET
19	C7	62	GLN
19	C7	67	ARG
19	C7	69	ILE
19	C7	72	LYS
19	C7	78	ARG
19	C7	88	VAL
19	C7	105	GLN
19	C7	113	LEU
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	13	HIS
20	C8	15	LEU
20	C8	17	LEU
20	C8	20	THR
20	C8	28	ILE
20	C8	40	ARG
20	C8	61	LEU
20	C8	65	GLU
20	C8	72	ILE
20	C8	74	GLN
20	C8	80	LYS

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Mol	Chain	Res	Type
20	C8	92	ILE
20	C8	93	THR
20	C8	97	ASP
20	C8	108	LYS
20	C8	132	ARG
20	C8	136	GLN
20	C8	138	THR
20	C8	143	ARG
21	C9	6	VAL
21	C9	22	LEU
21	C9	27	LYS
21	C9	28	LEU
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	38	LYS
21	C9	57	ARG
21	C9	60	SER
21	C9	67	MET
21	C9	71	VAL
21	C9	86	ARG
21	C9	94	ILE
21	C9	103	LYS
21	C9	116	ILE
21	C9	122	ARG
21	C9	130	ARG
21	C9	131	ASP
21	C9	133	ASP
21	C9	134	ARG
21	C9	143	ASP
21	C9	144	GLU
22	D0	15	GLN
22	D0	18	GLN
22	D0	19	ILE
22	D0	20	ILE
22	D0	23	ARG
22	D0	27	THR
22	D0	30	LYS
22	D0	31	VAL
22	D0	34	LEU
22	D0	47	GLN
22	D0	50	LEU

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Mol	Chain	Res	Type
22	D0	51	VAL
22	D0	57	ARG
22	D0	58	LEU
22	D0	60	THR
22	D0	61	LYS
22	D0	72	ASN
22	D0	74	GLU
22	D0	76	SER
22	D0	80	GLU
22	D0	81	THR
22	D0	89	ARG
22	D0	99	ILE
22	D0	103	ILE
22	D0	105	GLN
22	D0	108	ILE
22	D0	120	SER
22	D0	121	ASN
23	D1	3	ASN
23	D1	8	LEU
23	D1	11	LEU
23	D1	12	TYR
23	D1	18	SER
23	D1	21	ASN
23	D1	41	GLU
23	D1	49	GLU
23	D1	50	TYR
23	D1	52	THR
23	D1	69	LEU
23	D1	80	LYS
23	D1	87	ARG
24	D2	7	LEU
24	D2	12	ASN
24	D2	15	ASN
24	D2	20	THR
24	D2	23	ARG
24	D2	24	GLN
24	D2	27	ILE
24	D2	30	SER
24	D2	53	ILE
24	D2	56	HIS
24	D2	65	LEU
24	D2	66	ASN

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Mol	Chain	Res	Type
24	D2	81	VAL
24	D2	93	LEU
24	D2	98	GLN
24	D2	103	ILE
24	D2	105	THR
24	D2	117	ARG
24	D2	129	VAL
25	D3	5	LYS
25	D3	7	ARG
25	D3	9	LEU
25	D3	14	LYS
25	D3	16	ARG
25	D3	19	ARG
25	D3	26	GLU
25	D3	28	ASN
25	D3	31	LYS
25	D3	41	SER
25	D3	47	SER
25	D3	56	LYS
25	D3	82	LYS
25	D3	84	THR
25	D3	103	LEU
25	D3	107	PHE
25	D3	114	LYS
25	D3	117	ILE
25	D3	132	LEU
25	D3	135	LEU
25	D3	140	LYS
25	D3	144	ARG
26	D4	9	THR
26	D4	28	LEU
26	D4	32	ARG
26	D4	34	ASN
26	D4	51	GLU
26	D4	52	LYS
26	D4	61	ARG
26	D4	62	THR
26	D4	74	LEU
26	D4	75	VAL
26	D4	96	LEU
26	D4	100	VAL
26	D4	102	LYS

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Mol	Chain	Res	Type
26	D4	124	ARG
27	D5	40	VAL
27	D5	42	LEU
27	D5	48	ASP
27	D5	49	ARG
27	D5	50	ILE
27	D5	58	ARG
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	78	ILE
27	D5	85	LYS
27	D5	92	ILE
27	D5	95	HIS
27	D5	96	SER
27	D5	98	GLN
28	D6	5	ARG
28	D6	12	LYS
28	D6	21	VAL
28	D6	32	LYS
28	D6	36	ILE
28	D6	38	ARG
28	D6	41	ILE
28	D6	44	ILE
28	D6	57	SER
28	D6	58	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	66	LYS
28	D6	70	LYS
28	D6	76	SER
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
28	D6	88	SER
28	D6	90	GLU
29	D7	3	LEU
29	D7	29	ARG
29	D7	33	LEU

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Mol	Chain	Res	Type
29	D7	34	ASP
29	D7	41	LEU
29	D7	43	ILE
29	D7	60	SER
29	D7	61	THR
29	D7	62	ILE
29	D7	65	THR
29	D7	67	THR
30	D8	13	ILE
30	D8	19	THR
30	D8	22	ARG
30	D8	32	PHE
30	D8	33	LEU
30	D8	34	GLU
30	D8	36	THR
30	D8	49	ARG
30	D8	57	MET
30	D8	58	GLU
30	D8	61	ARG
30	D8	64	ARG
30	D8	65	ARG
31	D9	5	ASN
31	D9	7	TRP
31	D9	9	SER
31	D9	12	ARG
31	D9	21	CYS
31	D9	28	THR
31	D9	32	ARG
31	D9	48	ASN
32	E0	3	LYS
32	E0	20	LYS
32	E0	21	VAL
32	E0	22	GLU
32	E0	24	THR
32	E0	39	LEU
32	E0	42	ARG
32	E0	43	ARG
32	E0	47	VAL
32	E0	50	VAL
32	E0	56	MET
32	E0	58	PRO
33	E1	83	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	E1	84	VAL
33	E1	89	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	97	LYS
33	E1	108	VAL
33	E1	113	LYS
33	E1	118	ARG
33	E1	120	GLU
33	E1	130	VAL
33	E1	137	ASP
33	E1	138	ARG
33	E1	140	TYR
33	E1	145	HIS
33	E1	147	VAL
33	E1	151	ASN
34	SR	6	VAL
34	SR	21	THR
34	SR	22	SER
34	SR	29	GLN
34	SR	48	THR
34	SR	52	GLN
34	SR	59	ARG
34	SR	60	SER
34	SR	62	LYS
34	SR	69	GLN
34	SR	70	ASP
34	SR	76	ASP
34	SR	96	THR
34	SR	100	TYR
34	SR	102	ARG
34	SR	106	HIS
34	SR	109	ASP
34	SR	113	VAL
34	SR	117	LYS
34	SR	136	ILE
34	SR	141	LEU
34	SR	145	LEU
34	SR	148	ASN
34	SR	154	VAL
34	SR	159	ASN
34	SR	163	ASP

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Mol	Chain	Res	Type
34	SR	165	ASP
34	SR	184	ASN
34	SR	188	ILE
34	SR	191	ASP
34	SR	199	ILE
34	SR	200	ASN
34	SR	207	ASP
34	SR	229	LYS
34	SR	231	MET
34	SR	232	TYR
34	SR	238	ASP
34	SR	241	PHE
34	SR	242	SER
34	SR	258	THR
34	SR	265	LEU
34	SR	266	ASP
34	SR	268	GLN
34	SR	292	LEU
34	SR	300	THR
34	SR	309	VAL
34	SR	314	GLN
34	SR	316	MET
34	SR	317	THR
35	SM	34	LYS
35	SM	51	ARG
35	SM	53	ARG
35	SM	61	ILE
35	SM	64	LYS
35	SM	69	ARG
35	SM	72	ARG
35	SM	84	LYS
35	SM	89	ARG
35	SM	91	THR
35	SM	96	ARG
35	SM	102	THR
35	SM	103	LYS
35	SM	116	GLU
35	SM	121	LYS
35	SM	122	GLU
35	SM	139	GLU
39	L2	10	LYS
39	L2	14	SER

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Mol	Chain	Res	Type
39	L2	18	SER
39	L2	23	ARG
39	L2	32	LEU
39	L2	44	ILE
39	L2	45	VAL
39	L2	49	VAL
39	L2	64	ARG
39	L2	70	ARG
39	L2	74	GLU
39	L2	88	ILE
39	L2	95	SER
39	L2	96	LEU
39	L2	97	ASN
39	L2	101	VAL
39	L2	104	LEU
39	L2	109	GLU
39	L2	114	SER
39	L2	116	VAL
39	L2	119	LYS
39	L2	141	PRO
39	L2	142	ASP
39	L2	143	GLU
39	L2	157	VAL
39	L2	179	LEU
39	L2	180	LEU
39	L2	190	ARG
39	L2	191	LEU
39	L2	193	ARG
39	L2	202	VAL
39	L2	204	MET
39	L2	207	VAL
39	L2	226	SER
39	L2	227	ARG
39	L2	230	VAL
40	L3	2	SER
40	L3	7	GLU
40	L3	17	LEU
40	L3	19	ARG
40	L3	21	ARG
40	L3	24	SER
40	L3	25	ILE
40	L3	30	LYS

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Mol	Chain	Res	Type
40	L3	37	ARG
40	L3	44	THR
40	L3	47	LEU
40	L3	55	THR
40	L3	56	ILE
40	L3	70	ARG
40	L3	81	THR
40	L3	84	VAL
40	L3	85	VAL
40	L3	93	VAL
40	L3	103	THR
40	L3	112	ASP
40	L3	114	VAL
40	L3	116	ARG
40	L3	134	SER
40	L3	139	GLN
40	L3	146	ARG
40	L3	148	LEU
40	L3	150	ARG
40	L3	157	VAL
40	L3	165	GLN
40	L3	166	ILE
40	L3	184	ASN
40	L3	187	SER
40	L3	188	ILE
40	L3	192	VAL
40	L3	196	ARG
40	L3	202	THR
40	L3	208	VAL
40	L3	229	VAL
40	L3	232	ARG
40	L3	235	THR
40	L3	236	LYS
40	L3	237	LYS
40	L3	238	LEU
40	L3	241	LYS
40	L3	244	ARG
40	L3	252	ILE
40	L3	264	VAL
40	L3	266	ARG
40	L3	270	ARG
40	L3	274	SER

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Mol	Chain	Res	Type
40	L3	278	ILE
40	L3	284	ARG
40	L3	287	LYS
40	L3	296	THR
40	L3	304	THR
40	L3	305	ILE
40	L3	306	THR
40	L3	308	MET
40	L3	312	VAL
40	L3	324	VAL
40	L3	325	LYS
40	L3	332	ARG
40	L3	337	THR
40	L3	341	SER
40	L3	345	ASN
40	L3	347	SER
40	L3	353	GLU
40	L3	355	SER
41	L4	4	PRO
41	L4	20	LEU
41	L4	22	LEU
41	L4	37	THR
41	L4	40	THR
41	L4	41	SER
41	L4	63	GLU
41	L4	74	ILE
41	L4	93	MET
41	L4	99	MET
41	L4	108	LYS
41	L4	124	SER
41	L4	133	SER
41	L4	138	ARG
41	L4	145	ILE
41	L4	147	GLU
41	L4	150	LEU
41	L4	152	VAL
41	L4	156	LEU
41	L4	172	VAL
41	L4	179	LEU
41	L4	182	LEU
41	L4	185	LYS
41	L4	186	LYS

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Mol	Chain	Res	Type
41	L4	187	LEU
41	L4	188	ARG
41	L4	193	LYS
41	L4	194	TYR
41	L4	200	THR
41	L4	203	ARG
41	L4	206	LEU
41	L4	220	ARG
41	L4	222	VAL
41	L4	230	VAL
41	L4	246	ARG
41	L4	258	LEU
41	L4	259	ASP
41	L4	267	VAL
41	L4	283	THR
41	L4	289	ILE
41	L4	292	SER
41	L4	293	SER
41	L4	295	ILE
41	L4	297	SER
41	L4	306	THR
41	L4	307	GLN
41	L4	308	LYS
41	L4	311	HIS
41	L4	323	VAL
41	L4	332	LYS
41	L4	333	VAL
41	L4	343	LYS
41	L4	346	LYS
41	L4	349	THR
41	L4	350	LYS
41	L4	354	VAL
41	L4	356	THR
41	L4	362	ASP
42	L5	5	LYS
42	L5	8	LYS
42	L5	17	GLN
42	L5	23	ARG
42	L5	34	LYS
42	L5	35	ARG
42	L5	41	LYS
42	L5	58	LYS

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Mol	Chain	Res	Type
42	L5	75	LEU
42	L5	85	ARG
42	L5	89	THR
42	L5	105	ILE
42	L5	109	THR
42	L5	115	LEU
42	L5	118	THR
42	L5	131	LEU
42	L5	137	ASP
42	L5	140	ARG
42	L5	146	LEU
42	L5	148	ILE
42	L5	152	ARG
42	L5	155	THR
42	L5	177	GLU
42	L5	185	PHE
42	L5	187	THR
42	L5	188	GLU
42	L5	189	GLU
42	L5	190	ILE
42	L5	216	GLU
42	L5	232	ASP
42	L5	234	ASP
42	L5	235	SER
42	L5	257	GLU
42	L5	263	GLU
42	L5	268	GLU
42	L5	273	ARG
42	L5	275	THR
42	L5	276	LYS
43	L6	5	LYS
43	L6	21	THR
43	L6	33	SER
43	L6	35	VAL
43	L6	41	ILE
43	L6	52	VAL
43	L6	56	LYS
43	L6	65	ILE
43	L6	78	ARG
43	L6	79	VAL
43	L6	89	THR
43	L6	90	LYS

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Mol	Chain	Res	Type
43	L6	93	VAL
43	L6	98	VAL
43	L6	99	GLU
43	L6	134	ARG
43	L6	143	LYS
43	L6	152	THR
43	L6	155	LEU
43	L6	160	SER
44	L7	24	GLU
44	L7	26	VAL
44	L7	43	ILE
44	L7	59	GLU
44	L7	60	ARG
44	L7	80	GLN
44	L7	88	ARG
44	L7	89	ILE
44	L7	92	ILE
44	L7	93	ASN
44	L7	98	LYS
44	L7	100	ARG
44	L7	110	ARG
44	L7	124	LEU
44	L7	158	LYS
44	L7	164	SER
44	L7	173	LEU
44	L7	175	LYS
44	L7	178	ILE
44	L7	179	LEU
44	L7	184	LEU
44	L7	207	LEU
44	L7	234	GLU
44	L7	238	LYS
44	L7	239	LEU
44	L7	244	ASN
45	L8	26	LEU
45	L8	27	THR
45	L8	41	GLN
45	L8	47	SER
45	L8	57	ARG
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN

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Mol	Chain	Res	Type
45	L8	92	LYS
45	L8	95	ASN
45	L8	101	THR
45	L8	106	LYS
45	L8	118	GLU
45	L8	132	VAL
45	L8	136	LEU
45	L8	145	ASN
45	L8	150	LEU
45	L8	156	ASP
45	L8	160	ILE
45	L8	163	VAL
45	L8	169	LEU
45	L8	181	LYS
45	L8	185	ARG
45	L8	204	ARG
45	L8	211	LEU
45	L8	219	ASP
45	L8	221	ASN
45	L8	238	LEU
45	L8	241	LYS
45	L8	246	MET
46	L9	5	GLN
46	L9	6	THR
46	L9	14	GLU
46	L9	19	SER
46	L9	20	ILE
46	L9	22	SER
46	L9	33	THR
46	L9	34	LEU
46	L9	36	LYS
46	L9	41	ILE
46	L9	48	VAL
46	L9	52	LEU
46	L9	62	ARG
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	80	THR
46	L9	82	VAL
46	L9	90	MET
46	L9	91	ARG

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Mol	Chain	Res	Type
46	L9	102	ASN
46	L9	107	ASP
46	L9	114	VAL
46	L9	121	LYS
46	L9	124	ARG
46	L9	132	VAL
46	L9	133	THR
46	L9	135	GLU
46	L9	138	THR
46	L9	139	ASN
46	L9	141	LYS
46	L9	149	ASN
46	L9	151	VAL
46	L9	155	SER
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	164	ILE
46	L9	168	ARG
46	L9	172	ILE
46	L9	173	ARG
46	L9	188	THR
46	L9	189	GLU
47	M0	3	ARG
47	M0	7	ARG
47	M0	21	ARG
47	M0	24	ARG
47	M0	26	VAL
47	M0	28	ASP
47	M0	30	LYS
47	M0	31	ILE
47	M0	32	ARG
47	M0	33	ILE
47	M0	39	LYS
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	57	LEU
47	M0	63	GLU
47	M0	74	LYS
47	M0	87	LEU
47	M0	102	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
47	M0	128	ARG
47	M0	130	ASP
47	M0	138	VAL
47	M0	139	ARG
47	M0	145	LYS
47	M0	147	VAL
47	M0	156	ARG
47	M0	163	GLN
47	M0	164	LYS
47	M0	165	ILE
47	M0	169	LYS
47	M0	174	THR
47	M0	176	LEU
47	M0	177	ASP
47	M0	178	ARG
47	M0	189	GLU
47	M0	192	ASP
47	M0	203	LYS
47	M0	205	SER
48	M1	6	GLN
48	M1	9	MET
48	M1	10	ARG
48	M1	11	ASP
48	M1	12	LEU
48	M1	13	LYS
48	M1	19	LEU
48	M1	20	ASN
48	M1	22	SER
48	M1	23	VAL
48	M1	31	THR
48	M1	34	SER
48	M1	40	LEU
48	M1	44	THR
48	M1	46	VAL
48	M1	52	TYR
48	M1	56	THR
48	M1	63	GLU
48	M1	70	THR
48	M1	80	LEU
48	M1	82	ARG
48	M1	94	ARG
48	M1	99	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	M1	106	ILE
48	M1	107	ASP
48	M1	108	GLU
48	M1	112	LEU
48	M1	115	LYS
48	M1	130	VAL
48	M1	137	ARG
48	M1	140	ARG
48	M1	142	LYS
48	M1	155	THR
48	M1	158	ASP
48	M1	166	LYS
48	M1	168	ASP
48	M1	171	VAL
48	M1	173	ASP
49	M3	23	LYS
49	M3	24	VAL
49	M3	34	SER
49	M3	35	ARG
49	M3	41	THR
49	M3	54	LEU
49	M3	55	ARG
49	M3	57	VAL
49	M3	59	ARG
49	M3	67	ARG
49	M3	70	ARG
49	M3	85	LEU
49	M3	86	THR
49	M3	100	ARG
49	M3	106	GLN
49	M3	107	GLU
49	M3	108	ILE
49	M3	117	LYS
49	M3	121	SER
49	M3	124	ILE
49	M3	131	LYS
49	M3	136	GLU
49	M3	138	VAL
49	M3	144	THR
49	M3	154	VAL
49	M3	168	ARG
49	M3	169	THR

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Mol	Chain	Res	Type
49	M3	171	ARG
49	M3	190	LYS
49	M3	194	GLU
50	M4	5	SER
50	M4	8	LYS
50	M4	13	ARG
50	M4	25	LYS
50	M4	37	GLU
50	M4	38	ILE
50	M4	40	ASP
50	M4	43	LYS
50	M4	53	VAL
50	M4	55	ARG
50	M4	62	GLN
50	M4	63	VAL
50	M4	64	VAL
50	M4	72	LEU
50	M4	74	ARG
50	M4	90	VAL
50	M4	91	CYS
50	M4	102	LYS
50	M4	108	ARG
50	M4	135	LEU
51	M5	7	LEU
51	M5	10	LEU
51	M5	22	LEU
51	M5	35	VAL
51	M5	38	ARG
51	M5	46	ASP
51	M5	57	GLN
51	M5	68	ARG
51	M5	71	ARG
51	M5	80	THR
51	M5	83	LYS
51	M5	85	THR
51	M5	93	LYS
51	M5	96	ARG
51	M5	97	SER
51	M5	105	ARG
51	M5	109	ARG
51	M5	113	LEU
51	M5	117	ASN

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Mol	Chain	Res	Type
51	M5	133	ILE
51	M5	138	GLN
51	M5	142	ILE
51	M5	144	ARG
51	M5	151	ILE
51	M5	153	ASP
51	M5	155	VAL
51	M5	157	LYS
51	M5	159	ARG
51	M5	167	THR
51	M5	170	LYS
51	M5	182	ASN
51	M5	183	THR
51	M5	187	ARG
51	M5	190	THR
51	M5	196	THR
51	M5	197	LEU
52	M6	25	LYS
52	M6	34	VAL
52	M6	36	VAL
52	M6	41	LEU
52	M6	44	SER
52	M6	46	GLU
52	M6	51	LYS
52	M6	58	LEU
52	M6	68	ARG
52	M6	77	SER
52	M6	78	ARG
52	M6	84	LEU
52	M6	85	ARG
52	M6	103	LYS
52	M6	106	GLU
52	M6	110	PRO
52	M6	116	LYS
52	M6	117	ARG
52	M6	119	VAL
52	M6	124	LEU
52	M6	128	ARG
52	M6	129	LEU
52	M6	143	THR
52	M6	170	LYS
52	M6	175	THR

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Mol	Chain	Res	Type
52	M6	182	ASN
52	M6	189	ASP
52	M6	190	VAL
53	M7	3	ARG
53	M7	7	THR
53	M7	9	THR
53	M7	10	ASN
53	M7	14	SER
53	M7	16	SER
53	M7	23	ARG
53	M7	24	VAL
53	M7	32	THR
53	M7	36	ILE
53	M7	41	LEU
53	M7	52	LEU
53	M7	53	ASP
53	M7	65	SER
53	M7	67	ILE
53	M7	69	ARG
53	M7	87	SER
53	M7	112	LEU
53	M7	114	VAL
53	M7	119	VAL
53	M7	120	ASN
53	M7	126	ARG
53	M7	127	ARG
53	M7	128	ARG
53	M7	138	LYS
53	M7	142	SER
53	M7	144	SER
53	M7	152	GLU
53	M7	153	LYS
53	M7	157	VAL
53	M7	169	THR
53	M7	180	LYS
53	M7	181	ARG
53	M7	182	ILE
54	M8	3	ILE
54	M8	21	SER
54	M8	22	ASP
54	M8	24	VAL
54	M8	26	LEU

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Mol	Chain	Res	Type
54	M8	32	LEU
54	M8	46	LYS
54	M8	49	LEU
54	M8	55	SER
54	M8	57	ILE
54	M8	63	SER
54	M8	73	GLN
54	M8	74	GLU
54	M8	80	THR
54	M8	93	ILE
54	M8	95	GLU
54	M8	99	THR
54	M8	100	THR
54	M8	105	ARG
54	M8	129	VAL
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	150	VAL
54	M8	161	LYS
54	M8	168	THR
54	M8	178	ARG
54	M8	179	ARG
54	M8	180	ARG
55	M9	5	ARG
55	M9	31	GLU
55	M9	41	ILE
55	M9	46	LYS
55	M9	52	LYS
55	M9	55	VAL
55	M9	57	VAL
55	M9	60	LYS
55	M9	74	ARG
55	M9	81	ARG
55	M9	86	GLU
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	110	ARG
55	M9	115	ILE
55	M9	116	ASP
55	M9	134	HIS

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Mol	Chain	Res	Type
55	M9	135	LYS
55	M9	160	GLU
55	M9	176	ARG
55	M9	180	LYS
56	N0	1	MET
56	N0	8	GLN
56	N0	45	LEU
56	N0	51	VAL
56	N0	71	LYS
56	N0	81	TYR
56	N0	82	ASP
56	N0	85	SER
56	N0	87	THR
56	N0	92	LYS
56	N0	100	VAL
56	N0	105	THR
56	N0	113	ARG
56	N0	115	ARG
56	N0	122	HIS
56	N0	125	LYS
56	N0	130	GLU
56	N0	131	LYS
56	N0	132	THR
56	N0	137	ARG
56	N0	138	GLN
56	N0	142	GLN
56	N0	145	THR
56	N0	155	ARG
56	N0	156	VAL
56	N0	157	GLN
56	N0	160	THR
56	N0	162	THR
56	N0	166	LYS
57	N1	12	ARG
57	N1	26	HIS
57	N1	27	LEU
57	N1	55	LYS
57	N1	68	THR
57	N1	75	ILE
57	N1	79	MET
57	N1	83	ARG
57	N1	88	ARG

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Mol	Chain	Res	Type
57	N1	104	GLU
57	N1	106	LEU
57	N1	120	LYS
57	N1	122	GLN
57	N1	124	VAL
57	N1	126	VAL
57	N1	128	LEU
57	N1	136	ARG
57	N1	139	ARG
57	N1	141	VAL
57	N1	143	THR
57	N1	144	GLU
57	N1	149	GLN
57	N1	158	THR
57	N1	159	PHE
57	N1	160	ILE
58	N2	10	LYS
58	N2	11	ILE
58	N2	14	THR
58	N2	16	THR
58	N2	37	LEU
58	N2	38	ILE
58	N2	43	VAL
58	N2	52	ASN
58	N2	54	VAL
58	N2	55	THR
58	N2	58	GLU
58	N2	66	VAL
58	N2	70	LYS
58	N2	93	ILE
58	N2	100	THR
59	N3	9	THR
59	N3	13	ILE
59	N3	32	ARG
59	N3	44	SER
59	N3	45	ARG
59	N3	46	LEU
59	N3	48	ARG
59	N3	54	LEU
59	N3	64	LYS
59	N3	69	LEU
59	N3	73	VAL

