



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 06:31 PM BST

PDB ID : 4U3U
Title : Crystal structure of Cycloheximide bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-22
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

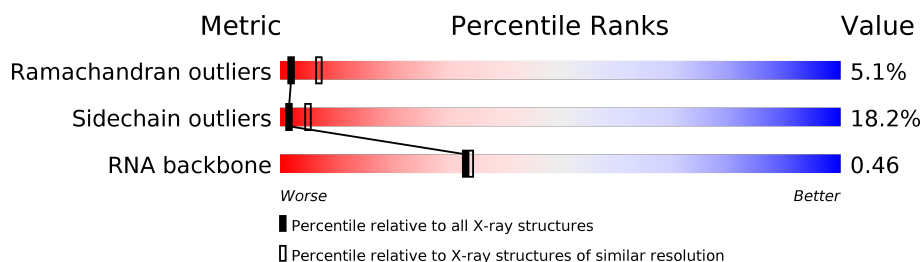
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)


























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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	
1	6	1800	
2	S0	251	
2	s0	251	
3	S1	254	
3	s1	254	
4	S2	253	
4	s2	253	















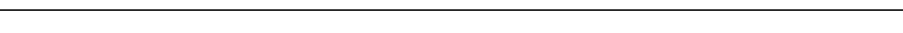




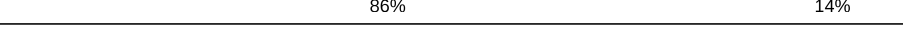
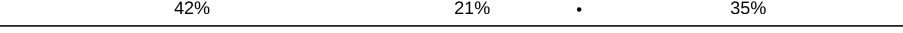




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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	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	
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	
43	L6	175	















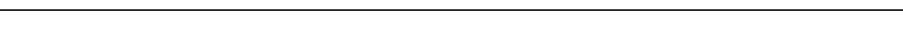




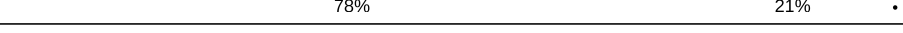





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Mol	Chain	Length	Quality of chain
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	















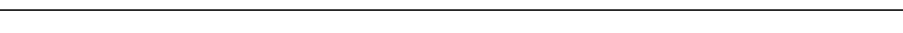




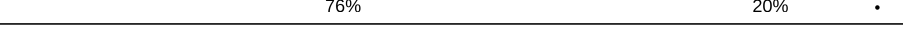





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Mol	Chain	Length	Quality of chain
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	

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Mol	Chain	Length	Quality of chain
68	o2	129	 78%19%..
69	O3	106	 88%11%.
69	o3	106	 85%14%.
70	O4	119	 76%17%6%.
70	o4	119	 81%13%6%.
71	O5	119	 80%18%.
71	o5	119	 82%18%
72	O6	99	 78%19%.
72	o6	99	 71%26%.
73	O7	87	 85%13%.
73	o7	87	 80%20%
74	O8	77	 79%19%.
74	o8	77	 83%16%.
75	O9	50	 88%12%
75	o9	50	 84%16%
76	Q0	52	 88%10%.
76	q0	52	 81%19%
77	Q1	25	 68%32%
77	q1	25	 76%20%.
78	Q2	105	 79%20%.
78	q2	105	 81%18%.
79	Q3	91	 82%18%
79	q3	91	 81%18%.
80	e0	62	 76%24%
81	e1	76	 58%34%7%.

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

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 411205 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	l2	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			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1764	1131	316	314	3			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	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				
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	S	0	0	0
			796	516	131	149				
58	n2	98	Total	C	N	O	S	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			

- 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			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O	S	0	0	0
			612	391	115	106				
74	o8	77	Total	C	N	O	S	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 Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

- Molecule 82 is a protein called UNKNOWN PROTEIN m2.

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

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

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

- Molecule 84 is a protein called UNKNOWN PROTEIN p1.

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

- Molecule 85 is a protein called UNKNOWN PROTEIN p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L7	3	Total	Mg	0	0
			3	3		
86	m7	4	Total	Mg	0	0
			4	4		
86	n8	3	Total	Mg	0	0
			3	3		
86	o1	2	Total	Mg	0	0
			2	2		
86	N5	1	Total	Mg	0	0
			1	1		
86	6	147	Total	Mg	0	0
			147	147		
86	sM	2	Total	Mg	0	0
			2	2		
86	O4	2	Total	Mg	0	0
			2	2		
86	m5	2	Total	Mg	0	0
			2	2		
86	l3	1	Total	Mg	0	0
			1	1		
86	M1	1	Total	Mg	0	0
			1	1		
86	n0	2	Total	Mg	0	0
			2	2		
86	d6	1	Total	Mg	0	0
			1	1		
86	2	122	Total	Mg	0	0
			122	122		
86	O3	1	Total	Mg	0	0
			1	1		
86	L4	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	l7	1	Total 1	Mg 1	0	0
86	M5	2	Total 2	Mg 2	0	0
86	l4	2	Total 2	Mg 2	0	0
86	S2	1	Total 1	Mg 1	0	0
86	L8	1	Total 1	Mg 1	0	0
86	D3	1	Total 1	Mg 1	0	0
86	o4	2	Total 2	Mg 2	0	0
86	M9	1	Total 1	Mg 1	0	0
86	q0	1	Total 1	Mg 1	0	0
86	SM	1	Total 1	Mg 1	0	0
86	c8	2	Total 2	Mg 2	0	0
86	M0	2	Total 2	Mg 2	0	0
86	c1	1	Total 1	Mg 1	0	0
86	5	505	Total 505	Mg 505	0	0
86	L5	1	Total 1	Mg 1	0	0
86	O7	1	Total 1	Mg 1	0	0
86	s6	1	Total 1	Mg 1	0	0
86	Q2	1	Total 1	Mg 1	0	0
86	1	471	Total 471	Mg 471	0	0
86	c4	1	Total 1	Mg 1	0	0
86	D0	1	Total 1	Mg 1	0	0