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Mol	Chain	Res	Type
59	N3	74	MET
59	N3	83	LYS
59	N3	87	ARG
59	N3	96	GLU
59	N3	102	ILE
59	N3	125	LEU
59	N3	128	ARG
59	N3	135	VAL
59	N3	137	VAL
60	N4	4	GLU
60	N4	5	ILE
60	N4	19	THR
60	N4	27	LYS
60	N4	39	LEU
60	N4	47	ARG
60	N4	64	THR
61	N5	27	ARG
61	N5	33	ARG
61	N5	37	THR
61	N5	38	LEU
61	N5	39	LYS
61	N5	45	LYS
61	N5	59	SER
61	N5	63	ILE
61	N5	74	LYS
61	N5	86	VAL
61	N5	92	LYS
61	N5	96	LYS
61	N5	105	VAL
61	N5	108	LEU
61	N5	109	LYS
61	N5	113	LEU
61	N5	115	ARG
61	N5	125	ARG
61	N5	127	THR
61	N5	134	ASP
61	N5	135	ILE
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS
62	N6	5	SER
62	N6	10	SER

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Mol	Chain	Res	Type
62	N6	13	ARG
62	N6	36	SER
62	N6	37	LYS
62	N6	38	GLU
62	N6	50	ILE
62	N6	55	GLU
62	N6	56	VAL
62	N6	57	LEU
62	N6	63	LYS
62	N6	70	ILE
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	83	ASP
62	N6	94	SER
62	N6	105	VAL
62	N6	115	ARG
62	N6	127	GLU
63	N7	9	LYS
63	N7	14	VAL
63	N7	24	VAL
63	N7	26	VAL
63	N7	35	SER
63	N7	46	ILE
63	N7	52	LYS
63	N7	53	VAL
63	N7	60	LYS
63	N7	72	ILE
63	N7	75	VAL
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	87	LEU
63	N7	99	GLU
63	N7	107	ARG
63	N7	108	GLU
63	N7	109	GLU
63	N7	121	ARG
63	N7	123	GLN
63	N7	134	LEU
63	N7	136	PHE
64	N8	6	THR

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Mol	Chain	Res	Type
64	N8	8	THR
64	N8	16	SER
64	N8	29	PRO
64	N8	34	MET
64	N8	42	ARG
64	N8	46	ASP
64	N8	47	LYS
64	N8	56	VAL
64	N8	60	TYR
64	N8	73	LEU
64	N8	78	LEU
64	N8	84	GLU
64	N8	91	LEU
64	N8	98	THR
64	N8	115	LYS
64	N8	123	VAL
64	N8	130	VAL
64	N8	133	LEU
64	N8	135	GLU
64	N8	139	ARG
65	N9	13	THR
65	N9	14	ARG
65	N9	23	LYS
65	N9	25	LYS
65	N9	28	LYS
65	N9	33	LYS
65	N9	50	THR
65	N9	59	LYS
66	O0	10	ILE
66	O0	12	GLN
66	O0	14	LEU
66	O0	16	LEU
66	O0	18	ILE
66	O0	34	LEU
66	O0	36	GLN
66	O0	40	LYS
66	O0	52	ARG
66	O0	61	MET
66	O0	65	THR
66	O0	66	LYS
66	O0	76	GLU
66	O0	83	LYS

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Mol	Chain	Res	Type
66	O0	86	ARG
66	O0	100	ILE
66	O0	101	LEU
66	O0	102	THR
67	O1	6	ASP
67	O1	8	VAL
67	O1	13	THR
67	O1	16	LEU
67	O1	24	SER
67	O1	26	LYS
67	O1	36	ILE
67	O1	42	LEU
67	O1	47	ASP
67	O1	64	VAL
67	O1	68	GLU
67	O1	73	LEU
67	O1	79	ARG
67	O1	84	ASP
67	O1	106	THR
67	O1	110	GLU
68	O2	3	SER
68	O2	18	LYS
68	O2	19	ARG
68	O2	33	ARG
68	O2	34	LYS
68	O2	35	GLN
68	O2	36	LYS
68	O2	41	VAL
68	O2	51	SER
68	O2	52	GLN
68	O2	54	LYS
68	O2	61	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	82	LEU
68	O2	84	THR
68	O2	90	LYS
68	O2	103	LYS
68	O2	109	LEU
68	O2	125	ARG
68	O2	126	LEU
68	O2	128	LEU

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Mol	Chain	Res	Type
69	O3	14	LEU
69	O3	15	SER
69	O3	37	THR
69	O3	48	ARG
69	O3	59	VAL
69	O3	60	ARG
69	O3	70	LYS
69	O3	81	VAL
69	O3	98	VAL
69	O3	106	ASN
70	O4	3	GLN
70	O4	8	ARG
70	O4	16	ARG
70	O4	20	ILE
70	O4	21	LYS
70	O4	24	LYS
70	O4	29	ILE
70	O4	51	LEU
70	O4	58	ARG
70	O4	65	VAL
70	O4	68	THR
70	O4	69	HIS
70	O4	71	THR
70	O4	73	SER
70	O4	81	CYS
70	O4	86	LYS
70	O4	103	LYS
70	O4	104	VAL
71	O5	4	VAL
71	O5	15	GLU
71	O5	21	LEU
71	O5	38	ARG
71	O5	41	LEU
71	O5	43	LYS
71	O5	45	LYS
71	O5	46	THR
71	O5	48	ARG
71	O5	49	LYS
71	O5	50	SER
71	O5	68	GLN
71	O5	71	LYS
71	O5	81	ARG

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Mol	Chain	Res	Type
71	O5	84	LYS
71	O5	85	THR
71	O5	89	ARG
71	O5	90	ARG
71	O5	93	THR
71	O5	100	VAL
71	O5	101	THR
71	O5	102	GLU
71	O5	105	ARG
71	O5	107	LYS
71	O5	111	PHE
71	O5	119	LYS
72	O6	11	LEU
72	O6	17	VAL
72	O6	18	THR
72	O6	20	MET
72	O6	21	THR
72	O6	25	LYS
72	O6	26	ILE
72	O6	29	LYS
72	O6	34	SER
72	O6	45	ARG
72	O6	56	ARG
72	O6	57	LEU
72	O6	58	ILE
72	O6	59	ASP
72	O6	68	ARG
72	O6	76	ARG
72	O6	81	THR
72	O6	88	GLU
72	O6	98	ARG
72	O6	99	ARG
73	O7	5	THR
73	O7	17	THR
73	O7	19	CYS
73	O7	24	ARG
73	O7	25	ARG
73	O7	33	THR
73	O7	36	SER
73	O7	44	THR
73	O7	54	LYS
73	O7	55	ARG

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Mol	Chain	Res	Type
73	O7	58	THR
73	O7	59	THR
73	O7	65	ARG
73	O7	75	LYS
73	O7	79	GLN
73	O7	82	SER
73	O7	84	SER
73	O7	85	LYS
74	O8	8	ILE
74	O8	12	LEU
74	O8	22	THR
74	O8	24	THR
74	O8	29	LYS
74	O8	32	ASN
74	O8	41	THR
74	O8	45	VAL
74	O8	46	ARG
74	O8	51	LEU
74	O8	52	TYR
74	O8	53	THR
74	O8	54	LEU
74	O8	58	ASP
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	77	ARG
74	O8	78	LEU
75	O9	5	LYS
75	O9	21	ARG
75	O9	23	LEU
75	O9	25	GLN
75	O9	28	ARG
75	O9	29	LEU
75	O9	48	LYS
75	O9	51	ILE
76	Q0	85	LEU
76	Q0	92	ASP
76	Q0	93	LYS
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	127	LEU
77	Q1	1	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
77	Q1	6	ARG
77	Q1	9	ARG
77	Q1	11	ARG
77	Q1	13	LEU
77	Q1	16	LYS
77	Q1	17	ARG
77	Q1	19	LYS
77	Q1	24	SER
78	Q2	4	VAL
78	Q2	8	ARG
78	Q2	13	LYS
78	Q2	21	THR
78	Q2	22	GLN
78	Q2	26	THR
78	Q2	45	ARG
78	Q2	47	GLN
78	Q2	48	SER
78	Q2	61	LYS
78	Q2	78	LYS
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	93	LEU
78	Q2	100	LYS
78	Q2	104	LEU
79	Q3	5	THR
79	Q3	11	THR
79	Q3	16	VAL
79	Q3	25	GLN
79	Q3	32	GLN
79	Q3	45	LYS
79	Q3	46	THR
79	Q3	56	THR
79	Q3	59	CYS
79	Q3	60	CYS
79	Q3	64	VAL
79	Q3	70	THR
79	Q3	73	THR
79	Q3	84	ARG
79	Q3	90	VAL
79	Q3	91	GLU
2	s0	10	THR
2	s0	12	GLU

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Mol	Chain	Res	Type
2	s0	18	LEU
2	s0	22	THR
2	s0	30	GLN
2	s0	34	GLU
2	s0	37	VAL
2	s0	41	ARG
2	s0	45	VAL
2	s0	50	VAL
2	s0	59	LEU
2	s0	62	ARG
2	s0	72	ASP
2	s0	87	LEU
2	s0	88	LYS
2	s0	93	THR
2	s0	96	THR
2	s0	101	ARG
2	s0	106	SER
2	s0	110	TYR
2	s0	111	ILE
2	s0	112	THR
2	s0	123	VAL
2	s0	131	GLN
2	s0	154	GLU
2	s0	158	VAL
2	s0	172	LEU
2	s0	179	ARG
2	s0	183	ARG
2	s0	184	LEU
2	s0	185	ARG
2	s0	189	VAL
2	s0	191	ARG
2	s0	198	MET
2	s0	202	TYR
3	s1	21	VAL
3	s1	25	THR
3	s1	37	THR
3	s1	47	LEU
3	s1	62	LYS
3	s1	70	LEU
3	s1	73	LEU
3	s1	74	GLN
3	s1	78	ASP

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Mol	Chain	Res	Type
3	s1	81	PHE
3	s1	83	LYS
3	s1	89	ASP
3	s1	90	GLU
3	s1	97	LEU
3	s1	105	PHE
3	s1	108	ASP
3	s1	114	VAL
3	s1	120	LEU
3	s1	131	ASP
3	s1	137	ILE
3	s1	146	GLN
3	s1	152	ARG
3	s1	159	SER
3	s1	169	SER
3	s1	173	THR
3	s1	177	GLN
3	s1	181	LEU
3	s1	183	GLN
3	s1	184	LEU
3	s1	193	ILE
3	s1	195	LYS
3	s1	197	ILE
3	s1	202	LYS
3	s1	206	PRO
3	s1	212	VAL
3	s1	214	LYS
3	s1	219	LYS
3	s1	222	LYS
3	s1	223	PHE
3	s1	228	LEU
3	s1	231	LEU
4	s2	41	LEU
4	s2	46	LYS
4	s2	51	THR
4	s2	52	THR
4	s2	53	ILE
4	s2	58	LEU
4	s2	60	SER
4	s2	61	LEU
4	s2	69	ILE
4	s2	73	LEU

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Mol	Chain	Res	Type
4	s2	77	GLN
4	s2	78	ASP
4	s2	80	VAL
4	s2	82	ASN
4	s2	83	ILE
4	s2	87	GLN
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	95	ARG
4	s2	96	THR
4	s2	106	ASP
4	s2	111	VAL
4	s2	113	LEU
4	s2	117	THR
4	s2	141	ARG
4	s2	146	THR
4	s2	148	LEU
4	s2	150	GLN
4	s2	159	THR
4	s2	164	SER
4	s2	166	THR
4	s2	170	ILE
4	s2	179	VAL
4	s2	185	LYS
4	s2	186	LYS
4	s2	199	GLN
4	s2	206	THR
4	s2	207	LEU
4	s2	222	TYR
4	s2	225	LEU
4	s2	229	LEU
4	s2	245	ASP
5	s3	4	LEU
5	s3	6	SER
5	s3	7	LYS
5	s3	9	ARG
5	s3	21	LEU
5	s3	23	GLU
5	s3	26	THR
5	s3	44	THR
5	s3	49	ILE

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Mol	Chain	Res	Type
5	s3	53	THR
5	s3	56	GLN
5	s3	61	GLU
5	s3	64	ARG
5	s3	69	LEU
5	s3	84	ILE
5	s3	90	ARG
5	s3	103	GLU
5	s3	115	ILE
5	s3	116	ARG
5	s3	120	TYR
5	s3	128	GLU
5	s3	129	SER
5	s3	139	SER
5	s3	142	LEU
5	s3	158	ILE
5	s3	162	GLN
5	s3	164	VAL
5	s3	166	ASP
5	s3	169	ASP
5	s3	172	THR
5	s3	176	LEU
5	s3	178	ARG
5	s3	189	MET
5	s3	202	LEU
5	s3	210	GLU
5	s3	212	LYS
5	s3	213	GLU
5	s3	223	LYS
6	s4	6	LYS
6	s4	9	LEU
6	s4	12	LEU
6	s4	23	LEU
6	s4	29	PRO
6	s4	37	LYS
6	s4	38	LEU
6	s4	42	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	69	HIS
6	s4	70	VAL
6	s4	72	VAL

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Mol	Chain	Res	Type
6	s4	93	ASP
6	s4	95	THR
6	s4	98	ASN
6	s4	102	VAL
6	s4	113	ARG
6	s4	115	THR
6	s4	116	ASP
6	s4	146	THR
6	s4	148	ARG
6	s4	159	THR
6	s4	160	VAL
6	s4	164	LEU
6	s4	170	THR
6	s4	176	ASP
6	s4	180	LEU
6	s4	182	TYR
6	s4	187	ARG
6	s4	196	VAL
6	s4	219	VAL
6	s4	221	ARG
6	s4	222	LEU
6	s4	227	VAL
6	s4	233	LYS
6	s4	252	ARG
6	s4	259	GLN
7	s5	23	VAL
7	s5	24	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	41	LYS
7	s5	43	PHE
7	s5	45	LYS
7	s5	58	LEU
7	s5	63	GLN
7	s5	66	GLN
7	s5	68	ILE
7	s5	76	ARG
7	s5	83	ARG
7	s5	84	LYS
7	s5	89	ILE
7	s5	93	LEU
7	s5	109	LYS

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Mol	Chain	Res	Type
7	s5	119	ASP
7	s5	125	THR
7	s5	128	ASN
7	s5	146	THR
7	s5	148	ARG
7	s5	157	ARG
7	s5	160	VAL
7	s5	163	SER
7	s5	166	ARG
7	s5	167	ARG
7	s5	170	GLN
7	s5	190	ILE
7	s5	194	LEU
7	s5	203	LYS
7	s5	206	SER
7	s5	216	GLU
8	s6	15	THR
8	s6	31	ARG
8	s6	69	LEU
8	s6	71	THR
8	s6	73	ILE
8	s6	76	LEU
8	s6	78	THR
8	s6	79	LYS
8	s6	89	ASP
8	s6	93	LYS
8	s6	96	SER
8	s6	108	VAL
8	s6	109	LEU
8	s6	111	LEU
8	s6	112	VAL
8	s6	121	LEU
8	s6	122	GLU
8	s6	126	ASP
8	s6	127	THR
8	s6	129	VAL
8	s6	143	LYS
8	s6	151	ASP
8	s6	156	PHE
8	s6	157	VAL
8	s6	162	VAL
8	s6	164	LYS

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Mol	Chain	Res	Type
8	s6	166	GLU
8	s6	170	THR
8	s6	171	LYS
8	s6	179	VAL
8	s6	193	LEU
8	s6	207	GLU
8	s6	212	LEU
8	s6	215	ARG
8	s6	216	LEU
9	s7	5	GLN
9	s7	9	LEU
9	s7	10	SER
9	s7	11	GLN
9	s7	14	THR
9	s7	16	LEU
9	s7	17	GLU
9	s7	18	LEU
9	s7	26	GLU
9	s7	33	GLU
9	s7	44	LYS
9	s7	49	ILE
9	s7	51	VAL
9	s7	58	LEU
9	s7	60	ILE
9	s7	62	VAL
9	s7	67	LEU
9	s7	77	LEU
9	s7	97	ARG
9	s7	110	GLN
9	s7	112	ARG
9	s7	114	ARG
9	s7	116	ARG
9	s7	117	THR
9	s7	126	LEU
9	s7	143	LEU
9	s7	149	ILE
9	s7	157	LYS
9	s7	166	LEU
9	s7	185	ILE
10	s8	7	SER
10	s8	10	LYS
10	s8	12	SER

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Mol	Chain	Res	Type
10	s8	18	ARG
10	s8	20	GLN
10	s8	22	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	41	LYS
10	s8	46	VAL
10	s8	58	LEU
10	s8	59	ARG
10	s8	62	THR
10	s8	73	SER
10	s8	76	THR
10	s8	77	ARG
10	s8	82	VAL
10	s8	89	GLU
10	s8	107	THR
10	s8	110	ARG
10	s8	117	TYR
10	s8	119	GLN
10	s8	120	THR
10	s8	121	LEU
10	s8	140	GLU
10	s8	141	ARG
10	s8	151	LYS
10	s8	155	SER
10	s8	183	ILE
10	s8	185	GLU
10	s8	197	THR
11	s9	3	ARG
11	s9	6	ARG
11	s9	7	THR
11	s9	16	LYS
11	s9	21	SER
11	s9	22	SER
11	s9	28	LEU
11	s9	39	LYS
11	s9	45	ILE
11	s9	78	ARG
11	s9	81	VAL
11	s9	82	ARG
11	s9	89	ASP
11	s9	90	LYS

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Mol	Chain	Res	Type
11	s9	93	LEU
11	s9	96	VAL
11	s9	101	VAL
11	s9	105	LEU
11	s9	109	LEU
11	s9	111	THR
11	s9	122	VAL
11	s9	126	ARG
11	s9	130	THR
11	s9	133	HIS
11	s9	134	ILE
11	s9	142	ASN
11	s9	152	SER
11	s9	154	LYS
11	s9	161	THR
11	s9	168	ARG
11	s9	172	VAL
11	s9	175	ARG
11	s9	180	LYS
11	s9	182	GLU
12	c0	2	LEU
12	c0	15	LEU
12	c0	20	VAL
12	c0	22	VAL
12	c0	28	ASN
12	c0	37	THR
12	c0	40	LEU
12	c0	55	VAL
12	c0	57	THR
12	c0	67	THR
12	c0	71	GLU
12	c0	73	VAL
13	c1	5	LEU
13	c1	21	ASN
13	c1	31	THR
13	c1	32	LYS
13	c1	40	LEU
13	c1	44	THR
13	c1	47	THR
13	c1	60	PHE
13	c1	64	VAL
13	c1	67	ARG

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Mol	Chain	Res	Type
13	c1	74	THR
13	c1	76	VAL
13	c1	77	SER
13	c1	82	ARG
13	c1	86	ILE
13	c1	118	GLN
13	c1	129	ARG
13	c1	138	ASN
13	c1	140	VAL
13	c1	141	LYS
14	c2	28	LEU
14	c2	30	VAL
14	c2	36	LEU
14	c2	38	HIS
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	86	VAL
14	c2	89	ILE
14	c2	97	LEU
14	c2	103	LEU
14	c2	116	VAL
14	c2	120	VAL
14	c2	121	VAL
14	c2	126	TRP
14	c2	132	GLU
14	c2	136	ILE
14	c2	137	MET
14	c2	138	GLU
14	c2	140	PHE
15	c3	12	SER
15	c3	14	SER
15	c3	16	ILE
15	c3	20	ARG
15	c3	46	THR
15	c3	66	ILE
15	c3	70	LYS
15	c3	72	MET

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Mol	Chain	Res	Type
15	c3	75	LEU
15	c3	80	LEU
15	c3	84	ILE
15	c3	87	ASP
15	c3	88	LEU
15	c3	97	SER
15	c3	102	LEU
15	c3	115	LEU
15	c3	125	LEU
15	c3	127	ARG
15	c3	134	VAL
15	c3	138	ASN
15	c3	149	LEU
15	c3	150	VAL
15	c3	151	ASN
16	c4	13	VAL
16	c4	14	PHE
16	c4	18	ARG
16	c4	20	TYR
16	c4	22	SER
16	c4	23	PHE
16	c4	26	THR
16	c4	28	VAL
16	c4	39	ILE
16	c4	49	LYS
16	c4	51	ASP
16	c4	52	ARG
16	c4	70	LYS
16	c4	76	ILE
16	c4	81	VAL
16	c4	84	ARG
16	c4	92	LYS
16	c4	102	LEU
16	c4	114	ARG
16	c4	119	THR
16	c4	121	VAL
16	c4	124	ASP
16	c4	127	ARG
16	c4	132	ARG
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU

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Mol	Chain	Res	Type
17	c5	10	ARG
17	c5	12	PHE
17	c5	22	LEU
17	c5	27	GLU
17	c5	28	MET
17	c5	35	LYS
17	c5	36	LEU
17	c5	49	MET
17	c5	52	LYS
17	c5	61	ARG
17	c5	69	GLU
17	c5	71	GLU
17	c5	77	ARG
17	c5	92	SER
17	c5	97	TYR
17	c5	110	GLU
17	c5	121	ILE
17	c5	122	THR
17	c5	124	THR
17	c5	127	ARG
18	c6	23	LYS
18	c6	28	LEU
18	c6	37	THR
18	c6	43	ILE
18	c6	48	VAL
18	c6	53	LEU
18	c6	54	LEU
18	c6	55	VAL
18	c6	57	LEU
18	c6	68	ARG
18	c6	69	VAL
18	c6	70	THR
18	c6	81	ILE
18	c6	83	GLN
18	c6	94	GLN
18	c6	106	LYS
18	c6	110	THR
18	c6	113	ASP
18	c6	115	THR
18	c6	118	ILE
18	c6	137	ARG
18	c6	143	ARG

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Mol	Chain	Res	Type
19	c7	3	ARG
19	c7	5	ARG
19	c7	6	THR
19	c7	8	THR
19	c7	25	THR
19	c7	34	LEU
19	c7	38	ILE
19	c7	46	LEU
19	c7	47	ARG
19	c7	49	LYS
19	c7	62	GLN
19	c7	69	ILE
19	c7	74	GLN
19	c7	83	GLN
19	c7	85	VAL
19	c7	87	GLU
19	c7	106	THR
19	c7	107	SER
19	c7	110	VAL
19	c7	113	LEU
20	c8	2	SER
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	8	GLN
20	c8	13	HIS
20	c8	15	LEU
20	c8	20	THR
20	c8	25	ASN
20	c8	26	ILE
20	c8	28	ILE
20	c8	33	THR
20	c8	36	LYS
20	c8	38	VAL
20	c8	40	ARG
20	c8	57	ARG
20	c8	61	LEU
20	c8	63	GLN
20	c8	80	LYS
20	c8	85	PHE
20	c8	105	VAL

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Mol	Chain	Res	Type
20	c8	106	GLU
20	c8	110	ARG
20	c8	116	LEU
20	c8	119	ILE
20	c8	136	GLN
20	c8	138	THR
20	c8	144	ARG
20	c8	145	ARG
21	c9	6	VAL
21	c9	13	ASP
21	c9	28	LEU
21	c9	29	GLU
21	c9	35	ASP
21	c9	51	GLU
21	c9	57	ARG
21	c9	68	ARG
21	c9	75	LYS
21	c9	84	LYS
21	c9	86	ARG
21	c9	88	VAL
21	c9	111	ILE
21	c9	115	GLU
21	c9	123	ARG
21	c9	126	GLU
21	c9	133	ASP
21	c9	139	THR
21	c9	140	LEU
21	c9	141	GLU
21	c9	142	GLU
22	d0	16	GLN
22	d0	23	ARG
22	d0	25	THR
22	d0	27	THR
22	d0	30	LYS
22	d0	31	VAL
22	d0	34	LEU
22	d0	44	ASN
22	d0	47	GLN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	63	LEU

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Mol	Chain	Res	Type
22	d0	66	SER
22	d0	70	THR
22	d0	72	ASN
22	d0	74	GLU
22	d0	88	LYS
22	d0	92	ASP
22	d0	99	ILE
22	d0	103	ILE
22	d0	107	THR
22	d0	108	ILE
22	d0	113	ASP
22	d0	116	VAL
22	d0	121	ASN
23	d1	1	MET
23	d1	2	GLU
23	d1	5	LYS
23	d1	10	GLU
23	d1	32	VAL
23	d1	49	GLU
23	d1	52	THR
23	d1	68	SER
23	d1	69	LEU
23	d1	74	GLN
23	d1	78	LEU
23	d1	86	SER
24	d2	2	THR
24	d2	6	VAL
24	d2	7	LEU
24	d2	22	LYS
24	d2	23	ARG
24	d2	25	VAL
24	d2	26	LEU
24	d2	68	ARG
24	d2	74	VAL
24	d2	93	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	105	THR
24	d2	119	LYS
24	d2	122	SER
24	d2	124	LYS
25	d3	9	LEU

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Mol	Chain	Res	Type
25	d3	16	ARG
25	d3	18	HIS
25	d3	19	ARG
25	d3	23	ARG
25	d3	31	LYS
25	d3	36	THR
25	d3	40	SER
25	d3	72	VAL
25	d3	73	ARG
25	d3	75	GLN
25	d3	84	THR
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	112	LYS
25	d3	121	ARG
25	d3	123	LYS
25	d3	131	SER
25	d3	133	LEU
25	d3	144	ARG
26	d4	5	VAL
26	d4	6	THR
26	d4	10	ARG
26	d4	13	ILE
26	d4	22	GLN
26	d4	26	ASP
26	d4	36	SER
26	d4	42	GLU
26	d4	43	LYS
26	d4	46	GLU
26	d4	47	VAL
26	d4	49	LYS
26	d4	62	THR
26	d4	77	ASN
26	d4	78	SER
26	d4	88	THR
26	d4	100	VAL
26	d4	116	LYS
26	d4	133	ASN
27	d5	48	ASP
27	d5	51	LEU
27	d5	60	VAL