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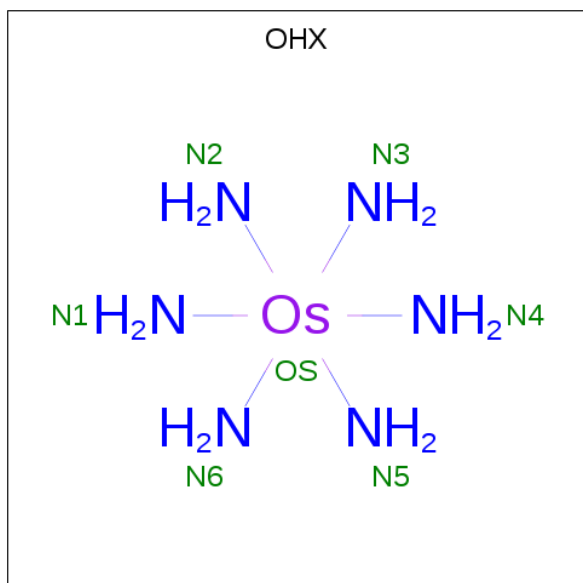
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	S8	1	Total 1	Mg 1	0	0
86	m1	2	Total 2	Mg 2	0	0
86	d3	1	Total 1	Mg 1	0	0
86	q3	2	Total 2	Mg 2	0	0
86	o3	1	Total 1	Mg 1	0	0
86	M3	4	Total 4	Mg 4	0	0
86	N3	3	Total 3	Mg 3	0	0
86	4	22	Total 22	Mg 22	0	0
86	n6	2	Total 2	Mg 2	0	0
86	S4	1	Total 1	Mg 1	0	0
86	L2	1	Total 1	Mg 1	0	0
86	o7	1	Total 1	Mg 1	0	0
86	l5	2	Total 2	Mg 2	0	0
86	C3	1	Total 1	Mg 1	0	0
86	M7	6	Total 6	Mg 6	0	0
86	N8	4	Total 4	Mg 4	0	0
86	s1	1	Total 1	Mg 1	0	0
86	m6	1	Total 1	Mg 1	0	0
86	O1	1	Total 1	Mg 1	0	0
86	s8	1	Total 1	Mg 1	0	0
86	l8	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	c7	2	Total	Mg	0	0
			2	2		
86	7	15	Total	Mg	0	0
			15	15		
86	n3	2	Total	Mg	0	0
			2	2		
86	L3	3	Total	Mg	0	0
			3	3		
86	d4	1	Total	Mg	0	0
			1	1		
86	l2	2	Total	Mg	0	0
			2	2		
86	8	13	Total	Mg	0	0
			13	13		
86	M6	1	Total	Mg	0	0
			1	1		
86	N0	1	Total	Mg	0	0
			1	1		
86	3	14	Total	Mg	0	0
			14	14		

- Molecule 87 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	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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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	4	1	Total	N	Os	0	0
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87	L3	1	Total	N	Os	0	0
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87	L3	1	Total	N	Os	0	0
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87	L4	1	Total	N	Os	0	0
			7	6	1		
87	M0	1	Total	N	Os	0	0
			7	6	1		
87	M5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	M7	1	Total	N	Os	0	0
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87	M9	1	Total	N	Os	0	0
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87	N1	1	Total	N	Os	0	0
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87	N9	1	Total	N	Os	0	0
			7	6	1		
87	O2	1	Total	N	Os	0	0
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87	O3	1	Total	N	Os	0	0
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87	O7	1	Total	N	Os	0	0
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87	O7	1	Total	N	Os	0	0
			7	6	1		
87	O9	1	Total	N	Os	0	0
			7	6	1		
87	Q2	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	13	1	Total	N	Os	0	0
			7	6	1		
87	13	1	Total	N	Os	0	0
			7	6	1		
87	13	1	Total	N	Os	0	0
			7	6	1		
87	14	1	Total	N	Os	0	0
			7	6	1		
87	14	1	Total	N	Os	0	0
			7	6	1		

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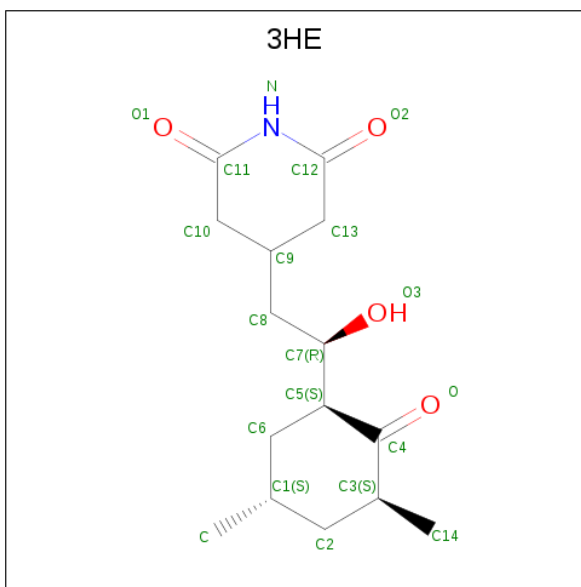
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l9	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m1	1	Total	N	Os	0	0
			7	6	1		
87	m4	1	Total	N	Os	0	0
			7	6	1		
87	m5	1	Total	N	Os	0	0
			7	6	1		
87	m6	1	Total	N	Os	0	0
			7	6	1		
87	m7	1	Total	N	Os	0	0
			7	6	1		
87	m8	1	Total	N	Os	0	0
			7	6	1		
87	n3	1	Total	N	Os	0	0
			7	6	1		
87	n9	1	Total	N	Os	0	0
			7	6	1		
87	o2	1	Total	N	Os	0	0
			7	6	1		
87	o3	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	o9	1	Total	N	Os	0	0
			7	6	1		
87	q2	1	Total	N	Os	0	0
			7	6	1		

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

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

- Molecule 89 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: C₁₅H₂₃NO₄).