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Mol	Chain	Res	Type
27	d5	61	SER
27	d5	62	VAL
27	d5	71	ILE
27	d5	81	ARG
27	d5	88	ILE
27	d5	90	LYS
27	d5	97	LYS
28	d6	4	LYS
28	d6	10	ARG
28	d6	12	LYS
28	d6	15	ARG
28	d6	18	VAL
28	d6	25	ASN
28	d6	28	LYS
28	d6	33	ASP
28	d6	39	MET
28	d6	44	ILE
28	d6	46	GLU
28	d6	51	ARG
28	d6	67	THR
28	d6	82	ARG
28	d6	85	ARG
28	d6	88	SER
28	d6	90	GLU
29	d7	3	LEU
29	d7	25	VAL
29	d7	36	LYS
29	d7	37	CYS
29	d7	41	LEU
29	d7	43	ILE
29	d7	52	THR
29	d7	63	LEU
29	d7	75	GLU
29	d7	77	THR
30	d8	22	ARG
30	d8	26	THR
30	d8	32	PHE
30	d8	33	LEU
30	d8	40	ILE
30	d8	45	LYS
30	d8	52	ASP
30	d8	54	LEU

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Mol	Chain	Res	Type
30	d8	58	GLU
30	d8	64	ARG
31	d9	6	VAL
31	d9	10	HIS
31	d9	19	ARG
31	d9	26	SER
31	d9	30	LEU
31	d9	32	ARG
31	d9	36	LEU
31	d9	38	ILE
31	d9	54	LYS
80	e0	13	LYS
80	e0	14	VAL
80	e0	21	VAL
80	e0	22	GLU
80	e0	26	LYS
80	e0	36	LYS
80	e0	41	THR
80	e0	45	VAL
80	e0	46	ASN
80	e0	49	LEU
80	e0	55	ARG
80	e0	56	MET
33	e1	80	ARG
33	e1	84	VAL
33	e1	87	THR
33	e1	90	LYS
33	e1	96	LYS
33	e1	100	LEU
33	e1	106	TYR
33	e1	109	ASP
33	e1	113	LYS
33	e1	115	THR
33	e1	118	ARG
33	e1	125	THR
33	e1	135	HIS
33	e1	147	VAL
33	e1	150	VAL
33	e1	151	ASN
34	sR	3	SER
34	sR	4	ASN
34	sR	8	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	sR	16	HIS
34	sR	21	THR
34	sR	23	LEU
34	sR	25	THR
34	sR	29	GLN
34	sR	42	LEU
34	sR	52	GLN
34	sR	66	HIS
34	sR	76	ASP
34	sR	96	THR
34	sR	145	LEU
34	sR	149	ASP
34	sR	152	SER
34	sR	176	LYS
34	sR	178	VAL
34	sR	188	ILE
34	sR	210	LEU
34	sR	232	TYR
34	sR	258	THR
34	sR	266	ASP
34	sR	275	ARG
34	sR	283	LYS
34	sR	286	GLU
34	sR	297	ASP
34	sR	299	GLN
34	sR	308	ASN
35	sM	23	LYS
35	sM	28	SER
35	sM	34	LYS
35	sM	41	SER
35	sM	43	ASP
35	sM	45	SER
35	sM	48	ARG
35	sM	53	ARG
35	sM	61	ILE
35	sM	64	LYS
35	sM	71	ASN
35	sM	74	LYS
35	sM	77	THR
39	l2	15	ILE
39	l2	23	ARG
39	l2	29	LEU

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Mol	Chain	Res	Type
39	12	30	ARG
39	12	32	LEU
39	12	44	ILE
39	12	48	ILE
39	12	49	VAL
39	12	61	VAL
39	12	62	VAL
39	12	70	ARG
39	12	74	GLU
39	12	80	GLU
39	12	82	VAL
39	12	101	VAL
39	12	104	LEU
39	12	112	ILE
39	12	132	ASN
39	12	137	ILE
39	12	142	ASP
39	12	158	ILE
39	12	168	VAL
39	12	179	LEU
39	12	180	LEU
39	12	193	ARG
39	12	200	ARG
39	12	204	MET
39	12	205	ASN
39	12	206	PRO
39	12	230	VAL
39	12	243	THR
39	12	246	LEU
39	12	249	SER
39	12	251	LYS
40	13	3	HIS
40	13	4	ARG
40	13	10	ARG
40	13	17	LEU
40	13	19	ARG
40	13	20	LYS
40	13	25	ILE
40	13	30	LYS
40	13	37	ARG
40	13	44	THR
40	13	47	LEU

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Mol	Chain	Res	Type
40	l3	55	THR
40	l3	56	ILE
40	l3	69	LYS
40	l3	70	ARG
40	l3	77	THR
40	l3	81	THR
40	l3	85	VAL
40	l3	90	VAL
40	l3	103	THR
40	l3	113	GLU
40	l3	114	VAL
40	l3	120	LYS
40	l3	125	SER
40	l3	128	LYS
40	l3	139	GLN
40	l3	145	GLU
40	l3	146	ARG
40	l3	148	LEU
40	l3	150	ARG
40	l3	157	VAL
40	l3	160	VAL
40	l3	167	ARG
40	l3	169	THR
40	l3	183	LEU
40	l3	192	VAL
40	l3	202	THR
40	l3	205	VAL
40	l3	208	VAL
40	l3	213	GLU
40	l3	215	ILE
40	l3	222	LYS
40	l3	232	ARG
40	l3	235	THR
40	l3	238	LEU
40	l3	248	LYS
40	l3	249	VAL
40	l3	252	ILE
40	l3	256	HIS
40	l3	266	ARG
40	l3	274	SER
40	l3	284	ARG
40	l3	287	LYS

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Mol	Chain	Res	Type
40	l3	293	ASN
40	l3	301	THR
40	l3	304	THR
40	l3	308	MET
40	l3	328	ILE
40	l3	332	ARG
40	l3	338	LEU
40	l3	340	LYS
40	l3	341	SER
40	l3	346	THR
40	l3	348	ARG
40	l3	363	SER
40	l3	370	PHE
40	l3	380	MET
40	l3	382	THR
40	l3	386	ASP
41	l4	3	ARG
41	l4	11	LEU
41	l4	16	THR
41	l4	18	ASN
41	l4	25	VAL
41	l4	31	ARG
41	l4	33	ASP
41	l4	47	ARG
41	l4	52	VAL
41	l4	73	ARG
41	l4	90	PHE
41	l4	93	MET
41	l4	99	MET
41	l4	112	LYS
41	l4	120	TYR
41	l4	144	LYS
41	l4	145	ILE
41	l4	148	ILE
41	l4	150	LEU
41	l4	156	LEU
41	l4	158	SER
41	l4	179	LEU
41	l4	182	LEU
41	l4	186	LYS
41	l4	187	LEU
41	l4	200	THR

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Mol	Chain	Res	Type
41	14	201	GLN
41	14	203	ARG
41	14	206	LEU
41	14	217	LYS
41	14	222	VAL
41	14	230	VAL
41	14	246	ARG
41	14	256	THR
41	14	258	LEU
41	14	260	GLN
41	14	265	GLU
41	14	267	VAL
41	14	289	ILE
41	14	292	SER
41	14	300	ARG
41	14	301	PRO
41	14	304	GLN
41	14	307	GLN
41	14	313	LEU
41	14	319	LYS
41	14	323	VAL
41	14	327	LEU
41	14	333	VAL
41	14	338	LYS
41	14	339	LEU
41	14	342	LYS
41	14	346	LYS
41	14	347	THR
41	14	357	GLU
41	14	358	THR
41	14	359	LEU
42	15	13	SER
42	15	34	LYS
42	15	51	LEU
42	15	52	VAL
42	15	58	LYS
42	15	70	THR
42	15	74	VAL
42	15	75	LEU
42	15	84	PRO
42	15	89	THR
42	15	93	THR

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Mol	Chain	Res	Type
42	15	110	LEU
42	15	111	GLN
42	15	112	LYS
42	15	113	LEU
42	15	115	LEU
42	15	118	THR
42	15	120	LYS
42	15	133	GLU
42	15	135	VAL
42	15	140	ARG
42	15	146	LEU
42	15	148	ILE
42	15	152	ARG
42	15	155	THR
42	15	158	ARG
42	15	159	VAL
42	15	164	LYS
42	15	177	GLU
42	15	185	PHE
42	15	186	GLU
42	15	187	THR
42	15	194	LEU
42	15	203	HIS
42	15	227	LEU
42	15	236	LEU
42	15	241	THR
42	15	254	LYS
42	15	258	LYS
42	15	259	LYS
42	15	260	PHE
42	15	261	THR
42	15	262	LYS
42	15	268	GLU
42	15	270	LYS
42	15	271	LYS
42	15	273	ARG
42	15	275	THR
42	15	278	SER
42	15	279	LYS
42	15	281	GLU
42	15	297	GLN
43	16	4	GLN

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Mol	Chain	Res	Type
43	16	8	LYS
43	16	21	THR
43	16	31	ARG
43	16	46	ARG
43	16	64	LEU
43	16	65	ILE
43	16	76	LEU
43	16	78	ARG
43	16	79	VAL
43	16	84	VAL
43	16	89	THR
43	16	98	VAL
43	16	109	GLU
43	16	131	LYS
43	16	152	THR
43	16	155	LEU
43	16	162	SER
43	16	164	SER
43	16	170	LYS
43	16	173	MET
44	17	24	GLU
44	17	29	GLU
44	17	40	LYS
44	17	41	ARG
44	17	45	LEU
44	17	46	GLU
44	17	54	GLU
44	17	56	GLU
44	17	60	ARG
44	17	77	VAL
44	17	83	LEU
44	17	93	ASN
44	17	98	LYS
44	17	101	LYS
44	17	110	ARG
44	17	124	LEU
44	17	130	ILE
44	17	156	ILE
44	17	157	ASN
44	17	158	LYS
44	17	159	GLN
44	17	173	LEU

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Mol	Chain	Res	Type
44	17	178	ILE
44	17	179	LEU
44	17	180	SER
44	17	184	LEU
44	17	199	ASN
44	17	229	PHE
44	17	234	GLU
44	17	239	LEU
45	18	27	THR
45	18	41	GLN
45	18	50	VAL
45	18	63	LYS
45	18	65	LEU
45	18	66	SER
45	18	67	ILE
45	18	68	ARG
45	18	74	THR
45	18	77	GLN
45	18	79	GLN
45	18	89	GLU
45	18	94	PHE
45	18	109	LEU
45	18	111	LYS
45	18	126	SER
45	18	136	LEU
45	18	149	LYS
45	18	150	LEU
45	18	157	VAL
45	18	160	ILE
45	18	164	VAL
45	18	169	LEU
45	18	172	LYS
45	18	183	LYS
45	18	185	ARG
45	18	200	LEU
45	18	203	VAL
45	18	208	GLU
45	18	211	LEU
45	18	213	LYS
45	18	219	ASP
45	18	221	ASN
45	18	222	PHE

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Mol	Chain	Res	Type
45	18	224	ASP
45	18	230	LYS
45	18	245	LYS
45	18	246	MET
45	18	248	LYS
46	19	4	ILE
46	19	5	GLN
46	19	6	THR
46	19	19	SER
46	19	31	ARG
46	19	33	THR
46	19	39	LYS
46	19	43	VAL
46	19	44	THR
46	19	48	VAL
46	19	52	LEU
46	19	55	VAL
46	19	62	ARG
46	19	68	LEU
46	19	69	ARG
46	19	70	THR
46	19	80	THR
46	19	105	GLU
46	19	107	ASP
46	19	115	ARG
46	19	122	LYS
46	19	123	ILE
46	19	129	ARG
46	19	130	ASP
46	19	132	VAL
46	19	133	THR
46	19	138	THR
46	19	144	ILE
46	19	151	VAL
46	19	157	ASN
46	19	161	LEU
46	19	162	GLN
46	19	163	GLN
46	19	177	ASP
46	19	179	ILE
47	m0	4	ARG
47	m0	21	ARG

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Mol	Chain	Res	Type
47	m0	24	ARG
47	m0	28	ASP
47	m0	36	LEU
47	m0	42	THR
47	m0	48	LEU
47	m0	52	LEU
47	m0	58	GLU
47	m0	63	GLU
47	m0	77	THR
47	m0	87	LEU
47	m0	90	ARG
47	m0	130	ASP
47	m0	139	ARG
47	m0	144	ASN
47	m0	145	LYS
47	m0	156	ARG
47	m0	169	LYS
47	m0	177	ASP
47	m0	182	LEU
47	m0	191	LYS
47	m0	197	VAL
47	m0	200	LEU
47	m0	203	LYS
47	m0	205	SER
47	m0	206	LEU
47	m0	211	ARG
47	m0	212	GLU
47	m0	217	PHE
48	m1	6	GLN
48	m1	10	ARG
48	m1	11	ASP
48	m1	13	LYS
48	m1	16	LYS
48	m1	23	VAL
48	m1	31	THR
48	m1	40	LEU
48	m1	44	THR
48	m1	46	VAL
48	m1	54	VAL
48	m1	56	THR
48	m1	59	ILE
48	m1	87	LYS

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Mol	Chain	Res	Type
48	m1	95	ASN
48	m1	107	ASP
48	m1	119	SER
48	m1	120	ILE
48	m1	122	ILE
48	m1	129	VAL
48	m1	130	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	145	LYS
48	m1	153	LYS
48	m1	155	THR
48	m1	156	LYS
48	m1	159	THR
48	m1	173	ASP
48	m1	174	LYS
49	m3	22	VAL
49	m3	28	GLN
49	m3	36	ARG
49	m3	45	LYS
49	m3	54	LEU
49	m3	57	VAL
49	m3	58	VAL
49	m3	59	ARG
49	m3	63	VAL
49	m3	67	ARG
49	m3	68	LYS
49	m3	69	VAL
49	m3	73	ARG
49	m3	75	PHE
49	m3	76	THR
49	m3	86	THR
49	m3	106	GLN
49	m3	107	GLU
49	m3	120	GLN
49	m3	123	ILE
49	m3	131	LYS
49	m3	149	GLN
49	m3	152	THR
49	m3	164	GLU
49	m3	165	SER
49	m3	168	ARG

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Mol	Chain	Res	Type
49	m3	176	GLU
49	m3	182	ILE
49	m3	194	GLU
50	m4	3	THR
50	m4	13	ARG
50	m4	15	VAL
50	m4	27	GLN
50	m4	42	LYS
50	m4	50	LYS
50	m4	53	VAL
50	m4	58	ILE
50	m4	62	GLN
50	m4	63	VAL
50	m4	66	THR
50	m4	72	LEU
50	m4	80	THR
50	m4	82	SER
50	m4	107	GLU
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	10	LEU
51	m5	12	ARG
51	m5	17	ASP
51	m5	19	LEU
51	m5	20	ARG
51	m5	22	LEU
51	m5	24	ARG
51	m5	27	VAL
51	m5	49	ARG
51	m5	65	ARG
51	m5	68	ARG
51	m5	72	LYS
51	m5	76	PRO
51	m5	80	THR
51	m5	85	THR
51	m5	92	LEU
51	m5	98	LEU
51	m5	105	ARG
51	m5	106	VAL
51	m5	138	GLN
51	m5	142	ILE

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Mol	Chain	Res	Type
51	m5	153	ASP
51	m5	155	VAL
51	m5	165	THR
51	m5	171	SER
51	m5	175	ASN
51	m5	176	LYS
51	m5	204	LYS
52	m6	22	VAL
52	m6	34	VAL
52	m6	41	LEU
52	m6	51	LYS
52	m6	58	LEU
52	m6	60	LYS
52	m6	66	LYS
52	m6	68	ARG
52	m6	74	ARG
52	m6	78	ARG
52	m6	100	GLU
52	m6	106	GLU
52	m6	110	PRO
52	m6	114	LYS
52	m6	117	ARG
52	m6	124	LEU
52	m6	126	VAL
52	m6	134	LYS
52	m6	143	THR
52	m6	152	VAL
52	m6	166	GLU
52	m6	171	LYS
52	m6	175	THR
52	m6	182	ASN
52	m6	184	THR
52	m6	197	LEU
53	m7	7	THR
53	m7	8	SER
53	m7	9	THR
53	m7	16	SER
53	m7	18	ARG
53	m7	32	THR
53	m7	42	THR
53	m7	52	LEU
53	m7	56	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	m7	69	ARG
53	m7	78	VAL
53	m7	79	THR
53	m7	89	LYS
53	m7	105	LYS
53	m7	112	LEU
53	m7	114	VAL
53	m7	119	VAL
53	m7	120	ASN
53	m7	124	LYS
53	m7	126	ARG
53	m7	127	ARG
53	m7	136	ILE
53	m7	144	SER
53	m7	153	LYS
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	39	ARG
54	m8	49	LEU
54	m8	57	ILE
54	m8	63	SER
54	m8	64	VAL
54	m8	69	ARG
54	m8	80	THR
54	m8	81	VAL
54	m8	93	ILE
54	m8	95	GLU
54	m8	97	PRO
54	m8	99	THR
54	m8	127	LEU
54	m8	135	GLN
54	m8	138	LEU
54	m8	146	SER
54	m8	165	ILE
54	m8	170	ARG

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Mol	Chain	Res	Type
54	m8	173	GLU
54	m8	178	ARG
55	m9	5	ARG
55	m9	8	LYS
55	m9	9	ARG
55	m9	10	LEU
55	m9	17	VAL
55	m9	20	ARG
55	m9	29	THR
55	m9	30	SER
55	m9	31	GLU
55	m9	32	ILE
55	m9	36	ASN
55	m9	43	LYS
55	m9	49	THR
55	m9	52	LYS
55	m9	53	LYS
55	m9	56	THR
55	m9	57	VAL
55	m9	63	THR
55	m9	70	LYS
55	m9	74	ARG
55	m9	76	SER
55	m9	88	ARG
55	m9	99	LEU
55	m9	116	ASP
55	m9	126	GLU
55	m9	138	LEU
55	m9	146	LYS
55	m9	152	GLU
55	m9	153	LYS
55	m9	156	ASN
55	m9	158	GLU
55	m9	167	ARG
55	m9	173	ARG
55	m9	177	VAL
56	n0	8	GLN
56	n0	16	THR
56	n0	19	VAL
56	n0	21	GLU
56	n0	23	LYS
56	n0	46	GLN

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Mol	Chain	Res	Type
56	n0	50	LYS
56	n0	58	ILE
56	n0	72	VAL
56	n0	73	LYS
56	n0	80	ARG
56	n0	87	THR
56	n0	92	LYS
56	n0	97	VAL
56	n0	105	THR
56	n0	115	ARG
56	n0	117	ARG
56	n0	120	SER
56	n0	130	GLU
56	n0	136	LYS
56	n0	137	ARG
56	n0	145	THR
56	n0	148	LEU
56	n0	149	LYS
56	n0	155	ARG
56	n0	157	GLN
56	n0	160	THR
56	n0	161	LYS
56	n0	162	THR
56	n0	166	LYS
56	n0	169	SER
56	n0	171	PHE
56	n0	172	TYR
57	n1	12	ARG
57	n1	17	ARG
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	55	LYS
57	n1	68	THR
57	n1	71	SER
57	n1	75	ILE
57	n1	80	VAL
57	n1	83	ARG
57	n1	88	ARG
57	n1	89	LEU
57	n1	96	ILE
57	n1	97	LYS

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Mol	Chain	Res	Type
57	n1	102	ARG
57	n1	104	GLU
57	n1	124	VAL
57	n1	126	VAL
57	n1	131	GLN
57	n1	139	ARG
57	n1	140	ILE
57	n1	141	VAL
57	n1	143	THR
57	n1	149	GLN
57	n1	150	THR
57	n1	154	VAL
57	n1	158	THR
57	n1	160	ILE
58	n2	15	PHE
58	n2	16	THR
58	n2	21	SER
58	n2	27	VAL
58	n2	28	PHE
58	n2	32	SER
58	n2	37	LEU
58	n2	38	ILE
58	n2	43	VAL
58	n2	50	LEU
58	n2	54	VAL
58	n2	55	THR
58	n2	63	VAL
58	n2	64	THR
58	n2	66	VAL
58	n2	72	SER
58	n2	74	LYS
58	n2	90	ARG
58	n2	98	THR
58	n2	100	THR
59	n3	7	GLN
59	n3	13	ILE
59	n3	14	SER
59	n3	45	ARG
59	n3	48	ARG
59	n3	69	LEU
59	n3	70	ARG
59	n3	73	VAL

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Mol	Chain	Res	Type
59	n3	93	LEU
59	n3	102	ILE
59	n3	104	ASN
59	n3	110	LYS
59	n3	115	THR
60	n4	1	MET
60	n4	19	THR
60	n4	34	SER
60	n4	39	LEU
60	n4	54	LEU
60	n4	57	LYS
60	n4	63	ILE
60	n4	89	LEU
60	n4	91	LYS
60	n4	96	LEU
60	n4	97	LYS
60	n4	105	ARG
60	n4	107	GLU
60	n4	119	GLU
60	n4	126	GLU
60	n4	135	SER
61	n5	24	LEU
61	n5	27	ARG
61	n5	37	THR
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	64	GLU
61	n5	86	VAL
61	n5	96	LYS
61	n5	104	GLU
61	n5	108	LEU
61	n5	109	LYS
61	n5	115	ARG
61	n5	117	ASN
61	n5	125	ARG
61	n5	133	LEU
61	n5	135	ILE
61	n5	137	ASN
62	n6	3	LYS
62	n6	9	SER
62	n6	12	ARG

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Mol	Chain	Res	Type
62	n6	13	ARG
62	n6	17	LYS
62	n6	37	LYS
62	n6	39	LEU
62	n6	40	ARG
62	n6	50	ILE
62	n6	51	ARG
62	n6	52	ARG
62	n6	56	VAL
62	n6	57	LEU
62	n6	59	VAL
62	n6	62	SER
62	n6	64	LYS
62	n6	66	GLN
62	n6	74	TYR
62	n6	80	VAL
62	n6	83	ASP
62	n6	88	GLU
62	n6	105	VAL
62	n6	108	LYS
63	n7	10	VAL
63	n7	14	VAL
63	n7	15	ARG
63	n7	17	ARG
63	n7	24	VAL
63	n7	34	LYS
63	n7	36	HIS
63	n7	46	ILE
63	n7	52	LYS
63	n7	56	LYS
63	n7	65	ARG
63	n7	66	THR
63	n7	72	ILE
63	n7	75	VAL
63	n7	81	LEU
63	n7	86	THR
63	n7	89	VAL
63	n7	90	GLU
63	n7	95	VAL
63	n7	98	THR
63	n7	102	GLU
63	n7	103	GLN

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Mol	Chain	Res	Type
63	n7	105	SER
63	n7	134	LEU
63	n7	135	ARG
64	n8	4	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	27	LYS
64	n8	42	ARG
64	n8	44	ASN
64	n8	46	ASP
64	n8	56	VAL
64	n8	60	TYR
64	n8	63	LYS
64	n8	70	LYS
64	n8	76	ASP
64	n8	80	THR
64	n8	91	LEU
64	n8	115	LYS
65	n9	13	THR
65	n9	14	ARG
65	n9	15	LYS
65	n9	22	LYS
65	n9	23	LYS
65	n9	25	LYS
65	n9	26	THR
65	n9	33	LYS
65	n9	38	LYS
65	n9	40	ARG
65	n9	44	LYS
65	n9	47	LEU
65	n9	58	LYS
65	n9	59	LYS
66	o0	8	GLU
66	o0	9	SER
66	o0	10	ILE
66	o0	12	GLN
66	o0	16	LEU
66	o0	18	ILE
66	o0	34	LEU
66	o0	40	LYS
66	o0	41	LEU
66	o0	44	ILE

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Mol	Chain	Res	Type
66	o0	48	THR
66	o0	55	GLU
66	o0	59	TYR
66	o0	61	MET
66	o0	66	LYS
66	o0	74	ASN
66	o0	81	VAL
66	o0	83	LYS
66	o0	86	ARG
66	o0	87	VAL
66	o0	97	ASP
67	o1	13	THR
67	o1	16	LEU
67	o1	26	LYS
67	o1	31	ARG
67	o1	34	LYS
67	o1	35	GLU
67	o1	36	ILE
67	o1	44	MET
67	o1	46	THR
67	o1	48	ASP
67	o1	55	LEU
67	o1	68	GLU
67	o1	73	LEU
67	o1	76	SER
67	o1	83	GLU
67	o1	84	ASP
67	o1	87	ASN
67	o1	89	LEU
67	o1	91	SER
67	o1	96	VAL
67	o1	97	LEU
67	o1	102	LYS
67	o1	104	LEU
67	o1	106	THR
67	o1	107	VAL
67	o1	112	ASP
68	o2	3	SER
68	o2	4	LEU
68	o2	6	HIS
68	o2	8	LYS
68	o2	10	VAL

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Mol	Chain	Res	Type
68	o2	19	ARG
68	o2	24	ARG
68	o2	33	ARG
68	o2	35	GLN
68	o2	41	VAL
68	o2	51	SER
68	o2	72	LYS
68	o2	73	THR
68	o2	75	LEU
68	o2	76	VAL
68	o2	82	LEU
68	o2	84	THR
68	o2	91	THR
68	o2	95	GLU
68	o2	109	LEU
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	10	LYS
69	o3	31	LYS
69	o3	37	THR
69	o3	56	SER
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	78	SER
69	o3	81	VAL
69	o3	84	THR
69	o3	86	ARG
69	o3	98	VAL
69	o3	105	SER
70	o4	5	VAL
70	o4	9	ARG
70	o4	20	ILE
70	o4	22	VAL
70	o4	23	VAL
70	o4	24	LYS
70	o4	25	THR

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Mol	Chain	Res	Type
70	o4	29	ILE
70	o4	30	LEU
70	o4	38	LEU
70	o4	47	CYS
70	o4	58	ARG
70	o4	64	THR
70	o4	68	THR
70	o4	71	THR
70	o4	79	SER
70	o4	83	ASN
70	o4	88	ARG
70	o4	98	GLN
71	o5	5	LYS
71	o5	15	GLU
71	o5	20	GLN
71	o5	21	LEU
71	o5	27	GLU
71	o5	28	LEU
71	o5	37	SER
71	o5	38	ARG
71	o5	40	SER
71	o5	47	VAL
71	o5	62	GLN
71	o5	69	LEU
71	o5	79	ASP
71	o5	81	ARG
71	o5	85	THR
71	o5	89	ARG
71	o5	101	THR
71	o5	104	GLN
71	o5	107	LYS
72	o6	2	THR
72	o6	7	ILE
72	o6	9	ILE
72	o6	16	LYS
72	o6	17	VAL
72	o6	18	THR
72	o6	26	ILE
72	o6	29	LYS
72	o6	34	SER
72	o6	36	ARG
72	o6	37	THR

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Mol	Chain	Res	Type
72	o6	38	LYS
72	o6	45	ARG
72	o6	46	GLU
72	o6	56	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	59	ASP
72	o6	60	LEU
72	o6	68	ARG
72	o6	76	ARG
72	o6	79	SER
72	o6	84	LYS
72	o6	88	GLU
72	o6	94	ILE
72	o6	98	ARG
73	o7	5	THR
73	o7	7	SER
73	o7	17	THR
73	o7	25	ARG
73	o7	33	THR
73	o7	36	SER
73	o7	44	THR
73	o7	55	ARG
73	o7	58	THR
73	o7	65	ARG
73	o7	67	LEU
73	o7	74	PHE
73	o7	80	THR
73	o7	82	SER
74	o8	5	ILE
74	o8	12	LEU
74	o8	13	GLU
74	o8	24	THR
74	o8	31	LEU
74	o8	32	ASN
74	o8	33	LYS
74	o8	41	THR
74	o8	45	VAL
74	o8	46	ARG
74	o8	53	THR
74	o8	61	LYS
74	o8	64	LYS

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Mol	Chain	Res	Type
74	o8	65	LEU
74	o8	67	GLN
74	o8	68	SER
75	o9	4	GLN
75	o9	11	GLN
75	o9	15	LYS
75	o9	21	ARG
75	o9	27	ILE
75	o9	28	ARG
75	o9	29	LEU
75	o9	45	ARG
76	q0	79	GLU
76	q0	85	LEU
76	q0	93	LYS
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	127	LEU
77	q1	6	ARG
77	q1	9	ARG
77	q1	13	LEU
77	q1	14	LYS
77	q1	19	LYS
77	q1	21	ARG
77	q1	23	ARG
78	q2	6	LYS
78	q2	7	THR
78	q2	8	ARG
78	q2	16	THR
78	q2	17	CYS
78	q2	20	HIS
78	q2	22	GLN
78	q2	26	THR
78	q2	45	ARG
78	q2	46	LYS
78	q2	61	LYS
78	q2	71	ARG
78	q2	72	LEU
78	q2	73	GLU
78	q2	78	LYS
78	q2	79	THR
78	q2	83	LEU

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Mol	Chain	Res	Type
78	q2	84	THR
78	q2	89	LYS
78	q2	93	LEU
78	q2	100	LYS
78	q2	104	LEU
78	q2	105	GLN
79	q3	3	LYS
79	q3	7	LYS
79	q3	20	SER
79	q3	21	SER
79	q3	24	ARG
79	q3	40	SER
79	q3	42	CYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	70	THR
79	q3	72	SER
79	q3	73	THR
79	q3	89	MET
82	p0	4	ILE
82	p0	25	LEU
82	p0	30	VAL
82	p0	31	ASP
82	p0	42	ARG
82	p0	43	LYS
82	p0	52	LEU
82	p0	55	LYS
82	p0	70	LEU
82	p0	72	ASP
82	p0	76	LEU
82	p0	81	LYS
82	p0	93	LEU
82	p0	94	THR
82	p0	95	GLU
82	p0	97	LYS
82	p0	101	VAL
82	p0	185	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
4	S2	89	GLN
4	S2	94	GLN
7	S5	200	ASN
7	S5	224	ASN
10	S8	116	HIS
12	C0	12	HIS
13	C1	110	HIS
13	C1	118	GLN
19	C7	29	GLN
22	D0	72	ASN
23	D1	74	GLN
24	D2	56	HIS
27	D5	38	HIS
35	SM	86	ASN
39	L2	209	HIS
41	L4	311	HIS
42	L5	40	HIS
42	L5	264	GLN
44	L7	225	GLN
44	L7	244	ASN
46	L9	59	ASN
47	M0	12	GLN
47	M0	163	GLN
48	M1	109	HIS
57	N1	26	HIS
59	N3	98	ASN
61	N5	80	ASN
64	N8	64	GLN
69	O3	106	ASN
70	O4	69	HIS
3	s1	74	GLN
3	s1	209	ASN
4	s2	220	ASN
5	s3	74	GLN
7	s5	104	ASN
8	s6	139	ASN
9	s7	71	HIS
11	s9	124	HIS
11	s9	142	ASN
12	c0	32	HIS
13	c1	18	HIS
13	c1	21	ASN
20	c8	6	GLN

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Mol	Chain	Res	Type
20	c8	12	GLN
24	d2	56	HIS
26	d4	22	GLN
34	sR	299	GLN
34	sR	314	GLN
41	l4	307	GLN
46	l9	169	ASN
61	n5	111	ASN
61	n5	117	ASN
64	n8	28	HIS
64	n8	44	ASN
82	p0	37	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	488 (27%)	54 (3%)
1	6	1792/1800 (99%)	440 (24%)	49 (2%)
36	1	3145/3396 (92%)	696 (22%)	89 (2%)
36	5	3145/3396 (92%)	666 (21%)	74 (2%)
37	3	120/121 (99%)	15 (12%)	0
37	7	120/121 (99%)	20 (16%)	0
38	4	157/158 (99%)	39 (24%)	2 (1%)
38	8	157/158 (99%)	36 (22%)	1 (0%)
All	All	10383/10950 (94%)	2400 (23%)	269 (2%)

All (2400) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	45	U
1	2	46	A
1	2	47	A
1	2	50	C
1	2	57	G

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Mol	Chain	Res	Type
1	2	60	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	101	U
1	2	104	A
1	2	114	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	161	U
1	2	167	U
1	2	169	A
1	2	176	C
1	2	178	U
1	2	185	U
1	2	186	C
1	2	187	G
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G

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Mol	Chain	Res	Type
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	231	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	236	A
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	242	U
1	2	250	C
1	2	260	U
1	2	261	U
1	2	265	A
1	2	266	A
1	2	271	A
1	2	272	U
1	2	274	G
1	2	275	C
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	284	G
1	2	288	A
1	2	290	G
1	2	299	A
1	2	302	U
1	2	303	U
1	2	314	C

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Mol	Chain	Res	Type
1	2	316	A
1	2	319	U
1	2	321	C
1	2	322	G
1	2	323	A
1	2	333	A
1	2	337	G
1	2	338	C
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	363	G
1	2	387	A
1	2	390	G
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	421	A
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	434	G
1	2	439	U
1	2	440	U
1	2	444	C
1	2	446	A
1	2	448	C
1	2	454	U
1	2	468	A
1	2	477	A
1	2	479	C
1	2	480	G
1	2	484	C
1	2	485	A
1	2	486	G

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Mol	Chain	Res	Type
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G
1	2	511	A
1	2	512	A
1	2	513	U
1	2	515	A
1	2	516	G
1	2	519	C
1	2	520	A
1	2	522	U
1	2	525	A
1	2	527	A
1	2	533	U
1	2	534	A
1	2	536	C
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	546	U
1	2	548	G
1	2	551	G
1	2	555	A
1	2	556	A

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Mol	Chain	Res	Type
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	578	U
1	2	579	A
1	2	580	A
1	2	585	A
1	2	594	A
1	2	595	G
1	2	609	U
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	630	A
1	2	639	U
1	2	640	U
1	2	650	U
1	2	653	C
1	2	655	G
1	2	656	G
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C
1	2	694	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	709	C

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Mol	Chain	Res	Type
1	2	710	U
1	2	711	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	744	U
1	2	745	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	779	U
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	789	A
1	2	790	U
1	2	793	A

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Mol	Chain	Res	Type
1	2	794	U
1	2	795	U
1	2	799	A
1	2	803	A
1	2	811	A
1	2	812	A
1	2	813	U
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	822	U
1	2	823	G
1	2	824	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	833	U
1	2	837	G
1	2	839	U
1	2	840	U
1	2	846	G
1	2	848	C
1	2	850	A
1	2	854	U
1	2	860	U
1	2	862	A
1	2	863	A
1	2	864	U
1	2	865	A
1	2	886	U
1	2	895	G
1	2	898	A
1	2	911	U
1	2	912	U
1	2	913	G
1	2	914	G
1	2	916	U
1	2	933	A

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Mol	Chain	Res	Type
1	2	935	U
1	2	942	G
1	2	944	A
1	2	951	A
1	2	960	U
1	2	966	A
1	2	991	G
1	2	992	A
1	2	993	A
1	2	995	A
1	2	997	G
1	2	999	U
1	2	1002	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1021	C
1	2	1026	A
1	2	1028	C
1	2	1031	U
1	2	1039	A
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	1074	G
1	2	1079	U
1	2	1082	C
1	2	1086	A
1	2	1087	A
1	2	1091	A
1	2	1092	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	1146	G

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Mol	Chain	Res	Type
1	2	1150	G
1	2	1151	A
1	2	1157	A
1	2	1158	C
1	2	1160	A
1	2	1163	A
1	2	1167	G
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1207	C
1	2	1208	A
1	2	1217	A
1	2	1218	G
1	2	1226	A
1	2	1227	A
1	2	1228	G
1	2	1235	C
1	2	1241	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1256	A
1	2	1257	U
1	2	1258	U
1	2	1260	U
1	2	1267	G
1	2	1284	C
1	2	1286	U
1	2	1291	G
1	2	1314	U
1	2	1315	U
1	2	1316	G
1	2	1321	A
1	2	1338	C
1	2	1339	C

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Mol	Chain	Res	Type
1	2	1340	U
1	2	1341	A
1	2	1342	C
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1361	U
1	2	1362	U
1	2	1363	U
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1379	C
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1412	G
1	2	1413	U
1	2	1418	G
1	2	1427	A
1	2	1428	G
1	2	1433	G
1	2	1446	A
1	2	1457	C
1	2	1459	C
1	2	1462	G
1	2	1466	G
1	2	1469	A
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1475	A
1	2	1478	G
1	2	1482	C
1	2	1486	G
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	1506	G
1	2	1510	U
1	2	1514	U
1	2	1516	A
1	2	1517	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1526	A
1	2	1530	C
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1540	G
1	2	1548	G
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1574	G
1	2	1584	G
1	2	1588	G
1	2	1590	G
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1631	A
1	2	1635	A
1	2	1639	C
1	2	1657	U
1	2	1658	G
1	2	1663	G
1	2	1681	A
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1731	A
1	2	1736	G
1	2	1756	A
1	2	1757	G
1	2	1759	C
1	2	1760	G

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Mol	Chain	Res	Type
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1768	G
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	14	U
36	1	16	A
36	1	26	A
36	1	37	U
36	1	40	A
36	1	42	C
36	1	43	A
36	1	45	A
36	1	49	A
36	1	59	G
36	1	60	A
36	1	61	A
36	1	65	A
36	1	66	A
36	1	73	C
36	1	83	U
36	1	92	G
36	1	93	C
36	1	94	G
36	1	99	A
36	1	108	A
36	1	109	A
36	1	110	G
36	1	111	C
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C

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Mol	Chain	Res	Type
36	1	136	G
36	1	147	U
36	1	156	G
36	1	157	A
36	1	160	G
36	1	163	C
36	1	166	C
36	1	169	U
36	1	170	G
36	1	173	G
36	1	181	U
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C
36	1	210	U
36	1	211	A
36	1	218	G
36	1	219	A
36	1	238	A
36	1	240	U
36	1	241	G
36	1	243	G
36	1	244	G
36	1	247	C
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	256	G
36	1	269	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	299	G
36	1	305	U
36	1	315	C
36	1	318	A
36	1	323	A
36	1	329	U
36	1	339	C

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Mol	Chain	Res	Type
36	1	349	A
36	1	350	C
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	421	G
36	1	422	A
36	1	438	A
36	1	440	A
36	1	495	G
36	1	498	A
36	1	507	U
36	1	520	U
36	1	521	A
36	1	525	C
36	1	535	G
36	1	544	C
36	1	546	C
36	1	547	G
36	1	548	G
36	1	552	G
36	1	555	U
36	1	556	U
36	1	557	A
36	1	559	A
36	1	560	G
36	1	568	G
36	1	578	A
36	1	579	G
36	1	592	A
36	1	594	U
36	1	600	G
36	1	604	G
36	1	609	G
36	1	611	A
36	1	619	A
36	1	620	U
36	1	621	A

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Mol	Chain	Res	Type
36	1	622	A
36	1	636	C
36	1	642	U
36	1	643	U
36	1	644	G
36	1	647	A
36	1	648	C
36	1	649	A
36	1	651	G
36	1	653	A
36	1	658	G
36	1	660	A
36	1	662	U
36	1	667	C
36	1	677	A
36	1	681	U
36	1	691	A
36	1	692	A
36	1	693	A
36	1	705	A
36	1	708	G
36	1	712	G
36	1	715	A
36	1	716	A
36	1	725	G
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	768	C
36	1	776	U
36	1	777	U
36	1	781	G
36	1	785	G
36	1	806	A
36	1	816	A
36	1	817	A
36	1	830	A
36	1	837	A
36	1	849	C
36	1	855	U
36	1	859	G

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Mol	Chain	Res	Type
36	1	861	C
36	1	874	U
36	1	879	U
36	1	883	A
36	1	885	U
36	1	887	G
36	1	890	C
36	1	896	A
36	1	897	U
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	923	C
36	1	937	G
36	1	938	C
36	1	943	U
36	1	944	C
36	1	959	C
36	1	960	U
36	1	962	A
36	1	974	G
36	1	979	U
36	1	981	U
36	1	982	C
36	1	993	G
36	1	994	G
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1015	U
36	1	1016	C
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A

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Mol	Chain	Res	Type
36	1	1037	C
36	1	1045	C
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1064	A
36	1	1065	A
36	1	1068	C
36	1	1069	C
36	1	1072	G
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1087	G
36	1	1093	A
36	1	1094	U
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	1116	G
36	1	1117	G
36	1	1128	U
36	1	1131	G
36	1	1153	A
36	1	1159	A
36	1	1160	C
36	1	1161	G
36	1	1178	G
36	1	1179	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1191	U
36	1	1192	C
36	1	1201	C
36	1	1202	A
36	1	1205	A
36	1	1209	G
36	1	1217	A

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Mol	Chain	Res	Type
36	1	1222	G
36	1	1226	G
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1235	U
36	1	1236	G
36	1	1237	G
36	1	1241	U
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1251	A
36	1	1258	U
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1274	A
36	1	1278	A
36	1	1279	C
36	1	1280	C
36	1	1285	G
36	1	1287	A
36	1	1292	C
36	1	1293	U
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1324	U
36	1	1329	U
36	1	1330	A
36	1	1332	A
36	1	1344	G
36	1	1345	G

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Mol	Chain	Res	Type
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	1379	G
36	1	1386	A
36	1	1398	U
36	1	1399	A
36	1	1400	G
36	1	1418	A
36	1	1419	A
36	1	1422	G
36	1	1425	U
36	1	1429	G
36	1	1434	G
36	1	1437	C
36	1	1446	A
36	1	1450	G
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1488	G
36	1	1490	A
36	1	1496	C
36	1	1503	A
36	1	1508	C
36	1	1526	U
36	1	1527	C
36	1	1528	G
36	1	1529	A
36	1	1555	U
36	1	1556	C
36	1	1557	A
36	1	1560	G
36	1	1561	G
36	1	1562	C
36	1	1563	C

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Mol	Chain	Res	Type
36	1	1564	U
36	1	1565	G
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	1576	G
36	1	1578	C
36	1	1579	C
36	1	1580	A
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1593	A
36	1	1605	A
36	1	1609	C
36	1	1620	U
36	1	1629	U
36	1	1633	C
36	1	1639	C
36	1	1643	A
36	1	1657	C
36	1	1683	A
36	1	1688	U
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1727	G
36	1	1729	A
36	1	1736	G
36	1	1741	A
36	1	1745	C
36	1	1746	U
36	1	1750	A
36	1	1751	G
36	1	1760	A
36	1	1761	C
36	1	1762	C
36	1	1763	U

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Mol	Chain	Res	Type
36	1	1764	U
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1769	G
36	1	1770	G
36	1	1775	G
36	1	1779	C
36	1	1780	G
36	1	1797	A
36	1	1809	A
36	1	1810	A
36	1	1811	G
36	1	1813	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	1841	A
36	1	1842	A
36	1	1845	G
36	1	1846	C
36	1	1849	C
36	1	1850	A
36	1	1866	C
36	1	1871	U
36	1	1879	A
36	1	1880	U
36	1	1886	A
36	1	1901	A
36	1	1906	G
36	1	1920	U
36	1	1927	G
36	1	1948	G
36	1	1951	C
36	1	1952	G
36	1	1953	G

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Mol	Chain	Res	Type
36	1	1954	G
36	1	2094	C
36	1	2097	U
36	1	2101	C
36	1	2102	U
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2114	C
36	1	2121	G
36	1	2122	G
36	1	2131	A
36	1	2134	G
36	1	2140	U
36	1	2158	A
36	1	2162	U
36	1	2165	G
36	1	2169	G
36	1	2186	U
36	1	2194	G
36	1	2201	G
36	1	2205	U
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2223	A
36	1	2244	A
36	1	2249	G
36	1	2250	G
36	1	2255	A
36	1	2256	A
36	1	2268	U
36	1	2272	G
36	1	2273	G
36	1	2281	A
36	1	2282	U
36	1	2298	U
36	1	2303	A
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2314	U

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Mol	Chain	Res	Type
36	1	2315	G
36	1	2319	U
36	1	2330	C
36	1	2334	U
36	1	2336	U
36	1	2341	A
36	1	2347	U
36	1	2360	C
36	1	2366	C
36	1	2370	G
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2393	G
36	1	2394	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2405	C
36	1	2406	C
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2424	A
36	1	2435	G
36	1	2437	G
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2504	U
36	1	2505	U
36	1	2509	U
36	1	2511	A
36	1	2513	U
36	1	2514	U
36	1	2515	A
36	1	2522	G
36	1	2523	A
36	1	2526	C
36	1	2532	U

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Mol	Chain	Res	Type
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	2547	A
36	1	2549	G
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2561	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2583	C
36	1	2585	G
36	1	2586	G
36	1	2593	A
36	1	2594	C
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2617	U
36	1	2628	A
36	1	2637	A
36	1	2638	C
36	1	2644	C
36	1	2652	U
36	1	2655	U
36	1	2656	A
36	1	2674	A
36	1	2677	G
36	1	2681	U
36	1	2689	A
36	1	2691	A

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Mol	Chain	Res	Type
36	1	2694	A
36	1	2696	A
36	1	2699	G
36	1	2705	A
36	1	2714	G
36	1	2728	G
36	1	2729	U
36	1	2733	A
36	1	2737	C
36	1	2744	U
36	1	2752	U
36	1	2753	G
36	1	2755	C
36	1	2762	A
36	1	2771	U
36	1	2772	C
36	1	2773	C
36	1	2777	G
36	1	2778	G
36	1	2780	A
36	1	2783	U
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2802	A
36	1	2810	C
36	1	2816	G
36	1	2817	A
36	1	2818	U
36	1	2828	G
36	1	2829	U
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2847	A
36	1	2860	U
36	1	2863	G
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2886	U

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Mol	Chain	Res	Type
36	1	2887	A
36	1	2889	C
36	1	2893	C
36	1	2898	G
36	1	2899	C
36	1	2904	U
36	1	2914	G
36	1	2922	G
36	1	2923	U
36	1	2925	C
36	1	2935	U
36	1	2936	A
36	1	2942	C
36	1	2947	G
36	1	2954	U
36	1	2955	U
36	1	2971	A
36	1	2974	U
36	1	2979	U
36	1	2980	U
36	1	2983	C
36	1	2990	G
36	1	2997	G
36	1	3006	A
36	1	3012	A
36	1	3040	A
36	1	3046	A
36	1	3058	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3086	A
36	1	3087	A
36	1	3090	U
36	1	3091	A
36	1	3092	C
36	1	3113	A
36	1	3119	U
36	1	3122	A
36	1	3129	A
36	1	3130	A
36	1	3131	U

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Mol	Chain	Res	Type
36	1	3142	A
36	1	3143	C
36	1	3150	A
36	1	3151	U
36	1	3152	U
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3164	C
36	1	3165	A
36	1	3168	A
36	1	3170	A
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3187	A
36	1	3195	U
36	1	3196	U
36	1	3207	U
36	1	3210	A
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3228	C
36	1	3229	G
36	1	3235	C
36	1	3236	U
36	1	3243	A
36	1	3244	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3259	U
36	1	3261	C
36	1	3265	C
36	1	3269	U
36	1	3270	U
36	1	3271	G

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Mol	Chain	Res	Type
36	1	3273	A
36	1	3276	G
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3288	G
36	1	3289	G
36	1	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	3341	U
36	1	3342	A
36	1	3343	G
36	1	3345	G
36	1	3347	A
36	1	3349	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	3375	A
36	1	3376	A
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3389	U
36	1	3390	G
36	1	3396	U
37	3	3	U
37	3	11	A
37	3	21	G
37	3	22	A

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Mol	Chain	Res	Type
37	3	26	C
37	3	42	A
37	3	54	U
37	3	65	G
37	3	74	C
37	3	76	A
37	3	91	G
37	3	102	A
37	3	103	A
37	3	112	G
37	3	121	U
38	4	3	A
38	4	17	A
38	4	26	U
38	4	34	U
38	4	35	C
38	4	48	A
38	4	50	C
38	4	51	G
38	4	52	A
38	4	57	C
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	84	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	97	A
38	4	102	U
38	4	104	A
38	4	105	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	122	U

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Mol	Chain	Res	Type
38	4	125	U
38	4	126	A
38	4	128	U
38	4	138	A
38	4	148	G
38	4	152	G
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	17	C
1	6	24	U
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	47	A
1	6	50	C
1	6	57	G
1	6	60	U
1	6	61	A
1	6	66	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	71	A
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	104	A
1	6	114	C
1	6	127	G
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	144	U
1	6	145	A
1	6	153	G

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Mol	Chain	Res	Type
1	6	158	U
1	6	159	U
1	6	166	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	195	G
1	6	196	G
1	6	197	A
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	230	C
1	6	232	U
1	6	233	C
1	6	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	261	U
1	6	265	A
1	6	270	C
1	6	271	A
1	6	272	U
1	6	273	G
1	6	275	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	287	G

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Mol	Chain	Res	Type
1	6	299	A
1	6	309	C
1	6	313	U
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	329	G
1	6	337	G
1	6	338	C
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	417	A
1	6	418	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	428	A
1	6	434	G
1	6	439	U
1	6	444	C
1	6	448	C
1	6	455	C
1	6	468	A
1	6	477	A
1	6	480	G
1	6	484	C
1	6	486	G
1	6	487	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A

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Mol	Chain	Res	Type
1	6	493	U
1	6	494	U
1	6	496	G
1	6	497	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	508	U
1	6	511	A
1	6	512	A
1	6	513	U
1	6	515	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	555	A
1	6	556	A
1	6	557	G
1	6	558	U
1	6	559	C
1	6	565	C
1	6	566	C
1	6	570	A
1	6	574	G
1	6	578	U
1	6	579	A
1	6	580	A
1	6	582	U
1	6	594	A
1	6	595	G
1	6	606	A
1	6	609	U
1	6	610	G

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Mol	Chain	Res	Type
1	6	617	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	630	A
1	6	637	C
1	6	639	U
1	6	640	U
1	6	645	C
1	6	651	G
1	6	652	G
1	6	653	C
1	6	658	C
1	6	659	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
1	6	669	G
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	680	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	691	C
1	6	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	717	C
1	6	718	U
1	6	719	U

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Mol	Chain	Res	Type
1	6	720	G
1	6	721	U
1	6	722	G
1	6	730	G
1	6	744	U
1	6	751	G
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	766	U
1	6	774	A
1	6	775	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	789	A
1	6	793	A
1	6	794	U
1	6	811	A
1	6	812	A
1	6	815	G
1	6	816	G
1	6	823	G
1	6	825	U
1	6	826	U
1	6	828	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	847	A
1	6	854	U
1	6	856	A
1	6	860	U
1	6	863	A
1	6	873	U
1	6	898	A
1	6	906	A