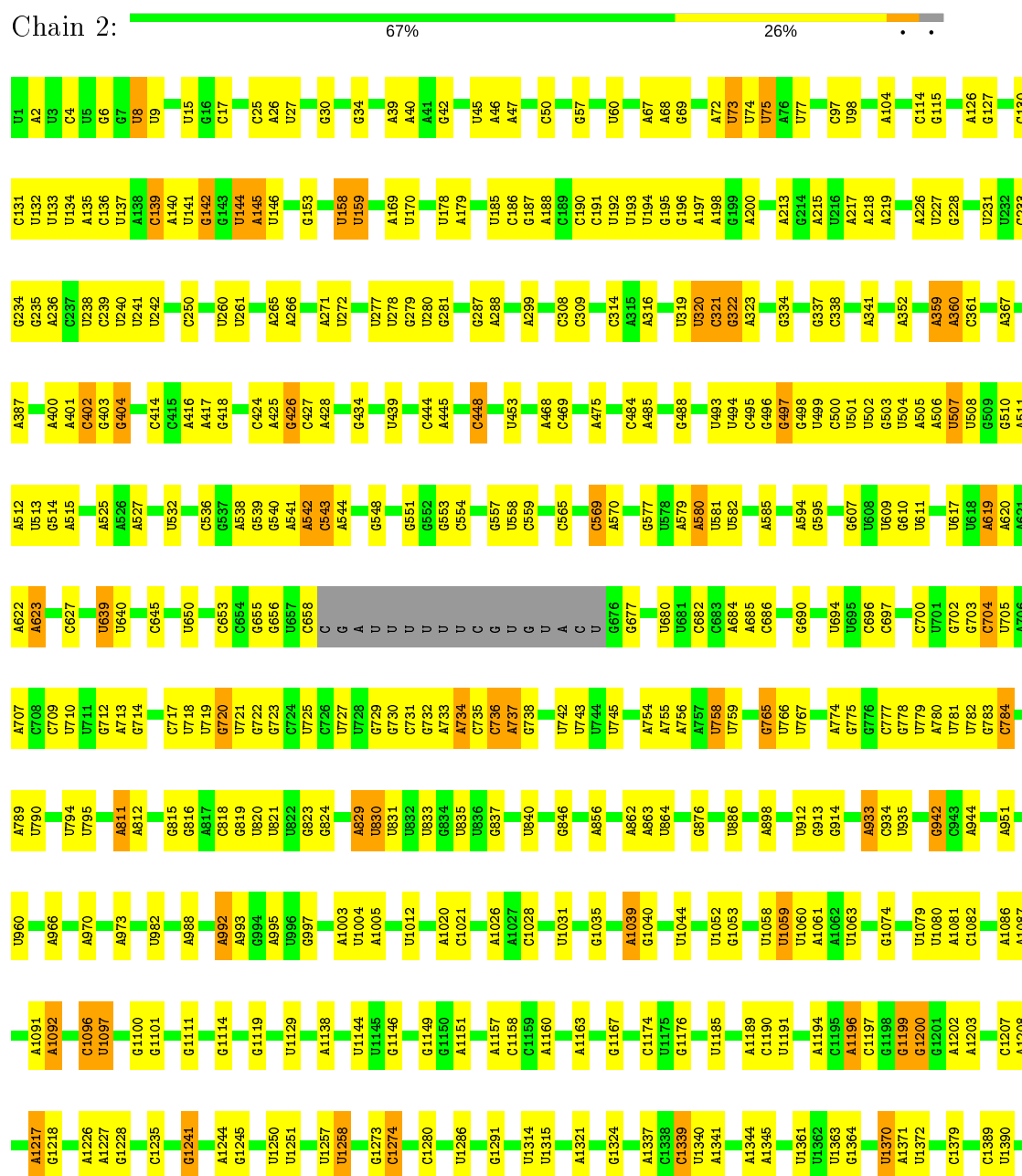
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	1	1	Total	C	N	O	0	0
			20	15	1	4		
89	5	1	Total	C	N	O	0	0
			20	15	1	4		