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Mol	Chain	Res	Type
1	6	910	C
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	959	U
1	6	960	U
1	6	966	A
1	6	970	A
1	6	971	A
1	6	992	A
1	6	993	A
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	1039	A
1	6	1040	G
1	6	1052	U
1	6	1053	G
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1063	U
1	6	1070	C
1	6	1072	C
1	6	1081	A
1	6	1082	C
1	6	1092	A
1	6	1093	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1100	G
1	6	1101	G
1	6	1104	U
1	6	1109	G

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Mol	Chain	Res	Type
1	6	1138	A
1	6	1146	G
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1167	G
1	6	1183	A
1	6	1185	U
1	6	1191	U
1	6	1194	A
1	6	1196	A
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1207	C
1	6	1208	A
1	6	1217	A
1	6	1218	G
1	6	1220	C
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1242	A
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1262	U
1	6	1273	G
1	6	1284	C
1	6	1286	U
1	6	1288	G
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A

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Mol	Chain	Res	Type
1	6	1327	C
1	6	1338	C
1	6	1341	A
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1354	G
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1371	A
1	6	1372	U
1	6	1373	C
1	6	1388	A
1	6	1389	C
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1413	U
1	6	1414	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1431	C
1	6	1433	G
1	6	1445	G
1	6	1446	A
1	6	1448	G
1	6	1458	G
1	6	1459	C
1	6	1460	A
1	6	1461	C
1	6	1471	A
1	6	1481	C
1	6	1482	C
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A

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Mol	Chain	Res	Type
1	6	1496	U
1	6	1506	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	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	1554	U
1	6	1555	A
1	6	1557	U
1	6	1559	A
1	6	1569	A
1	6	1573	A
1	6	1574	G
1	6	1575	G
1	6	1582	U
1	6	1584	G
1	6	1590	G
1	6	1600	A
1	6	1601	G
1	6	1616	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	1656	U
1	6	1657	U
1	6	1658	G
1	6	1696	G
1	6	1697	G
1	6	1698	G
1	6	1699	G

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Mol	Chain	Res	Type
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1712	A
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	1755	A
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A
1	6	1783	C
1	6	1789	G
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1795	U
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	11	A
36	5	16	A
36	5	21	G
36	5	26	A
36	5	40	A
36	5	44	U
36	5	45	A
36	5	49	A
36	5	60	A
36	5	65	A
36	5	66	A
36	5	67	A
36	5	74	G
36	5	76	G

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Mol	Chain	Res	Type
36	5	85	A
36	5	92	G
36	5	93	C
36	5	94	G
36	5	96	G
36	5	99	A
36	5	109	A
36	5	110	G
36	5	111	C
36	5	113	C
36	5	116	A
36	5	120	G
36	5	121	A
36	5	122	A
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G
36	5	142	C
36	5	150	A
36	5	156	G
36	5	157	A
36	5	165	A
36	5	170	G
36	5	171	G
36	5	172	G
36	5	173	G
36	5	174	C
36	5	179	C
36	5	180	C
36	5	182	U
36	5	186	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	200	C
36	5	206	G
36	5	210	U
36	5	211	A
36	5	213	A
36	5	218	G
36	5	219	A

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Mol	Chain	Res	Type
36	5	221	A
36	5	227	G
36	5	236	G
36	5	237	G
36	5	239	G
36	5	240	U
36	5	244	G
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	259	C
36	5	269	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	311	C
36	5	316	U
36	5	322	U
36	5	323	A
36	5	329	U
36	5	334	A
36	5	338	A
36	5	339	C
36	5	349	A
36	5	350	C
36	5	366	A
36	5	376	G
36	5	390	G
36	5	395	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	421	G
36	5	422	A
36	5	436	A
36	5	438	A

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Mol	Chain	Res	Type
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
36	5	529	A
36	5	532	A
36	5	535	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	551	A
36	5	552	G
36	5	553	U
36	5	555	U
36	5	557	A
36	5	559	A
36	5	560	G
36	5	578	A
36	5	579	G
36	5	592	A
36	5	600	G
36	5	604	G
36	5	607	A
36	5	609	G
36	5	611	A
36	5	619	A
36	5	620	U
36	5	621	A
36	5	636	C
36	5	649	A
36	5	651	G
36	5	656	A
36	5	660	A
36	5	661	G
36	5	675	C
36	5	677	A
36	5	681	U
36	5	689	U
36	5	691	A

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Mol	Chain	Res	Type
36	5	705	A
36	5	712	G
36	5	715	A
36	5	716	A
36	5	719	U
36	5	725	G
36	5	727	G
36	5	758	C
36	5	760	G
36	5	766	U
36	5	767	U
36	5	774	G
36	5	776	U
36	5	777	U
36	5	780	A
36	5	781	G
36	5	785	G
36	5	786	A
36	5	800	G
36	5	806	A
36	5	817	A
36	5	830	A
36	5	861	C
36	5	874	U
36	5	877	C
36	5	879	U
36	5	881	C
36	5	896	A
36	5	897	U
36	5	907	G
36	5	908	G
36	5	910	G
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	923	C
36	5	924	G
36	5	937	G
36	5	938	C
36	5	944	C
36	5	959	C

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Mol	Chain	Res	Type
36	5	960	U
36	5	961	C
36	5	963	G
36	5	964	G
36	5	979	U
36	5	984	G
36	5	993	G
36	5	994	G
36	5	1001	G
36	5	1002	A
36	5	1010	G
36	5	1014	U
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1019	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1027	A
36	5	1028	U
36	5	1029	G
36	5	1035	G
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1072	G
36	5	1081	U
36	5	1082	U
36	5	1085	A
36	5	1087	G
36	5	1088	U
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

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Mol	Chain	Res	Type
36	5	1116	G
36	5	1117	G
36	5	1129	A
36	5	1131	G
36	5	1144	U
36	5	1152	G
36	5	1153	A
36	5	1159	A
36	5	1160	C
36	5	1178	G
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1191	U
36	5	1192	C
36	5	1193	A
36	5	1196	C
36	5	1197	A
36	5	1201	C
36	5	1202	A
36	5	1209	G
36	5	1222	G
36	5	1232	C
36	5	1235	U
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1245	A
36	5	1246	G
36	5	1252	A
36	5	1253	U
36	5	1258	U
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1301	A
36	5	1307	G
36	5	1309	U

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Mol	Chain	Res	Type
36	5	1312	C
36	5	1330	A
36	5	1332	A
36	5	1348	U
36	5	1349	G
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1354	G
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1380	G
36	5	1386	A
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1428	A
36	5	1429	G
36	5	1431	G
36	5	1434	G
36	5	1437	C
36	5	1443	G
36	5	1446	A
36	5	1450	G
36	5	1465	A
36	5	1480	G
36	5	1481	A
36	5	1482	A
36	5	1488	G
36	5	1490	A
36	5	1495	U
36	5	1498	A
36	5	1508	C
36	5	1509	A
36	5	1526	U
36	5	1533	U
36	5	1536	G
36	5	1541	G
36	5	1554	U

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Mol	Chain	Res	Type
36	5	1555	U
36	5	1556	C
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1565	G
36	5	1566	A
36	5	1567	U
36	5	1570	U
36	5	1571	A
36	5	1573	G
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1581	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1605	A
36	5	1620	U
36	5	1621	A
36	5	1629	U
36	5	1635	G
36	5	1639	C
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1657	C
36	5	1661	G
36	5	1683	A
36	5	1684	U
36	5	1704	A
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1725	C
36	5	1736	G
36	5	1750	A
36	5	1751	G

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Mol	Chain	Res	Type
36	5	1761	C
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1770	G
36	5	1780	G
36	5	1795	U
36	5	1797	A
36	5	1810	A
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1818	U
36	5	1819	U
36	5	1820	U
36	5	1821	U
36	5	1839	A
36	5	1842	A
36	5	1846	C
36	5	1847	A
36	5	1849	C
36	5	1850	A
36	5	1866	C
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1886	A
36	5	1891	A
36	5	1893	A
36	5	1897	G
36	5	1906	G
36	5	1909	A
36	5	1918	C
36	5	1922	A
36	5	1932	A
36	5	1935	G
36	5	1947	G
36	5	1952	G
36	5	2101	C
36	5	2102	U
36	5	2111	G

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Mol	Chain	Res	Type
36	5	2112	U
36	5	2113	A
36	5	2117	A
36	5	2121	G
36	5	2122	G
36	5	2131	A
36	5	2133	U
36	5	2144	A
36	5	2158	A
36	5	2169	G
36	5	2170	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	2222	A
36	5	2223	A
36	5	2225	U
36	5	2244	A
36	5	2246	G
36	5	2250	G
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2258	U
36	5	2267	C
36	5	2268	U
36	5	2269	U
36	5	2273	G
36	5	2276	G
36	5	2279	A
36	5	2280	A
36	5	2281	A
36	5	2282	U
36	5	2283	G
36	5	2288	G
36	5	2303	A
36	5	2307	G
36	5	2310	U

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Mol	Chain	Res	Type
36	5	2313	A
36	5	2315	G
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2388	U
36	5	2392	C
36	5	2393	G
36	5	2397	A
36	5	2401	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2410	U
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2435	G
36	5	2436	U
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	2514	U
36	5	2515	A
36	5	2522	G
36	5	2523	A
36	5	2524	A
36	5	2526	C

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Mol	Chain	Res	Type
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	2549	G
36	5	2552	C
36	5	2555	G
36	5	2562	A
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2593	A
36	5	2606	G
36	5	2607	G
36	5	2614	G
36	5	2615	G
36	5	2637	A
36	5	2639	G
36	5	2652	U
36	5	2656	A
36	5	2674	A
36	5	2677	G
36	5	2681	U
36	5	2689	A
36	5	2691	A
36	5	2696	A
36	5	2704	A
36	5	2706	G
36	5	2707	C
36	5	2714	G

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Mol	Chain	Res	Type
36	5	2720	G
36	5	2728	G
36	5	2729	U
36	5	2752	U
36	5	2753	G
36	5	2755	C
36	5	2762	A
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2796	G
36	5	2800	G
36	5	2801	A
36	5	2802	A
36	5	2810	C
36	5	2814	G
36	5	2817	A
36	5	2818	U
36	5	2822	U
36	5	2839	G
36	5	2843	U
36	5	2845	A
36	5	2853	A
36	5	2865	U
36	5	2871	G
36	5	2872	A
36	5	2877	G
36	5	2886	U
36	5	2887	A
36	5	2889	C
36	5	2896	A
36	5	2899	C
36	5	2900	A
36	5	2921	U
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2939	G
36	5	2942	C
36	5	2946	A

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Mol	Chain	Res	Type
36	5	2947	G
36	5	2954	U
36	5	2971	A
36	5	2972	G
36	5	2983	C
36	5	2990	G
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3018	C
36	5	3028	G
36	5	3030	G
36	5	3046	A
36	5	3049	A
36	5	3056	U
36	5	3057	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3086	A
36	5	3092	C
36	5	3102	G
36	5	3104	U
36	5	3115	C
36	5	3119	U
36	5	3122	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3150	A
36	5	3153	U
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3164	C
36	5	3165	A
36	5	3166	C
36	5	3168	A
36	5	3171	U
36	5	3172	A

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Mol	Chain	Res	Type
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3177	G
36	5	3179	U
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3206	C
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3227	A
36	5	3229	G
36	5	3239	G
36	5	3243	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3270	U
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3279	A
36	5	3281	U
36	5	3282	U
36	5	3284	G
36	5	3285	C
36	5	3286	G
36	5	3287	U
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3295	A
36	5	3304	U
36	5	3313	U
36	5	3316	A

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Mol	Chain	Res	Type
36	5	3318	G
36	5	3319	U
36	5	3320	A
36	5	3332	U
36	5	3333	G
36	5	3342	A
36	5	3345	G
36	5	3348	G
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3356	G
36	5	3358	U
36	5	3369	G
36	5	3377	G
36	5	3378	C
36	5	3382	U
36	5	3383	G
36	5	3389	U
36	5	3393	U
36	5	3394	U
36	5	3396	U
37	7	7	G
37	7	22	A
37	7	29	C
37	7	33	U
37	7	38	U
37	7	51	A
37	7	52	G
37	7	54	U
37	7	55	A
37	7	60	G
37	7	65	G
37	7	73	C
37	7	74	C
37	7	76	A
37	7	99	G
37	7	101	G
37	7	102	A
37	7	103	A
37	7	110	G
37	7	112	G

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Mol	Chain	Res	Type
38	8	21	C
38	8	34	U
38	8	35	C
38	8	48	A
38	8	51	G
38	8	53	A
38	8	59	A
38	8	62	C
38	8	63	G
38	8	79	A
38	8	80	A
38	8	81	U
38	8	82	U
38	8	83	C
38	8	84	C
38	8	86	U
38	8	87	G
38	8	90	U
38	8	95	G
38	8	96	A
38	8	97	A
38	8	102	U
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	116	G
38	8	122	U
38	8	124	G
38	8	125	U
38	8	151	C
38	8	152	G
38	8	156	U
38	8	157	U
38	8	158	U

All (269) RNA pucker outliers are listed below:

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

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Mol	Chain	Res	Type
1	2	73	U
1	2	103	A
1	2	114	C
1	2	126	A
1	2	130	C
1	2	131	C
1	2	139	C
1	2	144	U
1	2	158	U
1	2	217	A
1	2	218	A
1	2	240	U
1	2	280	U
1	2	321	C
1	2	322	G
1	2	400	A
1	2	417	A
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	510	G
1	2	512	A
1	2	555	A
1	2	558	U
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	734	A
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	1196	A
1	2	1207	C
1	2	1226	A
1	2	1234	A
1	2	1244	A

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Mol	Chain	Res	Type
1	2	1250	U
1	2	1344	A
1	2	1370	U
1	2	1481	C
1	2	1521	G
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1657	U
1	2	1761	U
36	1	43	A
36	1	65	A
36	1	169	U
36	1	210	U
36	1	217	U
36	1	239	G
36	1	282	G
36	1	369	A
36	1	547	G
36	1	559	A
36	1	588	G
36	1	594	U
36	1	620	U
36	1	715	A
36	1	719	U
36	1	763	G
36	1	816	A
36	1	896	A
36	1	916	G
36	1	937	G
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1181	U
36	1	1196	C
36	1	1273	A
36	1	1307	G
36	1	1317	A
36	1	1329	U

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Mol	Chain	Res	Type
36	1	1331	U
36	1	1352	A
36	1	1355	A
36	1	1481	A
36	1	1484	U
36	1	1514	G
36	1	1554	U
36	1	1556	C
36	1	1562	C
36	1	1568	U
36	1	1589	A
36	1	1716	U
36	1	1751	G
36	1	1816	A
36	1	1820	U
36	1	1841	A
36	1	1842	A
36	1	1846	C
36	1	1849	C
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2249	G
36	1	2281	A
36	1	2297	U
36	1	2372	A
36	1	2374	C
36	1	2403	G
36	1	2418	G
36	1	2513	U
36	1	2537	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	2688	U
36	1	2689	A
36	1	2704	A
36	1	2728	G
36	1	2817	A
36	1	2818	U
36	1	3048	A

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Mol	Chain	Res	Type
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3195	U
36	1	3207	U
36	1	3217	C
36	1	3218	A
36	1	3228	C
36	1	3269	U
36	1	3275	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
36	1	3377	G
38	4	85	G
38	4	111	A
1	6	25	C
1	6	66	U
1	6	76	A
1	6	103	A
1	6	113	U
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	313	U
1	6	352	A
1	6	400	A
1	6	417	A
1	6	425	A
1	6	512	A
1	6	542	A
1	6	557	G
1	6	558	U
1	6	606	A
1	6	697	C
1	6	717	C
1	6	755	A

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Mol	Chain	Res	Type
1	6	829	A
1	6	834	G
1	6	1051	G
1	6	1058	U
1	6	1097	U
1	6	1098	U
1	6	1137	A
1	6	1207	C
1	6	1227	A
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1388	A
1	6	1481	C
1	6	1491	U
1	6	1535	U
1	6	1568	C
1	6	1572	G
1	6	1573	A
1	6	1615	C
1	6	1620	C
1	6	1657	U
1	6	1698	G
1	6	1700	C
36	5	43	A
36	5	93	C
36	5	210	U
36	5	217	U
36	5	238	A
36	5	283	G
36	5	397	A
36	5	438	A
36	5	588	G
36	5	594	U
36	5	715	A
36	5	765	C
36	5	816	A
36	5	896	A
36	5	916	G
36	5	960	U
36	5	993	G
36	5	1027	A

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Mol	Chain	Res	Type
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1160	C
36	5	1178	G
36	5	1181	U
36	5	1238	C
36	5	1241	U
36	5	1317	A
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1370	G
36	5	1481	A
36	5	1514	G
36	5	1554	U
36	5	1560	G
36	5	1580	A
36	5	1716	U
36	5	1750	A
36	5	1819	U
36	5	2101	C
36	5	2112	U
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2257	C
36	5	2282	U
36	5	2372	A
36	5	2374	C
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2572	C
36	5	2585	G
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2817	A
36	5	2818	U

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Mol	Chain	Res	Type
36	5	2896	A
36	5	2971	A
36	5	3078	U
36	5	3154	C
36	5	3167	A
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3242	G
36	5	3275	U
36	5	3289	G
36	5	3317	U
36	5	3341	U
36	5	3357	U
38	8	111	A

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
86	OHX	6	2139	-	0,6,6	0.00	-	-		
86	OHX	2	2042	-	0,6,6	0.00	-	-		
86	OHX	5	4045	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	15	303	-	0,6,6	0.00	-	-		
86	OHX	5	4008	-	0,6,6	0.00	-	-		
86	OHX	6	2153	-	0,6,6	0.00	-	-		
86	OHX	1	3952	-	0,6,6	0.00	-	-		
86	OHX	6	2129	-	0,6,6	0.00	-	-		
86	OHX	6	2144	-	0,6,6	0.00	-	-		
86	OHX	5	4100	-	0,6,6	0.00	-	-		
86	OHX	4	227	-	0,6,6	0.00	-	-		
86	OHX	M5	302	-	0,6,6	0.00	-	-		
86	OHX	6	2114	-	0,6,6	0.00	-	-		
86	OHX	6	2105	-	0,6,6	0.00	-	-		
86	OHX	1	3915	-	0,6,6	0.00	-	-		
86	OHX	1	4041	-	0,6,6	0.00	-	-		
86	OHX	5	3913	-	0,6,6	0.00	-	-		
86	OHX	5	4185	-	0,6,6	0.00	-	-		
86	OHX	1	4131	-	0,6,6	0.00	-	-		
86	OHX	5	4118	-	0,6,6	0.00	-	-		
86	OHX	2	2086	-	0,6,6	0.00	-	-		
86	OHX	5	4236	-	0,6,6	0.00	-	-		
86	OHX	5	4014	-	0,6,6	0.00	-	-		
86	OHX	1	4138	-	0,6,6	0.00	-	-		
86	OHX	M7	205	-	0,6,6	0.00	-	-		
86	OHX	1	3932	-	0,6,6	0.00	-	-		
86	OHX	1	3913	-	0,6,6	0.00	-	-		
86	OHX	1	4109	-	0,6,6	0.00	-	-		
86	OHX	5	3992	-	0,6,6	0.00	-	-		
86	OHX	1	4006	-	0,6,6	0.00	-	-		
86	OHX	1	4135	-	0,6,6	0.00	-	-		
86	OHX	5	4175	-	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	5	3995	-	0,6,6	0.00	-	-		
86	OHX	5	3899	-	0,6,6	0.00	-	-		
86	OHX	5	4123	-	0,6,6	0.00	-	-		
86	OHX	2	2069	-	0,6,6	0.00	-	-		
86	OHX	6	2074	-	0,6,6	0.00	-	-		
86	OHX	5	4129	-	0,6,6	0.00	-	-		
86	OHX	1	4011	-	0,6,6	0.00	-	-		
86	OHX	1	3978	-	0,6,6	0.00	-	-		
86	OHX	5	4202	-	0,6,6	0.00	-	-		
86	OHX	6	2156	-	0,6,6	0.00	-	-		
86	OHX	6	2159	-	0,6,6	0.00	-	-		
86	OHX	2	2081	-	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	4086	-	0,6,6	0.00	-	-		
86	OHX	1	4013	-	0,6,6	0.00	-	-		
86	OHX	2	2035	-	0,6,6	0.00	-	-		
86	OHX	5	4226	-	0,6,6	0.00	-	-		
86	OHX	s8	303	-	0,6,6	0.00	-	-		
86	OHX	1	4127	-	0,6,6	0.00	-	-		
86	OHX	5	4108	-	0,6,6	0.00	-	-		
86	OHX	1	3943	-	0,6,6	0.00	-	-		
86	OHX	5	4114	-	0,6,6	0.00	-	-		
86	OHX	5	4167	-	0,6,6	0.00	-	-		
86	OHX	1	3908	-	0,6,6	0.00	-	-		
86	OHX	6	2151	-	0,6,6	0.00	-	-		
86	OHX	6	2175	-	0,6,6	0.00	-	-		
86	OHX	5	3981	-	0,6,6	0.00	-	-		
86	OHX	5	4095	-	0,6,6	0.00	-	-		
86	OHX	5	4180	-	0,6,6	0.00	-	-		
86	OHX	2	2072	-	0,6,6	0.00	-	-		
86	OHX	5	3975	-	0,6,6	0.00	-	-		
86	OHX	1	4100	-	0,6,6	0.00	-	-		
86	OHX	5	3920	-	0,6,6	0.00	-	-		
86	OHX	1	3927	-	0,6,6	0.00	-	-		
86	OHX	5	4231	-	0,6,6	0.00	-	-		
86	OHX	1	3934	-	0,6,6	0.00	-	-		
86	OHX	5	3986	-	0,6,6	0.00	-	-		
86	OHX	6	2096	-	0,6,6	0.00	-	-		
86	OHX	5	4156	-	0,6,6	0.00	-	-		
86	OHX	6	2066	-	0,6,6	0.00	-	-		
86	OHX	8	228	-	0,6,6	0.00	-	-		
86	OHX	1	4007	-	0,6,6	0.00	-	-		
86	OHX	1	4149	-	0,6,6	0.00	-	-		
86	OHX	2	2048	-	0,6,6	0.00	-	-		
86	OHX	5	4240	-	0,6,6	0.00	-	-		
86	OHX	5	4233	-	0,6,6	0.00	-	-		
86	OHX	5	4232	-	0,6,6	0.00	-	-		
86	OHX	5	4172	-	0,6,6	0.00	-	-		
86	OHX	5	4168	-	0,6,6	0.00	-	-		
86	OHX	5	3994	-	0,6,6	0.00	-	-		
86	OHX	5	3923	-	0,6,6	0.00	-	-		
86	OHX	2	2070	-	0,6,6	0.00	-	-		
86	OHX	5	3944	-	0,6,6	0.00	-	-		
86	OHX	2	2137	-	0,6,6	0.00	-	-		
86	OHX	5	4085	-	0,6,6	0.00	-	-		
86	OHX	5	4072	-	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	4097	-	0,6,6	0.00	-	-		
86	OHX	1	4175	-	0,6,6	0.00	-	-		
86	OHX	6	2166	-	0,6,6	0.00	-	-		
86	OHX	6	2168	-	0,6,6	0.00	-	-		
86	OHX	1	4061	-	0,6,6	0.00	-	-		
86	OHX	1	4186	-	0,6,6	0.00	-	-		
86	OHX	5	4198	-	0,6,6	0.00	-	-		
86	OHX	2	2064	-	0,6,6	0.00	-	-		
86	OHX	2	2061	-	0,6,6	0.00	-	-		
86	OHX	6	2085	-	0,6,6	0.00	-	-		
86	OHX	5	4217	-	0,6,6	0.00	-	-		
86	OHX	2	2055	-	0,6,6	0.00	-	-		
86	OHX	6	2101	-	0,6,6	0.00	-	-		
86	OHX	1	4025	-	0,6,6	0.00	-	-		
86	OHX	1	4196	-	0,6,6	0.00	-	-		
86	OHX	6	2134	-	0,6,6	0.00	-	-		
86	OHX	5	3999	-	0,6,6	0.00	-	-		
86	OHX	2	2024	-	0,6,6	0.00	-	-		
86	OHX	6	2116	-	0,6,6	0.00	-	-		
86	OHX	1	4213	-	0,6,6	0.00	-	-		
86	OHX	6	2064	-	0,6,6	0.00	-	-		
86	OHX	6	2051	-	0,6,6	0.00	-	-		
86	OHX	4	238	-	0,6,6	0.00	-	-		
86	OHX	6	2076	-	0,6,6	0.00	-	-		
86	OHX	1	3967	-	0,6,6	0.00	-	-		
86	OHX	L4	403	-	0,6,6	0.00	-	-		
86	OHX	5	3949	-	0,6,6	0.00	-	-		
86	OHX	2	2066	-	0,6,6	0.00	-	-		
86	OHX	5	4021	-	0,6,6	0.00	-	-		
86	OHX	5	4243	-	0,6,6	0.00	-	-		
86	OHX	1	3949	-	0,6,6	0.00	-	-		
86	OHX	2	2057	-	0,6,6	0.00	-	-		
86	OHX	5	4020	-	0,6,6	0.00	-	-		
86	OHX	5	4142	-	0,6,6	0.00	-	-		
86	OHX	5	4219	-	0,6,6	0.00	-	-		
86	OHX	2	2171	-	0,6,6	0.00	-	-		
86	OHX	1	4015	-	0,6,6	0.00	-	-		
86	OHX	6	2192	-	0,6,6	0.00	-	-		
86	OHX	1	4046	-	0,6,6	0.00	-	-		
86	OHX	3	214	-	0,6,6	0.00	-	-		
86	OHX	2	2043	-	0,6,6	0.00	-	-		
86	OHX	4	226	-	0,6,6	0.00	-	-		
86	OHX	1	3986	-	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	4120	-	0,6,6	0.00	-	-		
86	OHX	5	4170	-	0,6,6	0.00	-	-		
86	OHX	1	3879	-	0,6,6	0.00	-	-		
86	OHX	2	2176	-	0,6,6	0.00	-	-		
86	OHX	5	4086	-	0,6,6	0.00	-	-		
86	OHX	1	3907	-	0,6,6	0.00	-	-		
86	OHX	5	4068	-	0,6,6	0.00	-	-		
86	OHX	1	3910	-	0,6,6	0.00	-	-		
86	OHX	1	3980	-	0,6,6	0.00	-	-		
86	OHX	6	2109	-	0,6,6	0.00	-	-		
86	OHX	1	3959	-	0,6,6	0.00	-	-		
86	OHX	C8	201	-	0,6,6	0.00	-	-		
86	OHX	4	230	-	0,6,6	0.00	-	-		
86	OHX	6	2061	-	0,6,6	0.00	-	-		
86	OHX	5	4018	-	0,6,6	0.00	-	-		
86	OHX	1	4206	-	0,6,6	0.00	-	-		
86	OHX	q1	102	-	0,6,6	0.00	-	-		
86	OHX	5	4196	-	0,6,6	0.00	-	-		
86	OHX	2	2040	-	0,6,6	0.00	-	-		
86	OHX	2	2131	-	0,6,6	0.00	-	-		
86	OHX	1	4195	-	0,6,6	0.00	-	-		
86	OHX	2	2166	-	0,6,6	0.00	-	-		
86	OHX	1	4056	-	0,6,6	0.00	-	-		
86	OHX	5	4103	-	0,6,6	0.00	-	-		
86	OHX	5	4076	-	0,6,6	0.00	-	-		
86	OHX	6	2079	-	0,6,6	0.00	-	-		
86	OHX	1	4023	-	0,6,6	0.00	-	-		
86	OHX	1	3951	-	0,6,6	0.00	-	-		
86	OHX	5	3993	-	0,6,6	0.00	-	-		
86	OHX	1	4125	-	0,6,6	0.00	-	-		
86	OHX	1	3882	-	0,6,6	0.00	-	-		
86	OHX	5	4070	-	0,6,6	0.00	-	-		
86	OHX	1	3888	-	0,6,6	0.00	-	-		
86	OHX	1	4176	-	0,6,6	0.00	-	-		
86	OHX	6	2048	-	0,6,6	0.00	-	-		
86	OHX	2	2132	-	0,6,6	0.00	-	-		
86	OHX	1	3975	-	0,6,6	0.00	-	-		
86	OHX	5	4139	-	0,6,6	0.00	-	-		
86	OHX	5	3976	-	0,6,6	0.00	-	-		
86	OHX	1	3935	-	0,6,6	0.00	-	-		
86	OHX	6	2152	-	0,6,6	0.00	-	-		
86	OHX	6	2157	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	n9	101	-	0,6,6	0.00	-	-		
86	OHX	7	222	-	0,6,6	0.00	-	-		
86	OHX	5	4087	-	0,6,6	0.00	-	-		
86	OHX	1	4037	-	0,6,6	0.00	-	-		
86	OHX	5	3950	-	0,6,6	0.00	-	-		
86	OHX	1	3881	-	0,6,6	0.00	-	-		
86	OHX	5	4190	-	0,6,6	0.00	-	-		
86	OHX	2	2052	-	0,6,6	0.00	-	-		
86	OHX	5	4207	-	0,6,6	0.00	-	-		
86	OHX	5	4047	-	0,6,6	0.00	-	-		
86	OHX	6	2130	-	0,6,6	0.00	-	-		
86	OHX	1	4169	-	0,6,6	0.00	-	-		
86	OHX	2	2163	-	0,6,6	0.00	-	-		
86	OHX	1	4215	-	0,6,6	0.00	-	-		
86	OHX	2	2108	-	0,6,6	0.00	-	-		
86	OHX	1	3894	-	0,6,6	0.00	-	-		
86	OHX	2	2153	-	0,6,6	0.00	-	-		
86	OHX	5	4225	-	0,6,6	0.00	-	-		
86	OHX	1	3973	-	0,6,6	0.00	-	-		
86	OHX	2	2179	-	0,6,6	0.00	-	-		
86	OHX	1	4009	-	0,6,6	0.00	-	-		
86	OHX	6	2172	-	0,6,6	0.00	-	-		
86	OHX	6	2113	-	0,6,6	0.00	-	-		
86	OHX	1	4177	-	0,6,6	0.00	-	-		
86	OHX	2	2104	-	0,6,6	0.00	-	-		
86	OHX	5	3984	-	0,6,6	0.00	-	-		
86	OHX	5	3924	-	0,6,6	0.00	-	-		
86	OHX	5	4223	-	0,6,6	0.00	-	-		
86	OHX	1	4064	-	0,6,6	0.00	-	-		
86	OHX	1	3962	-	0,6,6	0.00	-	-		
86	OHX	5	4063	-	0,6,6	0.00	-	-		
86	OHX	3	221	-	0,6,6	0.00	-	-		
86	OHX	6	2087	-	0,6,6	0.00	-	-		
86	OHX	1	4146	-	0,6,6	0.00	-	-		
86	OHX	6	2104	-	0,6,6	0.00	-	-		
86	OHX	5	4052	-	0,6,6	0.00	-	-		
86	OHX	5	3898	-	0,6,6	0.00	-	-		
86	OHX	6	2190	-	0,6,6	0.00	-	-		
86	OHX	5	4189	-	0,6,6	0.00	-	-		
86	OHX	2	2045	-	0,6,6	0.00	-	-		
86	OHX	2	2044	-	0,6,6	0.00	-	-		
86	OHX	6	2119	-	0,6,6	0.00	-	-		
86	OHX	5	4177	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	m5	305	-	0,6,6	0.00	-	-		
86	OHX	4	231	-	0,6,6	0.00	-	-		
86	OHX	6	2164	-	0,6,6	0.00	-	-		
86	OHX	o2	201	-	0,6,6	0.00	-	-		
86	OHX	6	2054	-	0,6,6	0.00	-	-		
86	OHX	5	4036	-	0,6,6	0.00	-	-		
86	OHX	5	4193	-	0,6,6	0.00	-	-		
86	OHX	1	3982	-	0,6,6	0.00	-	-		
86	OHX	5	4239	-	0,6,6	0.00	-	-		
86	OHX	5	4211	-	0,6,6	0.00	-	-		
86	OHX	1	4191	-	0,6,6	0.00	-	-		
86	OHX	1	3939	-	0,6,6	0.00	-	-		
86	OHX	1	4143	-	0,6,6	0.00	-	-		
86	OHX	5	3958	-	0,6,6	0.00	-	-		
86	OHX	6	2203	-	0,6,6	0.00	-	-		
86	OHX	5	3952	-	0,6,6	0.00	-	-		
86	OHX	1	3987	-	0,6,6	0.00	-	-		
86	OHX	6	2049	-	0,6,6	0.00	-	-		
86	OHX	1	4117	-	0,6,6	0.00	-	-		
86	OHX	2	2065	-	0,6,6	0.00	-	-		
86	OHX	1	3912	-	0,6,6	0.00	-	-		
86	OHX	5	3912	-	0,6,6	0.00	-	-		
86	OHX	1	4102	-	0,6,6	0.00	-	-		
86	OHX	1	4183	-	0,6,6	0.00	-	-		
86	OHX	5	3972	-	0,6,6	0.00	-	-		
86	OHX	1	4185	-	0,6,6	0.00	-	-		
86	OHX	3	219	-	0,6,6	0.00	-	-		
86	OHX	1	4010	-	0,6,6	0.00	-	-		
86	OHX	1	4018	-	0,6,6	0.00	-	-		
86	OHX	1	3905	-	0,6,6	0.00	-	-		
86	OHX	1	4053	-	0,6,6	0.00	-	-		
86	OHX	1	3958	-	0,6,6	0.00	-	-		
86	OHX	2	2135	-	0,6,6	0.00	-	-		
86	OHX	1	3933	-	0,6,6	0.00	-	-		
86	OHX	5	4144	-	0,6,6	0.00	-	-		
86	OHX	6	2204	-	0,6,6	0.00	-	-		
86	OHX	5	4112	-	0,6,6	0.00	-	-		
86	OHX	2	2080	-	0,6,6	0.00	-	-		
86	OHX	2	2142	-	0,6,6	0.00	-	-		
86	OHX	1	4189	-	0,6,6	0.00	-	-		
86	OHX	5	4106	-	0,6,6	0.00	-	-		
86	OHX	7	221	-	0,6,6	0.00	-	-		
86	OHX	5	3945	-	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	4200	-	0,6,6	0.00	-	-		
86	OHX	6	2089	-	0,6,6	0.00	-	-		
86	OHX	1	4182	-	0,6,6	0.00	-	-		
86	OHX	1	4044	-	0,6,6	0.00	-	-		
86	OHX	S8	302	-	0,6,6	0.00	-	-		
86	OHX	1	3960	-	0,6,6	0.00	-	-		
86	OHX	5	4120	-	0,6,6	0.00	-	-		
86	OHX	1	4049	-	0,6,6	0.00	-	-		
86	OHX	5	3967	-	0,6,6	0.00	-	-		
86	OHX	5	4143	-	0,6,6	0.00	-	-		
86	OHX	6	2182	-	0,6,6	0.00	-	-		
86	OHX	5	4218	-	0,6,6	0.00	-	-		
86	OHX	6	2097	-	0,6,6	0.00	-	-		
86	OHX	6	2199	-	0,6,6	0.00	-	-		
86	OHX	1	3969	-	0,6,6	0.00	-	-		
86	OHX	5	4116	-	0,6,6	0.00	-	-		
86	OHX	6	2112	-	0,6,6	0.00	-	-		
86	OHX	5	4088	-	0,6,6	0.00	-	-		
86	OHX	1	4197	-	0,6,6	0.00	-	-		
86	OHX	1	4158	-	0,6,6	0.00	-	-		
86	OHX	5	4013	-	0,6,6	0.00	-	-		
86	OHX	5	3985	-	0,6,6	0.00	-	-		
86	OHX	1	4134	-	0,6,6	0.00	-	-		
86	OHX	6	2091	-	0,6,6	0.00	-	-		
86	OHX	2	2159	-	0,6,6	0.00	-	-		
86	OHX	5	3929	-	0,6,6	0.00	-	-		
86	OHX	1	3930	-	0,6,6	0.00	-	-		
86	OHX	C3	201	-	0,6,6	0.00	-	-		
86	OHX	2	2083	-	0,6,6	0.00	-	-		
86	OHX	SR	401	-	0,6,6	0.00	-	-		
86	OHX	6	2171	-	0,6,6	0.00	-	-		
86	OHX	6	2145	-	0,6,6	0.00	-	-		
86	OHX	1	4091	-	0,6,6	0.00	-	-		
86	OHX	5	4011	-	0,6,6	0.00	-	-		
86	OHX	2	2116	-	0,6,6	0.00	-	-		
86	OHX	8	224	-	0,6,6	0.00	-	-		
86	OHX	2	2099	-	0,6,6	0.00	-	-		
86	OHX	5	3930	-	0,6,6	0.00	-	-		
86	OHX	1	3968	-	0,6,6	0.00	-	-		
88	3K5	5	4249	-	62,63,63	0.62	1 (1%)	82,95,95	1.38	11 (13%)
86	OHX	2	2140	-	0,6,6	0.00	-	-		
86	OHX	5	4038	-	0,6,6	0.00	-	-		
86	OHX	5	3939	-	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	4096	-	0,6,6	0.00	-	-		
86	OHX	5	4133	-	0,6,6	0.00	-	-		
86	OHX	1	3909	-	0,6,6	0.00	-	-		
86	OHX	1	4104	-	0,6,6	0.00	-	-		
86	OHX	1	4099	-	0,6,6	0.00	-	-		
86	OHX	6	2099	-	0,6,6	0.00	-	-		
86	OHX	2	2151	-	0,6,6	0.00	-	-		
86	OHX	5	3997	-	0,6,6	0.00	-	-		
86	OHX	5	3934	-	0,6,6	0.00	-	-		
86	OHX	1	4116	-	0,6,6	0.00	-	-		
86	OHX	1	4030	-	0,6,6	0.00	-	-		
86	OHX	2	2160	-	0,6,6	0.00	-	-		
86	OHX	1	3895	-	0,6,6	0.00	-	-		
86	OHX	2	2050	-	0,6,6	0.00	-	-		
86	OHX	1	4209	-	0,6,6	0.00	-	-		
86	OHX	1	3941	-	0,6,6	0.00	-	-		
86	OHX	1	4028	-	0,6,6	0.00	-	-		
86	OHX	1	4106	-	0,6,6	0.00	-	-		
86	OHX	1	3944	-	0,6,6	0.00	-	-		
86	OHX	1	4192	-	0,6,6	0.00	-	-		
86	OHX	1	4076	-	0,6,6	0.00	-	-		
86	OHX	5	4165	-	0,6,6	0.00	-	-		
86	OHX	5	4098	-	0,6,6	0.00	-	-		
86	OHX	5	4212	-	0,6,6	0.00	-	-		
86	OHX	6	2069	-	0,6,6	0.00	-	-		
86	OHX	5	4121	-	0,6,6	0.00	-	-		
86	OHX	6	2132	-	0,6,6	0.00	-	-		
86	OHX	6	2162	-	0,6,6	0.00	-	-		
86	OHX	2	2028	-	0,6,6	0.00	-	-		
86	OHX	4	236	-	0,6,6	0.00	-	-		
86	OHX	1	3897	-	0,6,6	0.00	-	-		
86	OHX	5	3926	-	0,6,6	0.00	-	-		
86	OHX	5	3980	-	0,6,6	0.00	-	-		
86	OHX	5	3937	-	0,6,6	0.00	-	-		
86	OHX	2	2133	-	0,6,6	0.00	-	-		
86	OHX	O3	202	-	0,6,6	0.00	-	-		
86	OHX	1	4032	-	0,6,6	0.00	-	-		
86	OHX	5	4135	-	0,6,6	0.00	-	-		
86	OHX	1	4068	-	0,6,6	0.00	-	-		
86	OHX	1	3874	-	0,6,6	0.00	-	-		
86	OHX	5	4186	-	0,6,6	0.00	-	-		
86	OHX	1	3917	-	0,6,6	0.00	-	-		
86	OHX	5	4157	-	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	3915	-	0,6,6	0.00	-	-		
86	OHX	2	2150	-	0,6,6	0.00	-	-		
86	OHX	2	2038	-	0,6,6	0.00	-	-		
86	OHX	1	3963	-	0,6,6	0.00	-	-		
86	OHX	1	4002	-	0,6,6	0.00	-	-		
86	OHX	2	2090	-	0,6,6	0.00	-	-		
86	OHX	5	4237	-	0,6,6	0.00	-	-		
86	OHX	1	3875	-	0,6,6	0.00	-	-		
86	OHX	5	4220	-	0,6,6	0.00	-	-		
86	OHX	6	2173	-	0,6,6	0.00	-	-		
86	OHX	1	4029	-	0,6,6	0.00	-	-		
86	OHX	1	4148	-	0,6,6	0.00	-	-		
86	OHX	1	3965	-	0,6,6	0.00	-	-		
86	OHX	1	4123	-	0,6,6	0.00	-	-		
86	OHX	2	2145	-	0,6,6	0.00	-	-		
86	OHX	1	4045	-	0,6,6	0.00	-	-		
86	OHX	2	2063	-	0,6,6	0.00	-	-		
86	OHX	1	3884	-	0,6,6	0.00	-	-		
86	OHX	5	4208	-	0,6,6	0.00	-	-		
86	OHX	6	2068	-	0,6,6	0.00	-	-		
86	OHX	5	4174	-	0,6,6	0.00	-	-		
86	OHX	5	4073	-	0,6,6	0.00	-	-		
86	OHX	2	2073	-	0,6,6	0.00	-	-		
86	OHX	5	4183	-	0,6,6	0.00	-	-		
86	OHX	1	4155	-	0,6,6	0.00	-	-		
86	OHX	5	3979	-	0,6,6	0.00	-	-		
86	OHX	1	4150	-	0,6,6	0.00	-	-		
86	OHX	D3	202	-	0,6,6	0.00	-	-		
86	OHX	5	4056	-	0,6,6	0.00	-	-		
86	OHX	5	4222	-	0,6,6	0.00	-	-		
86	OHX	5	4140	-	0,6,6	0.00	-	-		
86	OHX	1	4024	-	0,6,6	0.00	-	-		
86	OHX	5	4191	-	0,6,6	0.00	-	-		
86	OHX	1	4193	-	0,6,6	0.00	-	-		
86	OHX	5	4019	-	0,6,6	0.00	-	-		
86	OHX	2	2169	-	0,6,6	0.00	-	-		
86	OHX	5	4093	-	0,6,6	0.00	-	-		
86	OHX	5	4155	-	0,6,6	0.00	-	-		
86	OHX	4	239	-	0,6,6	0.00	-	-		
86	OHX	5	4077	-	0,6,6	0.00	-	-		
86	OHX	5	4224	-	0,6,6	0.00	-	-		
86	OHX	6	2170	-	0,6,6	0.00	-	-		
86	OHX	1	4159	-	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	4085	-	0,6,6	0.00	-	-		
86	OHX	6	2072	-	0,6,6	0.00	-	-		
86	OHX	1	4157	-	0,6,6	0.00	-	-		
86	OHX	5	4163	-	0,6,6	0.00	-	-		
86	OHX	1	3892	-	0,6,6	0.00	-	-		
86	OHX	1	4075	-	0,6,6	0.00	-	-		
86	OHX	1	4001	-	0,6,6	0.00	-	-		
86	OHX	1	4141	-	0,6,6	0.00	-	-		
86	OHX	1	3929	-	0,6,6	0.00	-	-		
86	OHX	5	4084	-	0,6,6	0.00	-	-		
86	OHX	5	3927	-	0,6,6	0.00	-	-		
86	OHX	2	2091	-	0,6,6	0.00	-	-		
86	OHX	5	4062	-	0,6,6	0.00	-	-		
86	OHX	6	2177	-	0,6,6	0.00	-	-		
86	OHX	5	4094	-	0,6,6	0.00	-	-		
86	OHX	6	2198	-	0,6,6	0.00	-	-		
86	OHX	6	2122	-	0,6,6	0.00	-	-		
86	OHX	5	3941	-	0,6,6	0.00	-	-		
86	OHX	1	4129	-	0,6,6	0.00	-	-		
86	OHX	5	4205	-	0,6,6	0.00	-	-		
86	OHX	1	4101	-	0,6,6	0.00	-	-		
86	OHX	5	3906	-	0,6,6	0.00	-	-		
86	OHX	L3	405	-	0,6,6	0.00	-	-		
86	OHX	1	3988	-	0,6,6	0.00	-	-		
86	OHX	1	3901	-	0,6,6	0.00	-	-		
86	OHX	5	4127	-	0,6,6	0.00	-	-		
86	OHX	6	2141	-	0,6,6	0.00	-	-		
86	OHX	5	3965	-	0,6,6	0.00	-	-		
86	OHX	1	4219	-	0,6,6	0.00	-	-		
86	OHX	8	230	-	0,6,6	0.00	-	-		
86	OHX	6	2163	-	0,6,6	0.00	-	-		
86	OHX	1	3997	-	0,6,6	0.00	-	-		
86	OHX	1	4083	-	0,6,6	0.00	-	-		
86	OHX	1	3984	-	0,6,6	0.00	-	-		
86	OHX	1	4187	-	0,6,6	0.00	-	-		
86	OHX	1	4094	-	0,6,6	0.00	-	-		
86	OHX	6	2106	-	0,6,6	0.00	-	-		
86	OHX	5	4104	-	0,6,6	0.00	-	-		
86	OHX	O7	104	-	0,6,6	0.00	-	-		
86	OHX	5	3971	-	0,6,6	0.00	-	-		
86	OHX	m8	201	-	0,6,6	0.00	-	-		
86	OHX	5	4111	-	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	5	4235	-	0,6,6	0.00	-	-		
86	OHX	5	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4110	-	0,6,6	0.00	-	-		
86	OHX	5	4058	-	0,6,6	0.00	-	-		
86	OHX	1	4174	-	0,6,6	0.00	-	-		
86	OHX	5	4210	-	0,6,6	0.00	-	-		
86	OHX	5	4024	-	0,6,6	0.00	-	-		
86	OHX	6	2100	-	0,6,6	0.00	-	-		
86	OHX	15	306	-	0,6,6	0.00	-	-		
86	OHX	1	4194	-	0,6,6	0.00	-	-		
86	OHX	1	4047	-	0,6,6	0.00	-	-		
86	OHX	1	4108	-	0,6,6	0.00	-	-		
86	OHX	m0	302	-	0,6,6	0.00	-	-		
86	OHX	1	4211	-	0,6,6	0.00	-	-		
86	OHX	2	2121	-	0,6,6	0.00	-	-		
86	OHX	5	3988	-	0,6,6	0.00	-	-		
86	OHX	5	3963	-	0,6,6	0.00	-	-		
86	OHX	O7	105	-	0,6,6	0.00	-	-		
86	OHX	5	4134	-	0,6,6	0.00	-	-		
86	OHX	5	3978	-	0,6,6	0.00	-	-		
86	OHX	5	3977	-	0,6,6	0.00	-	-		
86	OHX	1	4133	-	0,6,6	0.00	-	-		
86	OHX	5	4149	-	0,6,6	0.00	-	-		
86	OHX	6	2128	-	0,6,6	0.00	-	-		
86	OHX	6	2183	-	0,6,6	0.00	-	-		
86	OHX	m0	301	-	0,6,6	0.00	-	-		
86	OHX	5	3955	-	0,6,6	0.00	-	-		
86	OHX	1	3955	-	0,6,6	0.00	-	-		
86	OHX	6	2110	-	0,6,6	0.00	-	-		
86	OHX	5	4122	-	0,6,6	0.00	-	-		
86	OHX	6	2185	-	0,6,6	0.00	-	-		
86	OHX	5	4046	-	0,6,6	0.00	-	-		
86	OHX	6	2046	-	0,6,6	0.00	-	-		
86	OHX	1	4171	-	0,6,6	0.00	-	-		
86	OHX	2	2027	-	0,6,6	0.00	-	-		
86	OHX	5	4184	-	0,6,6	0.00	-	-		
86	OHX	5	4025	-	0,6,6	0.00	-	-		
86	OHX	6	2149	-	0,6,6	0.00	-	-		
86	OHX	2	2095	-	0,6,6	0.00	-	-		
86	OHX	5	3901	-	0,6,6	0.00	-	-		
86	OHX	15	305	-	0,6,6	0.00	-	-		
86	OHX	1	4070	-	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	3886	-	0,6,6	0.00	-	-		
86	OHX	1	4168	-	0,6,6	0.00	-	-		
86	OHX	1	3887	-	0,6,6	0.00	-	-		
86	OHX	1	4140	-	0,6,6	0.00	-	-		
86	OHX	5	4029	-	0,6,6	0.00	-	-		
86	OHX	1	4027	-	0,6,6	0.00	-	-		
86	OHX	2	2076	-	0,6,6	0.00	-	-		
86	OHX	19	202	-	0,6,6	0.00	-	-		
86	OHX	6	2071	-	0,6,6	0.00	-	-		
86	OHX	5	3961	-	0,6,6	0.00	-	-		
86	OHX	5	4141	-	0,6,6	0.00	-	-		
86	OHX	6	2090	-	0,6,6	0.00	-	-		
86	OHX	1	4111	-	0,6,6	0.00	-	-		
86	OHX	2	2037	-	0,6,6	0.00	-	-		
86	OHX	5	4053	-	0,6,6	0.00	-	-		
86	OHX	1	4107	-	0,6,6	0.00	-	-		
86	OHX	5	3943	-	0,6,6	0.00	-	-		
86	OHX	1	4066	-	0,6,6	0.00	-	-		
86	OHX	6	2195	-	0,6,6	0.00	-	-		
86	OHX	c8	203	-	0,6,6	0.00	-	-		
86	OHX	1	4167	-	0,6,6	0.00	-	-		
86	OHX	2	2088	-	0,6,6	0.00	-	-		
86	OHX	5	4131	-	0,6,6	0.00	-	-		
86	OHX	5	3983	-	0,6,6	0.00	-	-		
86	OHX	6	2176	-	0,6,6	0.00	-	-		
86	OHX	5	4176	-	0,6,6	0.00	-	-		
86	OHX	5	4188	-	0,6,6	0.00	-	-		
86	OHX	6	2205	-	0,6,6	0.00	-	-		
86	OHX	2	2129	-	0,6,6	0.00	-	-		
86	OHX	5	4242	-	0,6,6	0.00	-	-		
86	OHX	5	3956	-	0,6,6	0.00	-	-		
86	OHX	7	225	-	0,6,6	0.00	-	-		
86	OHX	5	4037	-	0,6,6	0.00	-	-		
86	OHX	1	3936	-	0,6,6	0.00	-	-		
86	OHX	5	4138	-	0,6,6	0.00	-	-		
86	OHX	5	3970	-	0,6,6	0.00	-	-		
86	OHX	5	3925	-	0,6,6	0.00	-	-		
86	OHX	5	4150	-	0,6,6	0.00	-	-		
86	OHX	2	2032	-	0,6,6	0.00	-	-		
86	OHX	2	2107	-	0,6,6	0.00	-	-		
86	OHX	1	4089	-	0,6,6	0.00	-	-		
86	OHX	6	2181	-	0,6,6	0.00	-	-		
86	OHX	2	2102	-	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	3962	-	0,6,6	0.00	-	-		
86	OHX	1	4154	-	0,6,6	0.00	-	-		
86	OHX	4	235	-	0,6,6	0.00	-	-		
86	OHX	1	4096	-	0,6,6	0.00	-	-		
86	OHX	8	229	-	0,6,6	0.00	-	-		
86	OHX	6	2174	-	0,6,6	0.00	-	-		
86	OHX	1	3904	-	0,6,6	0.00	-	-		
86	OHX	5	4162	-	0,6,6	0.00	-	-		
86	OHX	7	226	-	0,6,6	0.00	-	-		
86	OHX	5	4215	-	0,6,6	0.00	-	-		
86	OHX	7	223	-	0,6,6	0.00	-	-		
86	OHX	6	2107	-	0,6,6	0.00	-	-		
86	OHX	8	221	-	0,6,6	0.00	-	-		
86	OHX	1	3996	-	0,6,6	0.00	-	-		
86	OHX	c5	201	-	0,6,6	0.00	-	-		
86	OHX	1	3925	-	0,6,6	0.00	-	-		
86	OHX	1	4092	-	0,6,6	0.00	-	-		
86	OHX	1	3924	-	0,6,6	0.00	-	-		
86	OHX	8	232	-	0,6,6	0.00	-	-		
86	OHX	1	4112	-	0,6,6	0.00	-	-		
86	OHX	2	2105	-	0,6,6	0.00	-	-		
86	OHX	6	2124	-	0,6,6	0.00	-	-		
86	OHX	1	3899	-	0,6,6	0.00	-	-		
86	OHX	1	4130	-	0,6,6	0.00	-	-		
86	OHX	1	4122	-	0,6,6	0.00	-	-		
86	OHX	2	2054	-	0,6,6	0.00	-	-		
86	OHX	1	3976	-	0,6,6	0.00	-	-		
86	OHX	2	2175	-	0,6,6	0.00	-	-		
86	OHX	4	233	-	0,6,6	0.00	-	-		
86	OHX	2	2113	-	0,6,6	0.00	-	-		
86	OHX	1	4063	-	0,6,6	0.00	-	-		
86	OHX	6	2083	-	0,6,6	0.00	-	-		
86	OHX	1	3947	-	0,6,6	0.00	-	-		
86	OHX	5	4247	-	0,6,6	0.00	-	-		
86	OHX	1	3928	-	0,6,6	0.00	-	-		
86	OHX	2	2103	-	0,6,6	0.00	-	-		
86	OHX	m6	203	-	0,6,6	0.00	-	-		
86	OHX	1	4059	-	0,6,6	0.00	-	-		
86	OHX	5	4089	-	0,6,6	0.00	-	-		
86	OHX	1	4084	-	0,6,6	0.00	-	-		
88	3K5	1	4221	-	62,63,63	1.22	2 (3%)	82,95,95	1.47	11 (13%)
86	OHX	1	4042	-	0,6,6	0.00	-	-		
86	OHX	o7	503	-	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	4115	-	0,6,6	0.00	-	-		
86	OHX	2	2096	-	0,6,6	0.00	-	-		
86	OHX	d4	201	-	0,6,6	0.00	-	-		
86	OHX	1	3940	-	0,6,6	0.00	-	-		
86	OHX	1	4071	-	0,6,6	0.00	-	-		
86	OHX	1	4003	-	0,6,6	0.00	-	-		
86	OHX	5	4173	-	0,6,6	0.00	-	-		
86	OHX	1	4142	-	0,6,6	0.00	-	-		
86	OHX	5	3948	-	0,6,6	0.00	-	-		
86	OHX	1	4051	-	0,6,6	0.00	-	-		
86	OHX	1	4147	-	0,6,6	0.00	-	-		
86	OHX	1	4212	-	0,6,6	0.00	-	-		
86	OHX	5	4012	-	0,6,6	0.00	-	-		
86	OHX	6	2065	-	0,6,6	0.00	-	-		
86	OHX	5	4229	-	0,6,6	0.00	-	-		
86	OHX	1	4198	-	0,6,6	0.00	-	-		
86	OHX	1	4205	-	0,6,6	0.00	-	-		
86	OHX	2	2078	-	0,6,6	0.00	-	-		
86	OHX	1	4017	-	0,6,6	0.00	-	-		
86	OHX	2	2127	-	0,6,6	0.00	-	-		
86	OHX	1	4098	-	0,6,6	0.00	-	-		
86	OHX	2	2062	-	0,6,6	0.00	-	-		
86	OHX	2	2068	-	0,6,6	0.00	-	-		
86	OHX	3	222	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	6	2142	-	0,6,6	0.00	-	-		