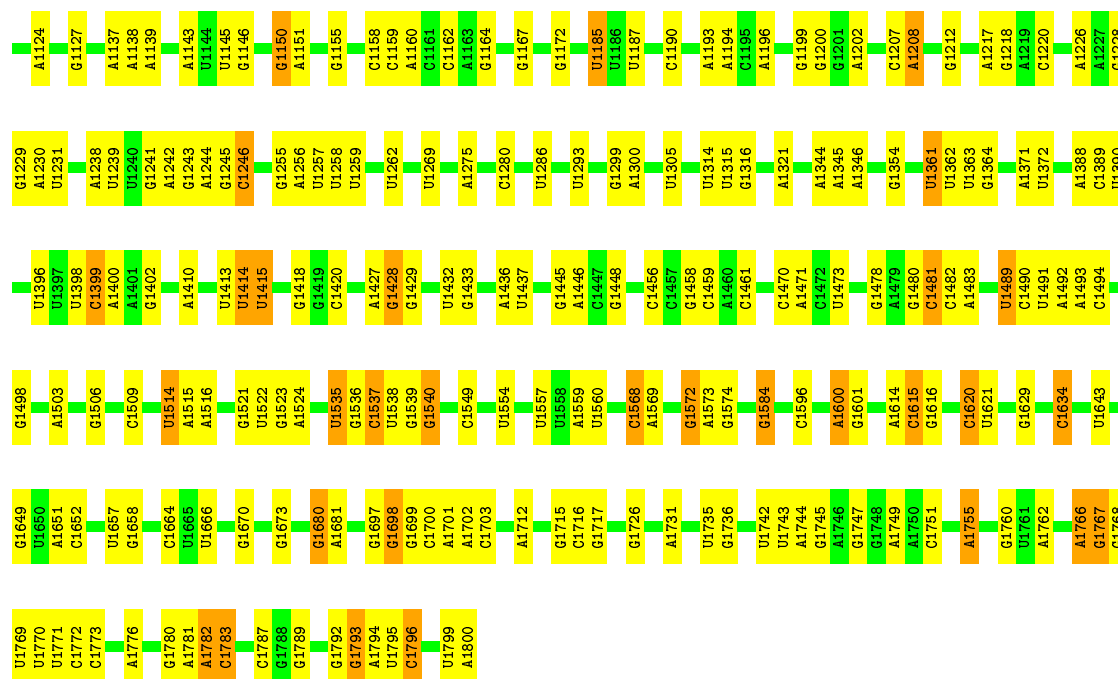
3 Residue-property plots

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.

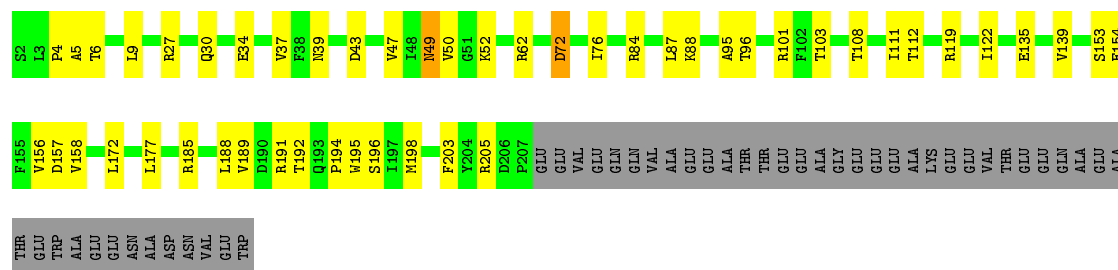
• Molecule 1: 18S ribosomal RNA





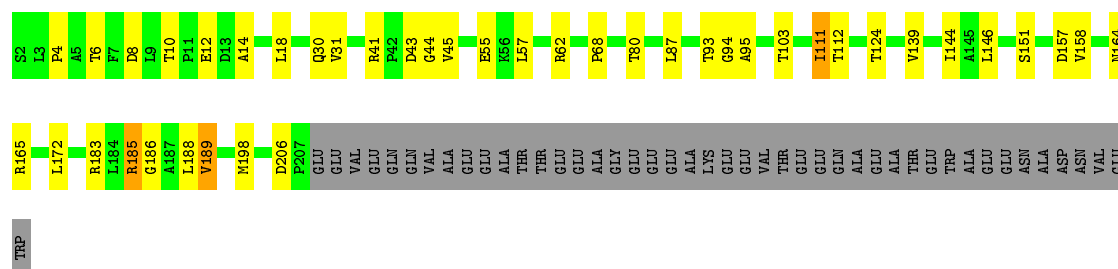
• Molecule 2: 40S ribosomal protein S0-A

Chain S0: 63% 19% 18%



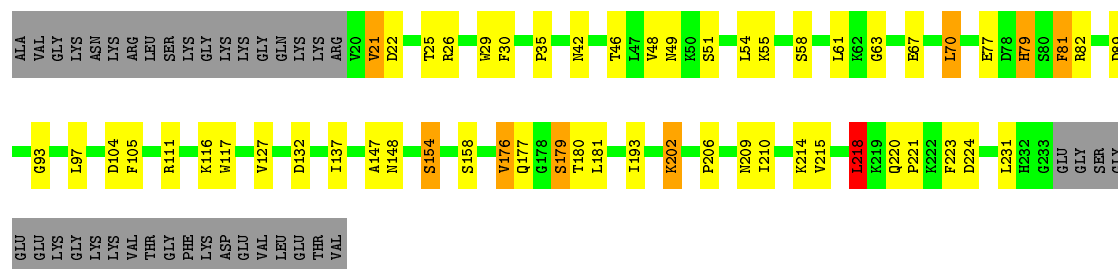
• Molecule 2: 40S ribosomal protein S0-A

Chain s0: 65% 16% 18%



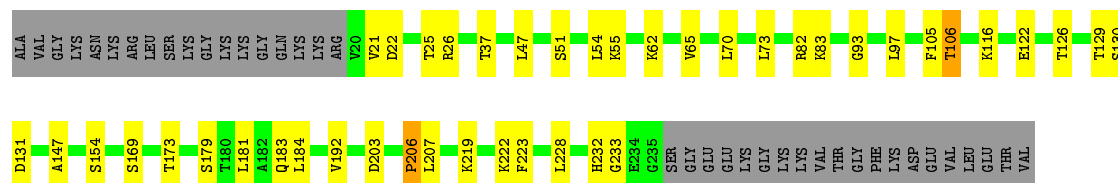
• Molecule 3: 40S ribosomal protein S1-A

Chain S1: 62% 19% 16%



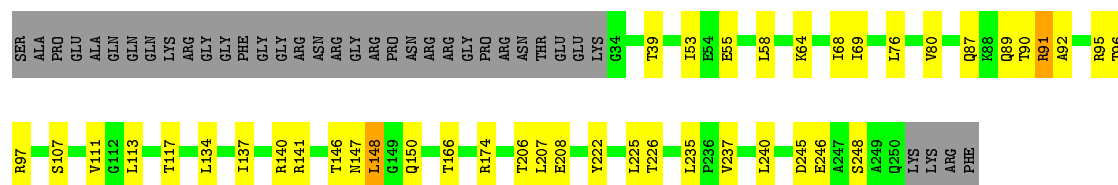
- Molecule 3: 40S ribosomal protein S1-A

Chain s1: 68% 16% 15%



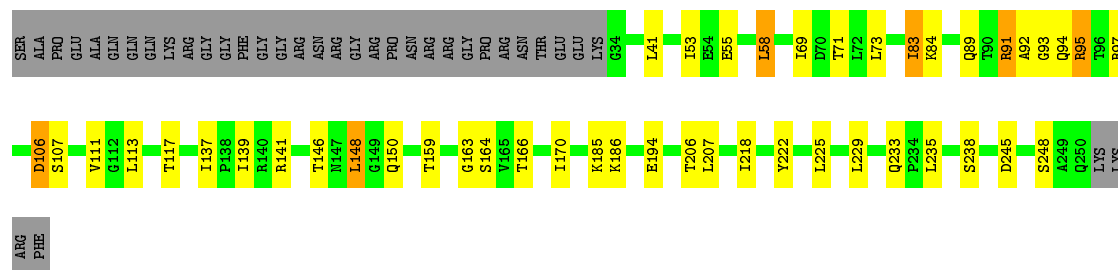
- Molecule 4: 40S ribosomal protein S2

Chain S2: 69% 16% 14%



- Molecule 4: 40S ribosomal protein S2

Chain s2: 68% 16% 14%



- Molecule 5: 40S ribosomal protein S3

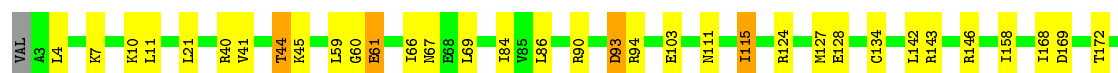
Chain S3: 74% 18% 7%





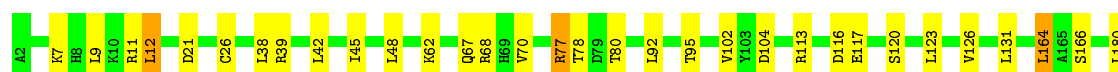
- Molecule 5: 40S ribosomal protein S3

Chain s3: 73% 18% 7%



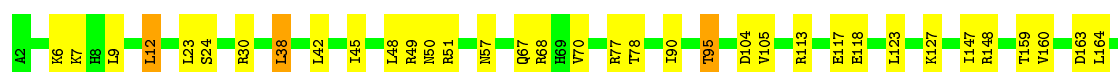
- Molecule 6: 40S ribosomal protein S4-A

Chain S4: 80% 19%



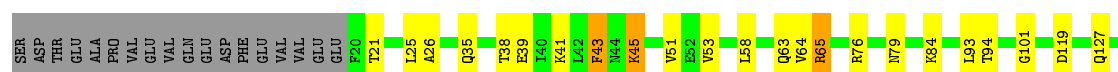
- Molecule 6: 40S ribosomal protein S4-A

Chain s4: 79% 20%



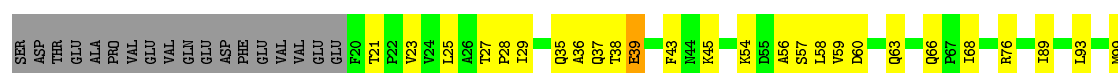
- Molecule 7: 40S ribosomal protein S5

Chain S5: 75% 16% 8%



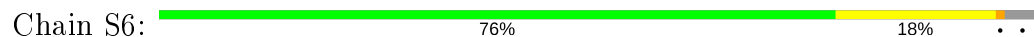
- Molecule 7: 40S ribosomal protein S5

Chain s5: 71% 21% 8%

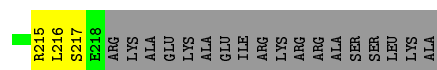
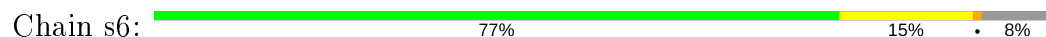




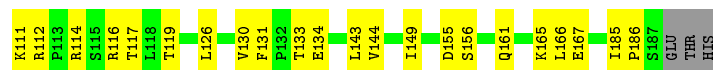
- Molecule 8: 40S ribosomal protein S6-A



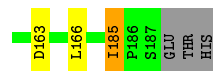
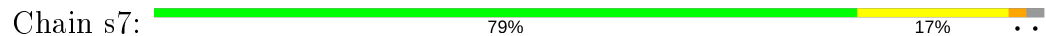
- Molecule 8: 40S ribosomal protein S6-A



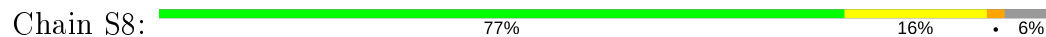
- Molecule 9: 40S ribosomal protein S7-A



- Molecule 9: 40S ribosomal protein S7-A



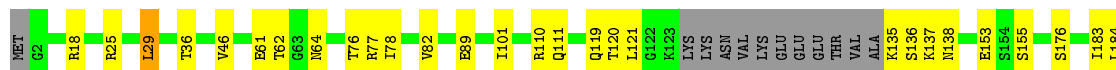
- Molecule 10: 40S ribosomal protein S8-A





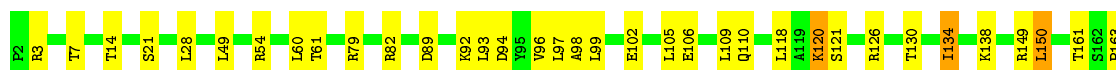
- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 80% 14% 6%



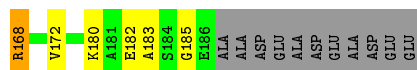
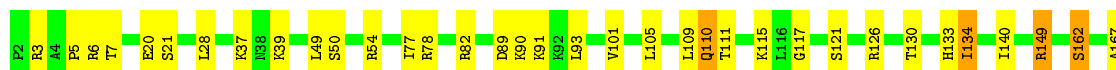
- Molecule 11: 40S ribosomal protein S9-A