86	OHX	1	4164	-	0,6,6	0.00	-	-		
86	OHX	5	4010	-	0,6,6	0.00	-	-		
86	OHX	8	227	-	0,6,6	0.00	-	-		
86	OHX	2	2046	-	0,6,6	0.00	-	-		
86	OHX	6	2084	-	0,6,6	0.00	-	-		
86	OHX	1	4172	-	0,6,6	0.00	-	-		
86	OHX	6	2137	-	0,6,6	0.00	-	-		
86	OHX	5	3907	-	0,6,6	0.00	-	-		
86	OHX	1	4207	-	0,6,6	0.00	-	-		
86	OHX	1	4208	-	0,6,6	0.00	-	-		
86	OHX	5	4067	-	0,6,6	0.00	-	-		
86	OHX	2	2143	-	0,6,6	0.00	-	-		
86	OHX	1	3974	-	0,6,6	0.00	-	-		
86	OHX	6	2056	-	0,6,6	0.00	-	-		
86	OHX	1	3979	-	0,6,6	0.00	-	-		
86	OHX	5	4158	-	0,6,6	0.00	-	-		
86	OHX	1	3903	-	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	2056	-	0,6,6	0.00	-	-		
86	OHX	2	2093	-	0,6,6	0.00	-	-		
86	OHX	1	3906	-	0,6,6	0.00	-	-		
86	OHX	5	4241	-	0,6,6	0.00	-	-		
86	OHX	2	2067	-	0,6,6	0.00	-	-		
86	OHX	1	4035	-	0,6,6	0.00	-	-		
86	OHX	5	3982	-	0,6,6	0.00	-	-		
86	OHX	2	2059	-	0,6,6	0.00	-	-		
86	OHX	5	3914	-	0,6,6	0.00	-	-		
86	OHX	1	3991	-	0,6,6	0.00	-	-		
86	OHX	5	4102	-	0,6,6	0.00	-	-		
86	OHX	6	2193	-	0,6,6	0.00	-	-		
86	OHX	N1	201	-	0,6,6	0.00	-	-		
86	OHX	6	2058	-	0,6,6	0.00	-	-		
86	OHX	5	4146	-	0,6,6	0.00	-	-		
86	OHX	s1	303	-	0,6,6	0.00	-	-		
86	OHX	1	4113	-	0,6,6	0.00	-	-		
86	OHX	2	2094	-	0,6,6	0.00	-	-		
86	OHX	5	3919	-	0,6,6	0.00	-	-		
86	OHX	5	3911	-	0,6,6	0.00	-	-		
86	OHX	1	4065	-	0,6,6	0.00	-	-		
86	OHX	2	2079	-	0,6,6	0.00	-	-		
86	OHX	2	2174	-	0,6,6	0.00	-	-		
86	OHX	5	4031	-	0,6,6	0.00	-	-		
86	OHX	2	2120	-	0,6,6	0.00	-	-		
86	OHX	6	2086	-	0,6,6	0.00	-	-		
86	OHX	1	4181	-	0,6,6	0.00	-	-		
86	OHX	3	224	-	0,6,6	0.00	-	-		
86	OHX	5	3960	-	0,6,6	0.00	-	-		
86	OHX	1	4069	-	0,6,6	0.00	-	-		
86	OHX	1	4093	-	0,6,6	0.00	-	-		
86	OHX	1	3916	-	0,6,6	0.00	-	-		
86	OHX	2	2155	-	0,6,6	0.00	-	-		
86	OHX	1	3921	-	0,6,6	0.00	-	-		
86	OHX	2	2089	-	0,6,6	0.00	-	-		
86	OHX	2	2123	-	0,6,6	0.00	-	-		
86	OHX	5	4002	-	0,6,6	0.00	-	-		
86	OHX	5	4039	-	0,6,6	0.00	-	-		
86	OHX	5	4228	-	0,6,6	0.00	-	-		
86	OHX	6	2136	-	0,6,6	0.00	-	-		
86	OHX	1	4210	-	0,6,6	0.00	-	-		
86	OHX	2	2039	-	0,6,6	0.00	-	-		
86	OHX	5	4054	-	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	4012	-	0,6,6	0.00	-	-		
86	OHX	4	225	-	0,6,6	0.00	-	-		
86	OHX	1	4178	-	0,6,6	0.00	-	-		
86	OHX	1	3964	-	0,6,6	0.00	-	-		
86	OHX	1	3873	-	0,6,6	0.00	-	-		
86	OHX	1	4152	-	0,6,6	0.00	-	-		
86	OHX	5	4159	-	0,6,6	0.00	-	-		
86	OHX	5	3959	-	0,6,6	0.00	-	-		
86	OHX	1	4202	-	0,6,6	0.00	-	-		
86	OHX	14	402	-	0,6,6	0.00	-	-		
86	OHX	2	2060	-	0,6,6	0.00	-	-		
86	OHX	2	2141	-	0,6,6	0.00	-	-		
86	OHX	5	4119	-	0,6,6	0.00	-	-		
86	OHX	2	2106	-	0,6,6	0.00	-	-		
86	OHX	5	4201	-	0,6,6	0.00	-	-		
86	OHX	5	4026	-	0,6,6	0.00	-	-		
86	OHX	5	4028	-	0,6,6	0.00	-	-		
86	OHX	5	4145	-	0,6,6	0.00	-	-		
86	OHX	5	3996	-	0,6,6	0.00	-	-		
86	OHX	5	3954	-	0,6,6	0.00	-	-		
86	OHX	1	3948	-	0,6,6	0.00	-	-		
86	OHX	1	4110	-	0,6,6	0.00	-	-		
86	OHX	1	4072	-	0,6,6	0.00	-	-		
86	OHX	8	223	-	0,6,6	0.00	-	-		
86	OHX	4	234	-	0,6,6	0.00	-	-		
86	OHX	1	4077	-	0,6,6	0.00	-	-		
86	OHX	1	3914	-	0,6,6	0.00	-	-		
86	OHX	7	219	-	0,6,6	0.00	-	-		
86	OHX	5	4061	-	0,6,6	0.00	-	-		
86	OHX	s1	302	-	0,6,6	0.00	-	-		
86	OHX	6	2123	-	0,6,6	0.00	-	-		
86	OHX	5	4040	-	0,6,6	0.00	-	-		
86	OHX	5	3909	-	0,6,6	0.00	-	-		
86	OHX	6	2133	-	0,6,6	0.00	-	-		
86	OHX	5	4209	-	0,6,6	0.00	-	-		
86	OHX	2	2030	-	0,6,6	0.00	-	-		
86	OHX	5	4203	-	0,6,6	0.00	-	-		
86	OHX	5	3900	-	0,6,6	0.00	-	-		
86	OHX	5	4033	-	0,6,6	0.00	-	-		
86	OHX	5	4003	-	0,6,6	0.00	-	-		
86	OHX	6	2179	-	0,6,6	0.00	-	-		
86	OHX	1	4034	-	0,6,6	0.00	-	-		
86	OHX	5	3910	-	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	4132	-	0,6,6	0.00	-	-		
86	OHX	5	4099	-	0,6,6	0.00	-	-		
86	OHX	1	4043	-	0,6,6	0.00	-	-		
86	OHX	1	4126	-	0,6,6	0.00	-	-		
86	OHX	5	3917	-	0,6,6	0.00	-	-		
86	OHX	sR	401	-	0,6,6	0.00	-	-		
86	OHX	1	3876	-	0,6,6	0.00	-	-		
86	OHX	5	4166	-	0,6,6	0.00	-	-		
86	OHX	5	3966	-	0,6,6	0.00	-	-		
86	OHX	6	2184	-	0,6,6	0.00	-	-		
86	OHX	5	4048	-	0,6,6	0.00	-	-		
86	OHX	5	4016	-	0,6,6	0.00	-	-		
86	OHX	6	2053	-	0,6,6	0.00	-	-		
86	OHX	1	4114	-	0,6,6	0.00	-	-		
86	OHX	6	2194	-	0,6,6	0.00	-	-		
86	OHX	1	3878	-	0,6,6	0.00	-	-		
86	OHX	5	4171	-	0,6,6	0.00	-	-		
86	OHX	5	3973	-	0,6,6	0.00	-	-		
86	OHX	5	4182	-	0,6,6	0.00	-	-		
86	OHX	1	4163	-	0,6,6	0.00	-	-		
86	OHX	2	2125	-	0,6,6	0.00	-	-		
86	OHX	2	2173	-	0,6,6	0.00	-	-		
86	OHX	6	2158	-	0,6,6	0.00	-	-		
86	OHX	1	3985	-	0,6,6	0.00	-	-		
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	1	3893	-	0,6,6	0.00	-	-		
86	OHX	5	4051	-	0,6,6	0.00	-	-		
86	OHX	1	3971	-	0,6,6	0.00	-	-		
86	OHX	1	3911	-	0,6,6	0.00	-	-		
86	OHX	6	2178	-	0,6,6	0.00	-	-		
86	OHX	1	4162	-	0,6,6	0.00	-	-		
86	OHX	6	2180	-	0,6,6	0.00	-	-		
86	OHX	1	3885	-	0,6,6	0.00	-	-		
86	OHX	1	3999	-	0,6,6	0.00	-	-		
86	OHX	1	3877	-	0,6,6	0.00	-	-		
86	OHX	5	4057	-	0,6,6	0.00	-	-		
86	OHX	5	4059	-	0,6,6	0.00	-	-		
86	OHX	2	2110	-	0,6,6	0.00	-	-		
86	OHX	8	226	-	0,6,6	0.00	-	-		
86	OHX	6	2191	-	0,6,6	0.00	-	-		
86	OHX	2	2161	-	0,6,6	0.00	-	-		
86	OHX	1	4097	-	0,6,6	0.00	-	-		
86	OHX	5	4227	-	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	4248	-	0,6,6	0.00	-	-		
86	OHX	2	2097	-	0,6,6	0.00	-	-		
86	OHX	1	4021	-	0,6,6	0.00	-	-		
86	OHX	2	2092	-	0,6,6	0.00	-	-		
86	OHX	5	3932	-	0,6,6	0.00	-	-		
86	OHX	1	3922	-	0,6,6	0.00	-	-		
86	OHX	5	4148	-	0,6,6	0.00	-	-		
86	OHX	5	4060	-	0,6,6	0.00	-	-		
86	OHX	1	4058	-	0,6,6	0.00	-	-		
86	OHX	2	2162	-	0,6,6	0.00	-	-		
86	OHX	6	2186	-	0,6,6	0.00	-	-		
86	OHX	6	2161	-	0,6,6	0.00	-	-		
86	OHX	5	4206	-	0,6,6	0.00	-	-		
86	OHX	2	2053	-	0,6,6	0.00	-	-		
86	OHX	1	4190	-	0,6,6	0.00	-	-		
86	OHX	1	3945	-	0,6,6	0.00	-	-		
86	OHX	5	4042	-	0,6,6	0.00	-	-		
86	OHX	6	2111	-	0,6,6	0.00	-	-		
86	OHX	5	3916	-	0,6,6	0.00	-	-		
86	OHX	1	3880	-	0,6,6	0.00	-	-		
86	OHX	5	4192	-	0,6,6	0.00	-	-		
86	OHX	1	3998	-	0,6,6	0.00	-	-		
86	OHX	5	4246	-	0,6,6	0.00	-	-		
86	OHX	1	3992	-	0,6,6	0.00	-	-		
86	OHX	8	222	-	0,6,6	0.00	-	-		
86	OHX	5	4007	-	0,6,6	0.00	-	-		
86	OHX	2	2025	-	0,6,6	0.00	-	-		
86	OHX	1	3942	-	0,6,6	0.00	-	-		
86	OHX	2	2168	-	0,6,6	0.00	-	-		
86	OHX	6	2093	-	0,6,6	0.00	-	-		
86	OHX	2	2031	-	0,6,6	0.00	-	-		
86	OHX	2	2136	-	0,6,6	0.00	-	-		
86	OHX	6	2138	-	0,6,6	0.00	-	-		
86	OHX	2	2047	-	0,6,6	0.00	-	-		
86	OHX	5	4179	-	0,6,6	0.00	-	-		
86	OHX	l3	404	-	0,6,6	0.00	-	-		
86	OHX	m5	304	-	0,6,6	0.00	-	-		
86	OHX	n3	203	-	0,6,6	0.00	-	-		
86	OHX	1	4124	-	0,6,6	0.00	-	-		
86	OHX	2	2074	-	0,6,6	0.00	-	-		
86	OHX	5	4030	-	0,6,6	0.00	-	-		
86	OHX	5	3946	-	0,6,6	0.00	-	-		
86	OHX	5	4065	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	O1	201	-	0,6,6	0.00	-	-		
86	OHX	d9	102	-	0,6,6	0.00	-	-		
86	OHX	3	220	-	0,6,6	0.00	-	-		
86	OHX	1	4067	-	0,6,6	0.00	-	-		
86	OHX	m1	202	-	0,6,6	0.00	-	-		
86	OHX	1	4000	-	0,6,6	0.00	-	-		
86	OHX	2	2109	-	0,6,6	0.00	-	-		
86	OHX	5	4115	-	0,6,6	0.00	-	-		
86	OHX	1	4166	-	0,6,6	0.00	-	-		
86	OHX	2	2128	-	0,6,6	0.00	-	-		
86	OHX	5	4137	-	0,6,6	0.00	-	-		
86	OHX	2	2100	-	0,6,6	0.00	-	-		
86	OHX	1	4139	-	0,6,6	0.00	-	-		
86	OHX	1	3977	-	0,6,6	0.00	-	-		
86	OHX	1	4121	-	0,6,6	0.00	-	-		
86	OHX	1	3937	-	0,6,6	0.00	-	-		
86	OHX	c3	201	-	0,6,6	0.00	-	-		
86	OHX	1	3989	-	0,6,6	0.00	-	-		
86	OHX	1	4050	-	0,6,6	0.00	-	-		
86	OHX	5	4049	-	0,6,6	0.00	-	-		
86	OHX	2	2022	-	0,6,6	0.00	-	-		
86	OHX	6	2070	-	0,6,6	0.00	-	-		
86	OHX	2	2149	-	0,6,6	0.00	-	-		
86	OHX	14	403	-	0,6,6	0.00	-	-		
86	OHX	5	4101	-	0,6,6	0.00	-	-		
86	OHX	6	2062	-	0,6,6	0.00	-	-		
86	OHX	5	4105	-	0,6,6	0.00	-	-		
86	OHX	6	2140	-	0,6,6	0.00	-	-		
86	OHX	6	2050	-	0,6,6	0.00	-	-		
86	OHX	3	216	-	0,6,6	0.00	-	-		
86	OHX	1	4080	-	0,6,6	0.00	-	-		
86	OHX	1	4137	-	0,6,6	0.00	-	-		
86	OHX	2	2130	-	0,6,6	0.00	-	-		
86	OHX	5	4027	-	0,6,6	0.00	-	-		
86	OHX	1	4132	-	0,6,6	0.00	-	-		
86	OHX	5	4050	-	0,6,6	0.00	-	-		
86	OHX	2	2156	-	0,6,6	0.00	-	-		
86	OHX	3	223	-	0,6,6	0.00	-	-		
86	OHX	5	4109	-	0,6,6	0.00	-	-		
86	OHX	1	3920	-	0,6,6	0.00	-	-		
86	OHX	1	4119	-	0,6,6	0.00	-	-		
86	OHX	1	4052	-	0,6,6	0.00	-	-		
86	OHX	5	3931	-	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	2075	-	0,6,6	0.00	-	-		
86	OHX	1	4199	-	0,6,6	0.00	-	-		
86	OHX	5	4107	-	0,6,6	0.00	-	-		
86	OHX	2	2082	-	0,6,6	0.00	-	-		
86	OHX	2	2178	-	0,6,6	0.00	-	-		
86	OHX	5	3964	-	0,6,6	0.00	-	-		
86	OHX	6	2118	-	0,6,6	0.00	-	-		
86	OHX	1	3926	-	0,6,6	0.00	-	-		
86	OHX	6	2092	-	0,6,6	0.00	-	-		
86	OHX	1	4054	-	0,6,6	0.00	-	-		
86	OHX	1	4039	-	0,6,6	0.00	-	-		
86	OHX	6	2127	-	0,6,6	0.00	-	-		
86	OHX	5	4194	-	0,6,6	0.00	-	-		
86	OHX	1	4160	-	0,6,6	0.00	-	-		
86	OHX	2	2152	-	0,6,6	0.00	-	-		
86	OHX	1	4165	-	0,6,6	0.00	-	-		
86	OHX	1	4026	-	0,6,6	0.00	-	-		
86	OHX	5	3974	-	0,6,6	0.00	-	-		
86	OHX	2	2115	-	0,6,6	0.00	-	-		
86	OHX	1	4088	-	0,6,6	0.00	-	-		
86	OHX	6	2120	-	0,6,6	0.00	-	-		
86	OHX	1	4036	-	0,6,6	0.00	-	-		
86	OHX	1	3931	-	0,6,6	0.00	-	-		
86	OHX	2	2154	-	0,6,6	0.00	-	-		
86	OHX	5	3908	-	0,6,6	0.00	-	-		
86	OHX	5	4082	-	0,6,6	0.00	-	-		
86	OHX	2	2033	-	0,6,6	0.00	-	-		
86	OHX	2	2117	-	0,6,6	0.00	-	-		
86	OHX	2	2036	-	0,6,6	0.00	-	-		
86	OHX	5	4043	-	0,6,6	0.00	-	-		
86	OHX	5	4022	-	0,6,6	0.00	-	-		
86	OHX	5	4147	-	0,6,6	0.00	-	-		
86	OHX	1	4040	-	0,6,6	0.00	-	-		
86	OHX	5	4154	-	0,6,6	0.00	-	-		
86	OHX	5	3969	-	0,6,6	0.00	-	-		
86	OHX	5	4023	-	0,6,6	0.00	-	-		
86	OHX	5	4055	-	0,6,6	0.00	-	-		
86	OHX	6	2200	-	0,6,6	0.00	-	-		
86	OHX	O2	201	-	0,6,6	0.00	-	-		
86	OHX	5	3991	-	0,6,6	0.00	-	-		
86	OHX	1	4161	-	0,6,6	0.00	-	-		
86	OHX	5	4164	-	0,6,6	0.00	-	-		
86	OHX	7	220	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	M9	203	-	0,6,6	0.00	-	-		
86	OHX	5	4032	-	0,6,6	0.00	-	-		
86	OHX	5	3938	-	0,6,6	0.00	-	-		
86	OHX	6	2103	-	0,6,6	0.00	-	-		
86	OHX	6	2143	-	0,6,6	0.00	-	-		
86	OHX	1	4153	-	0,6,6	0.00	-	-		
86	OHX	4	237	-	0,6,6	0.00	-	-		
86	OHX	5	4152	-	0,6,6	0.00	-	-		
86	OHX	2	2071	-	0,6,6	0.00	-	-		
86	OHX	5	4015	-	0,6,6	0.00	-	-		
86	OHX	5	3903	-	0,6,6	0.00	-	-		
86	OHX	6	2094	-	0,6,6	0.00	-	-		
86	OHX	6	2135	-	0,6,6	0.00	-	-		
86	OHX	7	224	-	0,6,6	0.00	-	-		
86	OHX	8	225	-	0,6,6	0.00	-	-		
86	OHX	6	2146	-	0,6,6	0.00	-	-		
86	OHX	1	3883	-	0,6,6	0.00	-	-		
86	OHX	6	2167	-	0,6,6	0.00	-	-		
86	OHX	5	4204	-	0,6,6	0.00	-	-		
86	OHX	5	4071	-	0,6,6	0.00	-	-		
86	OHX	5	4136	-	0,6,6	0.00	-	-		
86	OHX	1	4220	-	0,6,6	0.00	-	-		
86	OHX	6	2202	-	0,6,6	0.00	-	-		
86	OHX	1	4033	-	0,6,6	0.00	-	-		
86	OHX	5	4066	-	0,6,6	0.00	-	-		
86	OHX	1	4188	-	0,6,6	0.00	-	-		
86	OHX	2	2098	-	0,6,6	0.00	-	-		
86	OHX	1	4014	-	0,6,6	0.00	-	-		
86	OHX	1	4055	-	0,6,6	0.00	-	-		
86	OHX	5	4078	-	0,6,6	0.00	-	-		
86	OHX	2	2146	-	0,6,6	0.00	-	-		
86	OHX	1	3919	-	0,6,6	0.00	-	-		
86	OHX	1	4087	-	0,6,6	0.00	-	-		
86	OHX	6	2057	-	0,6,6	0.00	-	-		
86	OHX	5	4001	-	0,6,6	0.00	-	-		
86	OHX	5	4161	-	0,6,6	0.00	-	-		
86	OHX	5	3990	-	0,6,6	0.00	-	-		
86	OHX	5	4035	-	0,6,6	0.00	-	-		
86	OHX	2	2148	-	0,6,6	0.00	-	-		
86	OHX	1	3902	-	0,6,6	0.00	-	-		
86	OHX	6	2121	-	0,6,6	0.00	-	-		
86	OHX	6	2081	-	0,6,6	0.00	-	-		
86	OHX	5	4079	-	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	2144	-	0,6,6	0.00	-	-		
86	OHX	1	4144	-	0,6,6	0.00	-	-		
86	OHX	7	217	-	0,6,6	0.00	-	-		
86	OHX	8	216	-	0,6,6	0.00	-	-		
86	OHX	2	2058	-	0,6,6	0.00	-	-		
86	OHX	5	4178	-	0,6,6	0.00	-	-		
86	OHX	2	2112	-	0,6,6	0.00	-	-		
86	OHX	1	3900	-	0,6,6	0.00	-	-		
86	OHX	5	4006	-	0,6,6	0.00	-	-		
86	OHX	o3	203	-	0,6,6	0.00	-	-		
86	OHX	7	227	-	0,6,6	0.00	-	-		
86	OHX	2	2077	-	0,6,6	0.00	-	-		
86	OHX	8	231	-	0,6,6	0.00	-	-		
86	OHX	5	4080	-	0,6,6	0.00	-	-		
86	OHX	1	3891	-	0,6,6	0.00	-	-		
86	OHX	3	215	-	0,6,6	0.00	-	-		
86	OHX	5	4117	-	0,6,6	0.00	-	-		
86	OHX	5	4187	-	0,6,6	0.00	-	-		
86	OHX	5	4075	-	0,6,6	0.00	-	-		
86	OHX	5	3940	-	0,6,6	0.00	-	-		
86	OHX	2	2172	-	0,6,6	0.00	-	-		
86	OHX	6	2148	-	0,6,6	0.00	-	-		
86	OHX	M0	304	-	0,6,6	0.00	-	-		
86	OHX	1	4020	-	0,6,6	0.00	-	-		
86	OHX	6	2095	-	0,6,6	0.00	-	-		
86	OHX	5	3922	-	0,6,6	0.00	-	-		
86	OHX	6	2155	-	0,6,6	0.00	-	-		
86	OHX	2	2126	-	0,6,6	0.00	-	-		
86	OHX	5	4074	-	0,6,6	0.00	-	-		
86	OHX	6	2160	-	0,6,6	0.00	-	-		
86	OHX	1	4184	-	0,6,6	0.00	-	-		
86	OHX	5	4124	-	0,6,6	0.00	-	-		
86	OHX	1	3970	-	0,6,6	0.00	-	-		
86	OHX	1	4022	-	0,6,6	0.00	-	-		
86	OHX	N9	101	-	0,6,6	0.00	-	-		
86	OHX	2	2118	-	0,6,6	0.00	-	-		
86	OHX	8	217	-	0,6,6	0.00	-	-		
86	OHX	1	3889	-	0,6,6	0.00	-	-		
86	OHX	1	3981	-	0,6,6	0.00	-	-		
86	OHX	6	2169	-	0,6,6	0.00	-	-		
86	OHX	2	2167	-	0,6,6	0.00	-	-		
86	OHX	1	3918	-	0,6,6	0.00	-	-		
86	OHX	1	4218	-	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	3872	-	0,6,6	0.00	-	-		
86	OHX	2	2177	-	0,6,6	0.00	-	-		
86	OHX	5	4090	-	0,6,6	0.00	-	-		
86	OHX	1	4180	-	0,6,6	0.00	-	-		
86	OHX	1	4016	-	0,6,6	0.00	-	-		
86	OHX	1	4048	-	0,6,6	0.00	-	-		
86	OHX	1	4031	-	0,6,6	0.00	-	-		
86	OHX	5	3989	-	0,6,6	0.00	-	-		
86	OHX	2	2029	-	0,6,6	0.00	-	-		
86	OHX	2	2139	-	0,6,6	0.00	-	-		
86	OHX	1	3995	-	0,6,6	0.00	-	-		
86	OHX	5	3998	-	0,6,6	0.00	-	-		
86	OHX	1	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4169	-	0,6,6	0.00	-	-		
86	OHX	6	2059	-	0,6,6	0.00	-	-		
86	OHX	6	2187	-	0,6,6	0.00	-	-		
86	OHX	6	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4041	-	0,6,6	0.00	-	-		
86	OHX	1	4156	-	0,6,6	0.00	-	-		
86	OHX	M7	206	-	0,6,6	0.00	-	-		
86	OHX	1	4090	-	0,6,6	0.00	-	-		
86	OHX	7	218	-	0,6,6	0.00	-	-		
86	OHX	1	4082	-	0,6,6	0.00	-	-		
86	OHX	8	219	-	0,6,6	0.00	-	-		
86	OHX	6	2073	-	0,6,6	0.00	-	-		
86	OHX	1	3993	-	0,6,6	0.00	-	-		
86	OHX	5	4064	-	0,6,6	0.00	-	-		
86	OHX	5	3918	-	0,6,6	0.00	-	-		
86	OHX	5	3987	-	0,6,6	0.00	-	-		
86	OHX	6	2102	-	0,6,6	0.00	-	-		
86	OHX	5	4092	-	0,6,6	0.00	-	-		
86	OHX	5	3968	-	0,6,6	0.00	-	-		
86	OHX	1	4081	-	0,6,6	0.00	-	-		
86	OHX	l3	406	-	0,6,6	0.00	-	-		
86	OHX	2	2087	-	0,6,6	0.00	-	-		
86	OHX	6	2154	-	0,6,6	0.00	-	-		
86	OHX	6	2080	-	0,6,6	0.00	-	-		
86	OHX	2	2034	-	0,6,6	0.00	-	-		
86	OHX	1	4151	-	0,6,6	0.00	-	-		
86	OHX	1	4060	-	0,6,6	0.00	-	-		
86	OHX	2	2114	-	0,6,6	0.00	-	-		
86	OHX	5	4083	-	0,6,6	0.00	-	-		
86	OHX	s4	302	-	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	2111	-	0,6,6	0.00	-	-		
86	OHX	2	2051	-	0,6,6	0.00	-	-		
86	OHX	5	4234	-	0,6,6	0.00	-	-		
86	OHX	4	228	-	0,6,6	0.00	-	-		
86	OHX	6	2047	-	0,6,6	0.00	-	-		
86	OHX	1	4217	-	0,6,6	0.00	-	-		
86	OHX	8	220	-	0,6,6	0.00	-	-		
86	OHX	5	3947	-	0,6,6	0.00	-	-		
86	OHX	1	4216	-	0,6,6	0.00	-	-		
86	OHX	5	3904	-	0,6,6	0.00	-	-		
86	OHX	5	4151	-	0,6,6	0.00	-	-		
86	OHX	2	2134	-	0,6,6	0.00	-	-		
86	OHX	1	3956	-	0,6,6	0.00	-	-		
86	OHX	2	2085	-	0,6,6	0.00	-	-		
86	OHX	6	2125	-	0,6,6	0.00	-	-		
86	OHX	1	4095	-	0,6,6	0.00	-	-		
86	OHX	5	3905	-	0,6,6	0.00	-	-		
86	OHX	1	4145	-	0,6,6	0.00	-	-		
86	OHX	1	4074	-	0,6,6	0.00	-	-		
86	OHX	L3	404	-	0,6,6	0.00	-	-		
86	OHX	1	3961	-	0,6,6	0.00	-	-		
86	OHX	2	2023	-	0,6,6	0.00	-	-		
86	OHX	1	3896	-	0,6,6	0.00	-	-		
86	OHX	1	3950	-	0,6,6	0.00	-	-		
86	OHX	2	2101	-	0,6,6	0.00	-	-		
86	OHX	1	4204	-	0,6,6	0.00	-	-		
86	OHX	6	2078	-	0,6,6	0.00	-	-		
86	OHX	8	218	-	0,6,6	0.00	-	-		
86	OHX	C5	201	-	0,6,6	0.00	-	-		
86	OHX	1	4173	-	0,6,6	0.00	-	-		
86	OHX	3	218	-	0,6,6	0.00	-	-		
86	OHX	1	4179	-	0,6,6	0.00	-	-		
86	OHX	2	2164	-	0,6,6	0.00	-	-		
86	OHX	5	4230	-	0,6,6	0.00	-	-		
86	OHX	6	2055	-	0,6,6	0.00	-	-		
86	OHX	5	4004	-	0,6,6	0.00	-	-		
86	OHX	1	3938	-	0,6,6	0.00	-	-		
86	OHX	5	4005	-	0,6,6	0.00	-	-		
86	OHX	15	304	-	0,6,6	0.00	-	-		
86	OHX	5	4000	-	0,6,6	0.00	-	-		
86	OHX	1	4128	-	0,6,6	0.00	-	-		
86	OHX	1	3923	-	0,6,6	0.00	-	-		
86	OHX	Q2	503	-	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	4195	-	0,6,6	0.00	-	-		
86	OHX	1	4079	-	0,6,6	0.00	-	-		
86	OHX	6	2131	-	0,6,6	0.00	-	-		
86	OHX	1	4078	-	0,6,6	0.00	-	-		
86	OHX	l3	405	-	0,6,6	0.00	-	-		
86	OHX	5	4128	-	0,6,6	0.00	-	-		
86	OHX	1	4008	-	0,6,6	0.00	-	-		
86	OHX	6	2115	-	0,6,6	0.00	-	-		
86	OHX	1	3966	-	0,6,6	0.00	-	-		
86	OHX	5	4113	-	0,6,6	0.00	-	-		
86	OHX	6	2189	-	0,6,6	0.00	-	-		
86	OHX	5	4009	-	0,6,6	0.00	-	-		
86	OHX	6	2067	-	0,6,6	0.00	-	-		
86	OHX	1	3972	-	0,6,6	0.00	-	-		
86	OHX	5	3957	-	0,6,6	0.00	-	-		
86	OHX	2	2170	-	0,6,6	0.00	-	-		
86	OHX	q2	502	-	0,6,6	0.00	-	-		
86	OHX	1	4004	-	0,6,6	0.00	-	-		
86	OHX	5	4160	-	0,6,6	0.00	-	-		
86	OHX	6	2150	-	0,6,6	0.00	-	-		
86	OHX	1	4062	-	0,6,6	0.00	-	-		
86	OHX	4	224	-	0,6,6	0.00	-	-		
86	OHX	5	4069	-	0,6,6	0.00	-	-		
86	OHX	5	4044	-	0,6,6	0.00	-	-		
86	OHX	2	2165	-	0,6,6	0.00	-	-		
86	OHX	5	4245	-	0,6,6	0.00	-	-		
86	OHX	1	4073	-	0,6,6	0.00	-	-		
86	OHX	5	3921	-	0,6,6	0.00	-	-		
86	OHX	1	4136	-	0,6,6	0.00	-	-		
86	OHX	5	4244	-	0,6,6	0.00	-	-		
86	OHX	1	3983	-	0,6,6	0.00	-	-		
86	OHX	2	2049	-	0,6,6	0.00	-	-		
86	OHX	1	4118	-	0,6,6	0.00	-	-		
86	OHX	5	4130	-	0,6,6	0.00	-	-		
86	OHX	6	2088	-	0,6,6	0.00	-	-		
86	OHX	5	4081	-	0,6,6	0.00	-	-		
86	OHX	1	4214	-	0,6,6	0.00	-	-		
86	OHX	2	2084	-	0,6,6	0.00	-	-		
86	OHX	2	2119	-	0,6,6	0.00	-	-		
86	OHX	6	2077	-	0,6,6	0.00	-	-		
86	OHX	1	3990	-	0,6,6	0.00	-	-		
86	OHX	1	3946	-	0,6,6	0.00	-	-		
86	OHX	6	2165	-	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	2041	-	0,6,6	0.00	-	-		
86	OHX	2	2122	-	0,6,6	0.00	-	-		
86	OHX	6	2108	-	0,6,6	0.00	-	-		
86	OHX	1	4105	-	0,6,6	0.00	-	-		
86	OHX	2	2075	-	0,6,6	0.00	-	-		
86	OHX	5	4238	-	0,6,6	0.00	-	-		
86	OHX	2	2157	-	0,6,6	0.00	-	-		
86	OHX	2	2026	-	0,6,6	0.00	-	-		
86	OHX	5	3935	-	0,6,6	0.00	-	-		
86	OHX	L3	406	-	0,6,6	0.00	-	-		
86	OHX	1	4057	-	0,6,6	0.00	-	-		
86	OHX	1	3994	-	0,6,6	0.00	-	-		
86	OHX	6	2147	-	0,6,6	0.00	-	-		
86	OHX	1	3954	-	0,6,6	0.00	-	-		
86	OHX	m4	202	-	0,6,6	0.00	-	-		
86	OHX	1	4203	-	0,6,6	0.00	-	-		
86	OHX	5	3928	-	0,6,6	0.00	-	-		
86	OHX	5	4216	-	0,6,6	0.00	-	-		
86	OHX	6	2052	-	0,6,6	0.00	-	-		
86	OHX	5	4197	-	0,6,6	0.00	-	-		
86	OHX	5	4213	-	0,6,6	0.00	-	-		
86	OHX	4	229	-	0,6,6	0.00	-	-		
86	OHX	5	4091	-	0,6,6	0.00	-	-		
86	OHX	5	4153	-	0,6,6	0.00	-	-		
86	OHX	1	3890	-	0,6,6	0.00	-	-		
86	OHX	3	217	-	0,6,6	0.00	-	-		
86	OHX	5	4017	-	0,6,6	0.00	-	-		
86	OHX	6	2201	-	0,6,6	0.00	-	-		
86	OHX	1	4103	-	0,6,6	0.00	-	-		
86	OHX	2	2147	-	0,6,6	0.00	-	-		
86	OHX	5	4199	-	0,6,6	0.00	-	-		
86	OHX	5	3936	-	0,6,6	0.00	-	-		
86	OHX	6	2188	-	0,6,6	0.00	-	-		
86	OHX	2	2138	-	0,6,6	0.00	-	-		
86	OHX	5	3933	-	0,6,6	0.00	-	-		
86	OHX	1	4019	-	0,6,6	0.00	-	-		
86	OHX	5	4221	-	0,6,6	0.00	-	-		
86	OHX	1	4038	-	0,6,6	0.00	-	-		
86	OHX	2	2124	-	0,6,6	0.00	-	-		
86	OHX	1	4201	-	0,6,6	0.00	-	-		
86	OHX	5	4034	-	0,6,6	0.00	-	-		
86	OHX	5	3951	-	0,6,6	0.00	-	-		
86	OHX	5	4214	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	4	232	-	0,6,6	0.00	-	-		
86	OHX	D9	102	-	0,6,6	0.00	-	-		
86	OHX	6	2196	-	0,6,6	0.00	-	-		
86	OHX	5	4200	-	0,6,6	0.00	-	-		
86	OHX	5	4181	-	0,6,6	0.00	-	-		
86	OHX	1	3898	-	0,6,6	0.00	-	-		
86	OHX	1	4005	-	0,6,6	0.00	-	-		
86	OHX	m7	206	-	0,6,6	0.00	-	-		
86	OHX	6	2197	-	0,6,6	0.00	-	-		
86	OHX	1	4170	-	0,6,6	0.00	-	-		
86	OHX	6	2126	-	0,6,6	0.00	-	-		
86	OHX	6	2098	-	0,6,6	0.00	-	-		
86	OHX	2	2158	-	0,6,6	0.00	-	-		
86	OHX	5	3902	-	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	3K5	1	4221	-	-	2/29/121/121	0/7/7/7
88	3K5	5	4249	-	-	7/29/121/121	0/7/7/7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4221	3K5	O3-C15	8.97	1.60	1.44
88	5	4249	3K5	O3-C15	-3.50	1.38	1.44
88	1	4221	3K5	C17-C22	-2.16	1.49	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4221	3K5	O3-C16-C15	7.82	67.35	59.35
88	5	4249	3K5	O14-C34-C35	5.62	120.52	107.70
88	5	4249	3K5	C3-C15-C17	4.49	111.30	103.01
88	1	4221	3K5	O3-C15-C16	-4.41	55.88	59.74
88	5	4249	3K5	O3-C15-C16	3.88	63.14	59.74
88	1	4221	3K5	O14-C34-C35	3.58	115.86	107.70
88	5	4249	3K5	C4-C3-C15	-3.25	108.80	114.34
88	1	4221	3K5	C16-O3-C15	-3.16	56.77	60.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4221	3K5	O9-C26-C27	2.68	113.81	107.70
88	5	4249	3K5	O3-C16-C15	-2.60	56.68	59.35
88	1	4221	3K5	O14-C34-C33	-2.53	101.93	107.70
88	1	4221	3K5	O7-C24-O6	-2.49	101.25	107.97
88	5	4249	3K5	C34-C35-C36	-2.44	104.82	110.12
88	5	4249	3K5	C2-O-C3	2.39	115.34	113.66
88	5	4249	3K5	O-C3-C15	2.33	111.87	107.32
88	5	4249	3K5	O14-C34-C33	-2.09	102.94	107.70
88	1	4221	3K5	O4-C22-C21	2.06	116.61	111.36
88	5	4249	3K5	O11-C25-C26	2.03	112.64	107.48
88	5	4249	3K5	O1-C5-C1	2.03	110.10	107.23
88	1	4221	3K5	O13-C35-C34	2.02	115.30	109.94
88	1	4221	3K5	C32-O12-C36	2.02	117.14	113.67
88	1	4221	3K5	C26-C27-C28	-2.01	105.76	110.12