Chain S9: 73% 20% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 73% 18% 6%



- Molecule 12: 40S ribosomal protein S10-A

Chain C0: 71% 18% 9%




- Molecule 12: 40S ribosomal protein S10-A

Chain c0: 72% 14% 5% 9%



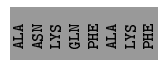
- Molecule 13: 40S ribosomal protein S11-A

Chain C1:  79% 19% 2%



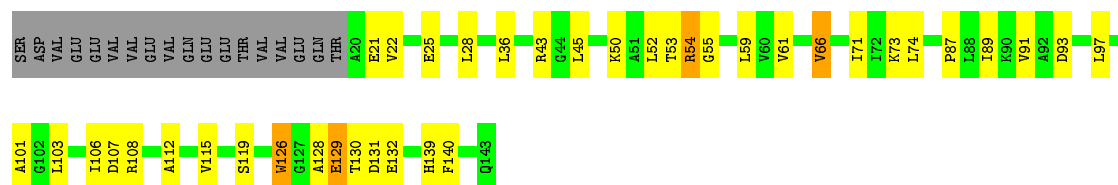
- Molecule 13: 40S ribosomal protein S11-A

Chain c1:  75% 19% • 6%



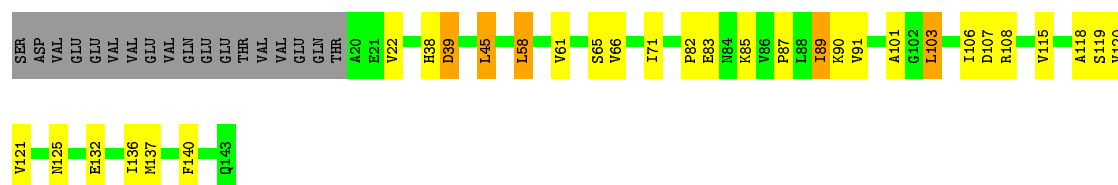
- Molecule 14: 40S ribosomal protein S12

Chain C2: 




- Molecule 14: 40S ribosomal protein S12

Chain c2:  65% 18% • 13%

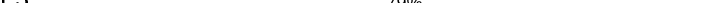


- Molecule 15: 40S ribosomal protein S13

Chain C3:  83% 14% .



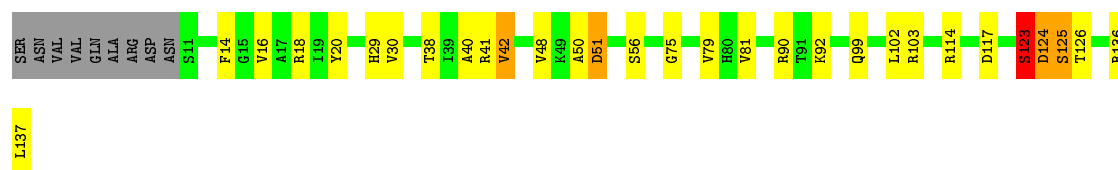
- Molecule 15: 40S ribosomal protein S13

Chain c3:  79% 19%



- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 



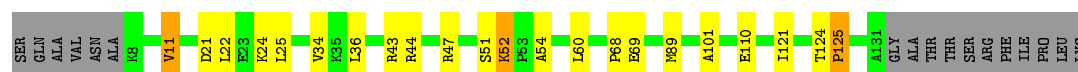
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 



- Molecule 17: 40S ribosomal protein S15

Chain C5: 




- Molecule 17: 40S ribosomal protein S15

Chain c5: 




- Molecule 18: 40S ribosomal protein S16-A

Chain C6: 



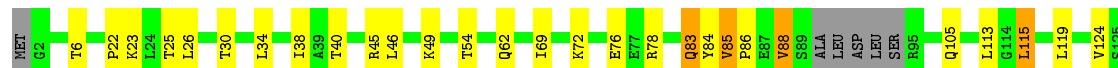
- Molecule 18: 40S ribosomal protein S16-A

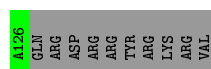
Chain c6: 



- Molecule 19: 40S ribosomal protein S17-A

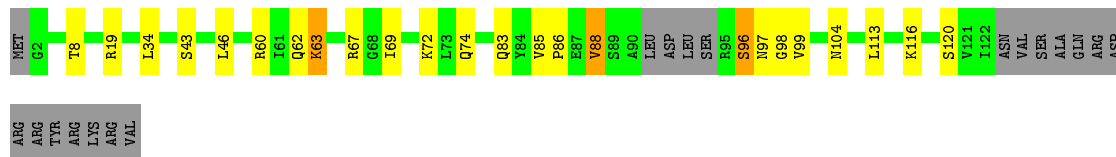
Chain C7: 





- Molecule 19: 40S ribosomal protein S17-A

Chain c7: 68% 15% 14%



- Molecule 20: 40S ribosomal protein S18-A

Chain C8: 77% 19%



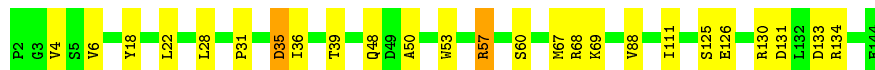
- Molecule 20: 40S ribosomal protein S18-A

Chain c8: 76% 21%



- Molecule 21: 40S ribosomal protein S19-A

Chain C9: 83% 16%



- Molecule 21: 40S ribosomal protein S19-A

Chain c9: 83% 15%

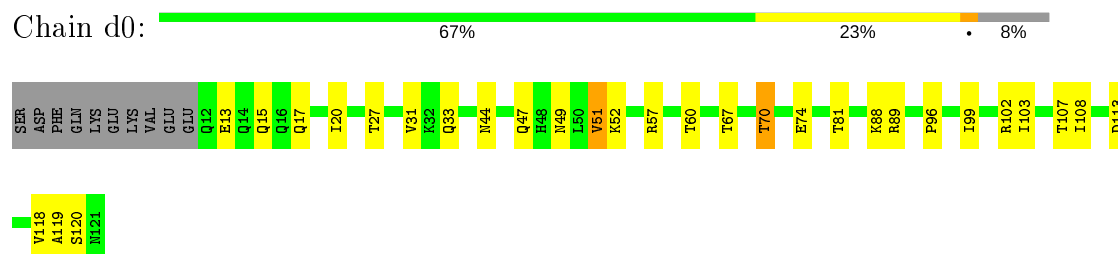


- Molecule 22: 40S ribosomal protein S20

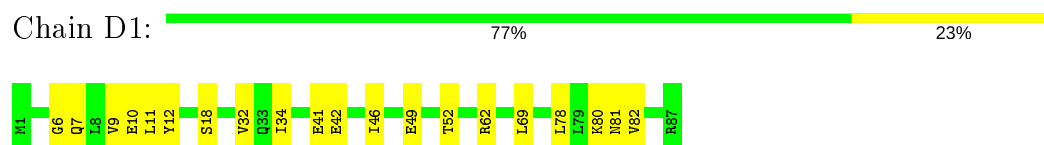
Chain D0: 67% 22% 11%



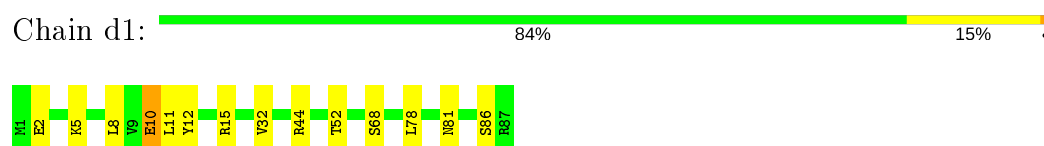
- Molecule 22: 40S ribosomal protein S20



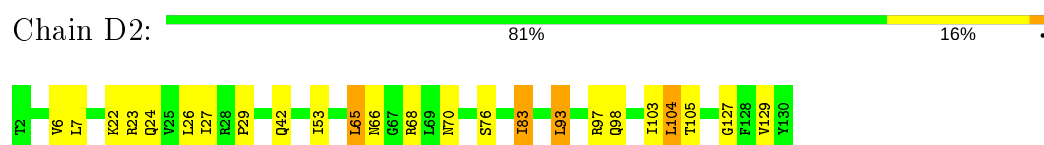
- Molecule 23: 40S ribosomal protein S21-A



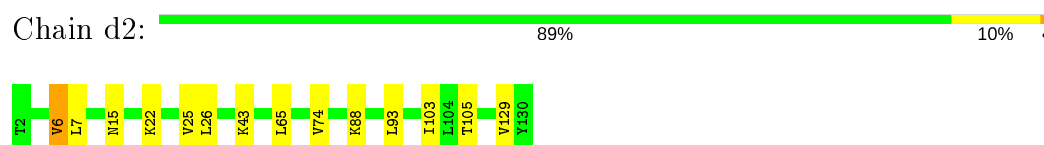
- Molecule 23: 40S ribosomal protein S21-A



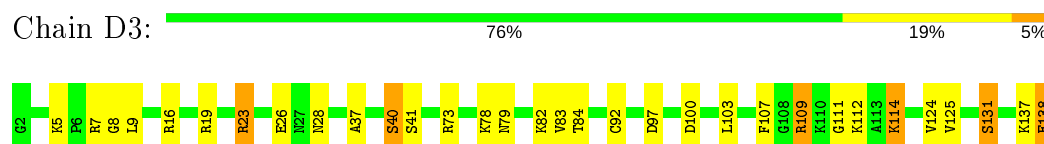
- Molecule 24: 40S ribosomal protein S22-A



- Molecule 24: 40S ribosomal protein S22-A



- Molecule 25: 40S ribosomal protein S23-A

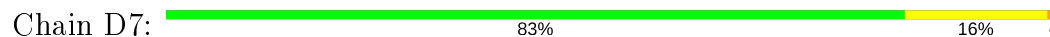


- Molecule 25: 40S ribosomal protein S23-A

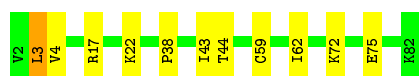
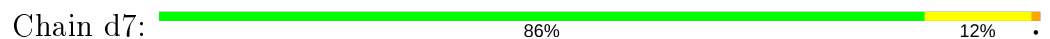




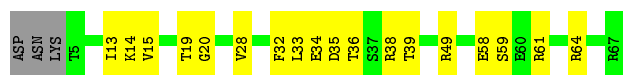
- Molecule 29: 40S ribosomal protein S27-A



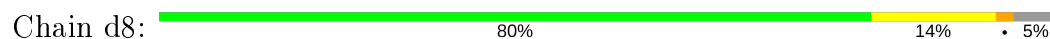
- Molecule 29: 40S ribosomal protein S27-A



- Molecule 30: 40S ribosomal protein S28-A



- Molecule 30: 40S ribosomal protein S28-A



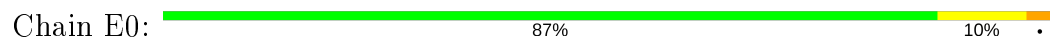
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 31: 40S ribosomal protein S29-A



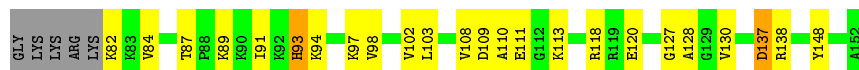
- Molecule 32: 40S ribosomal protein S30-A