There are no chirality outliers.

All (9) torsion outliers are listed below:

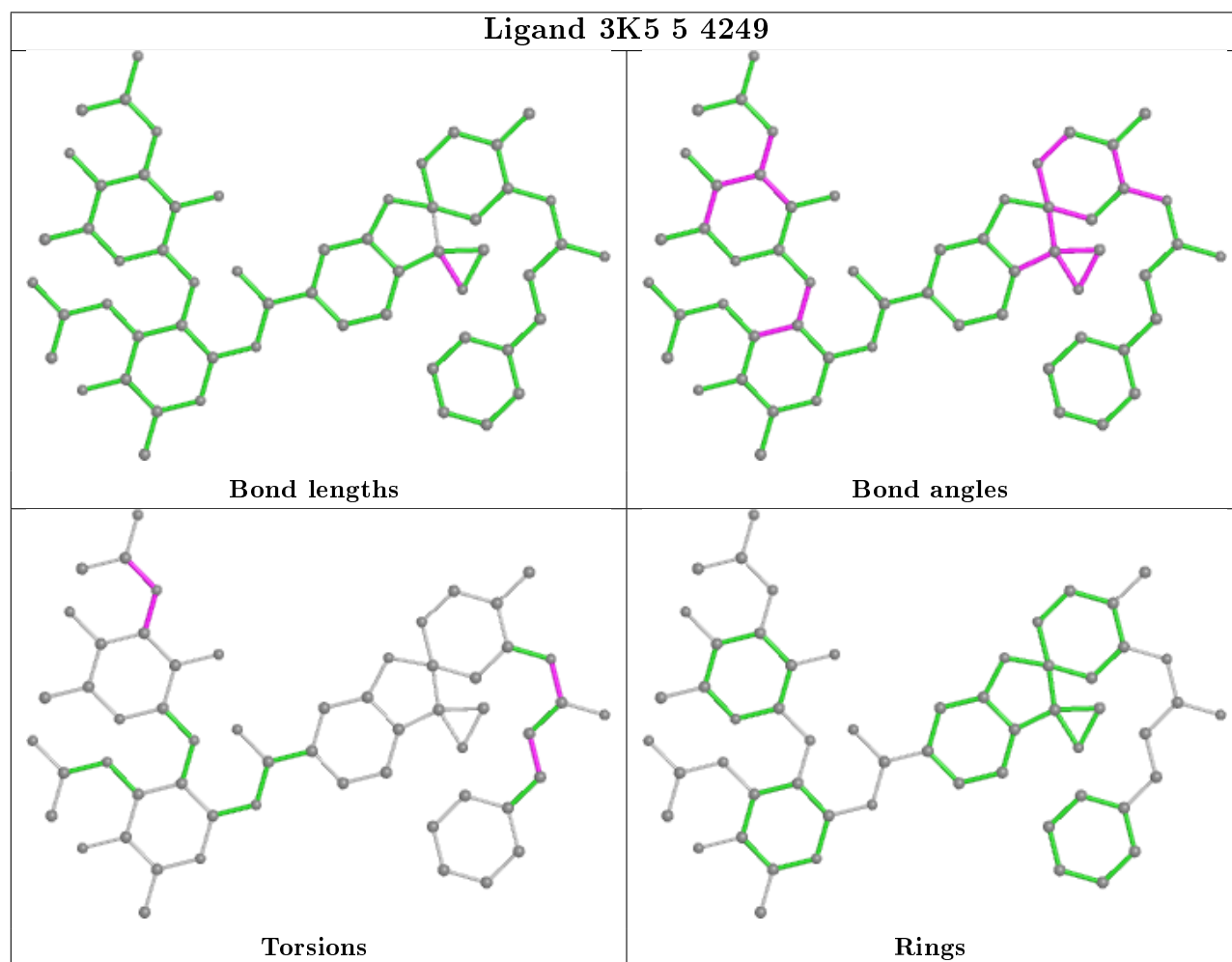
Mol	Chain	Res	Type	Atoms
88	5	4249	3K5	C6-C7-C8-C9
88	5	4249	3K5	C35-C34-O14-C38
88	5	4249	3K5	C39-C38-O14-C34
88	5	4249	3K5	C33-C34-O14-C38
88	5	4249	3K5	O15-C38-O14-C34
88	5	4249	3K5	O2-C6-O1-C5
88	1	4221	3K5	C31-C30-O9-C26
88	1	4221	3K5	C19-C20-C23-O6
88	5	4249	3K5	C7-C6-O1-C5

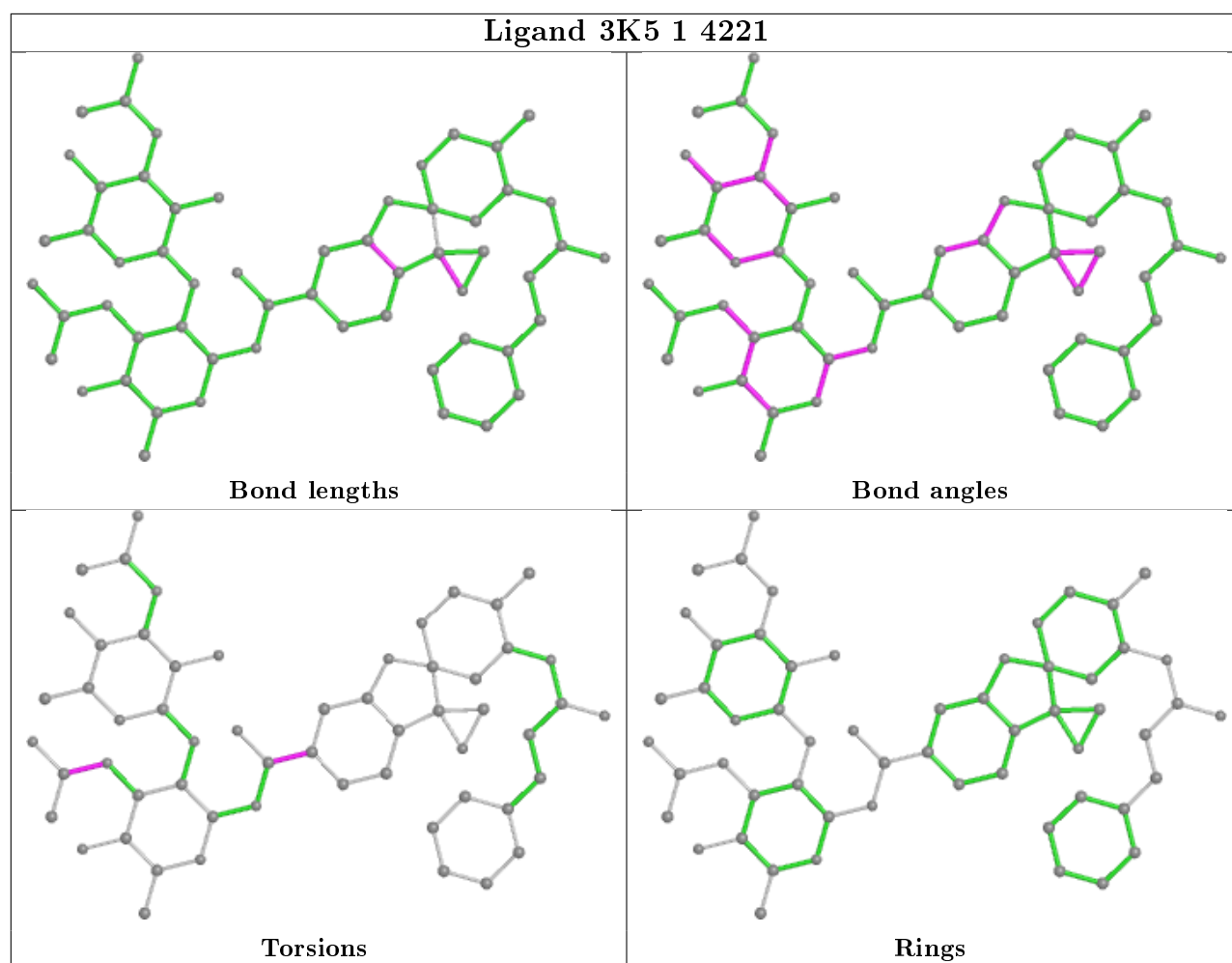
There are no ring outliers.

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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