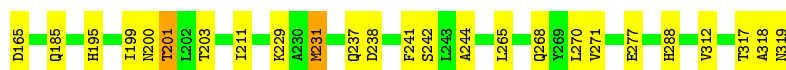
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:

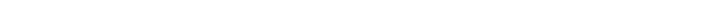


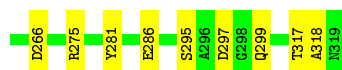
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:  81% 18%



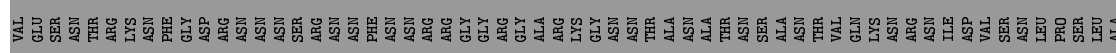
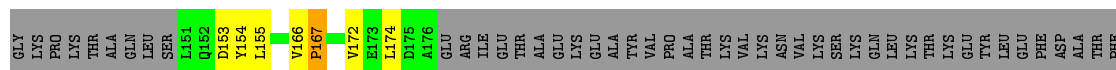
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:  87% 13%



- Molecule 35: Suppressor protein STM1

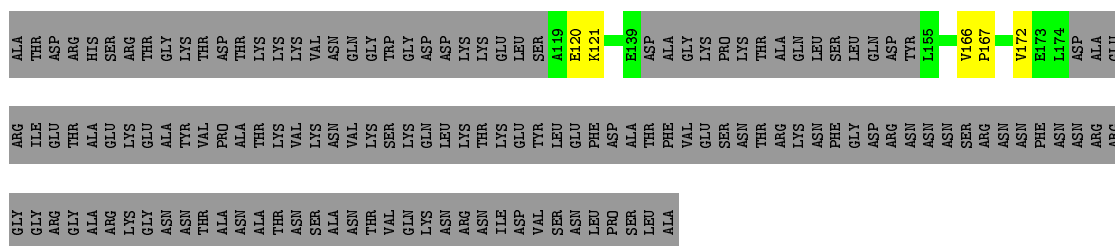
Chain SM: 



- Molecule 35: Suppressor protein STM1

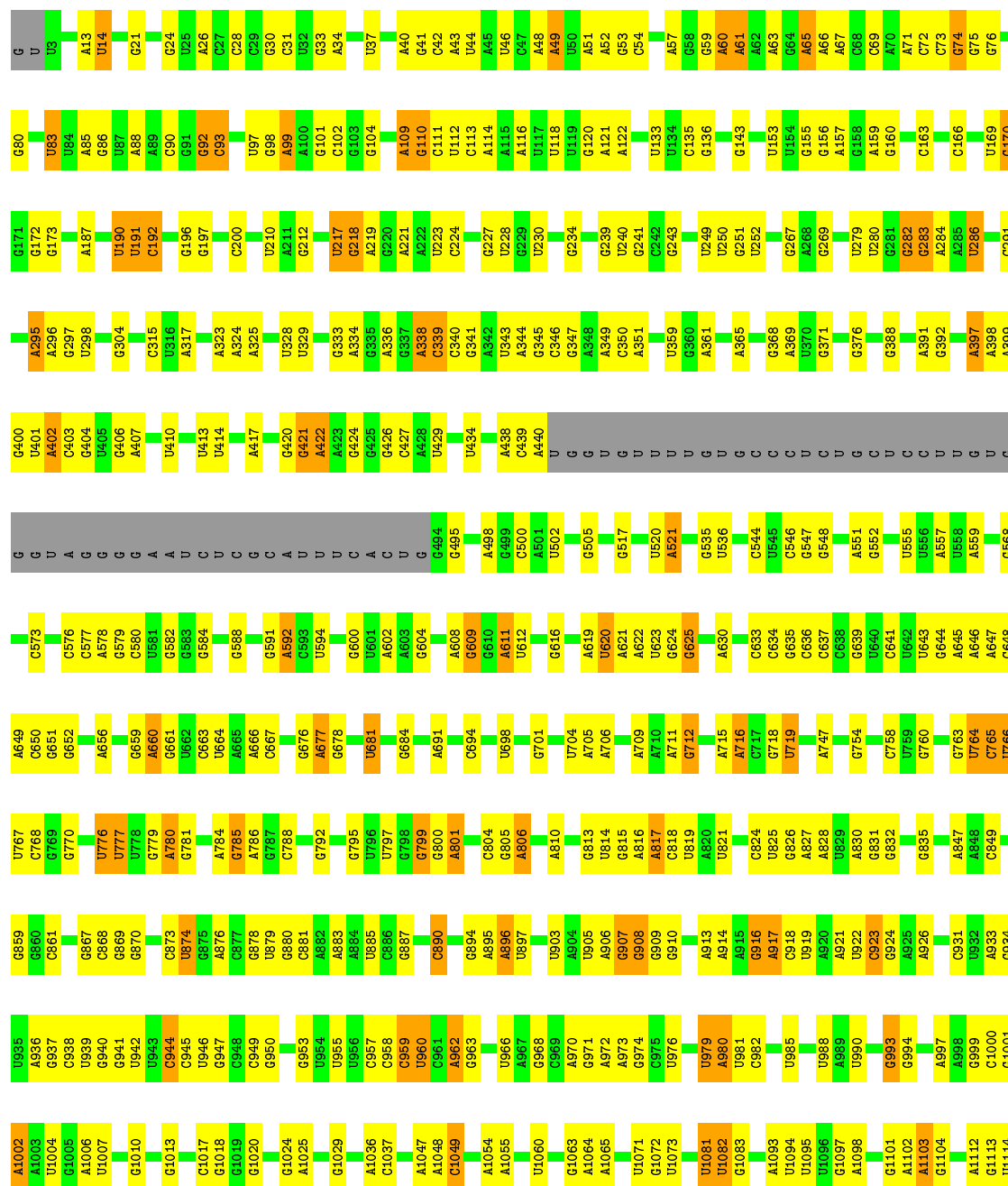
Chain sM: 



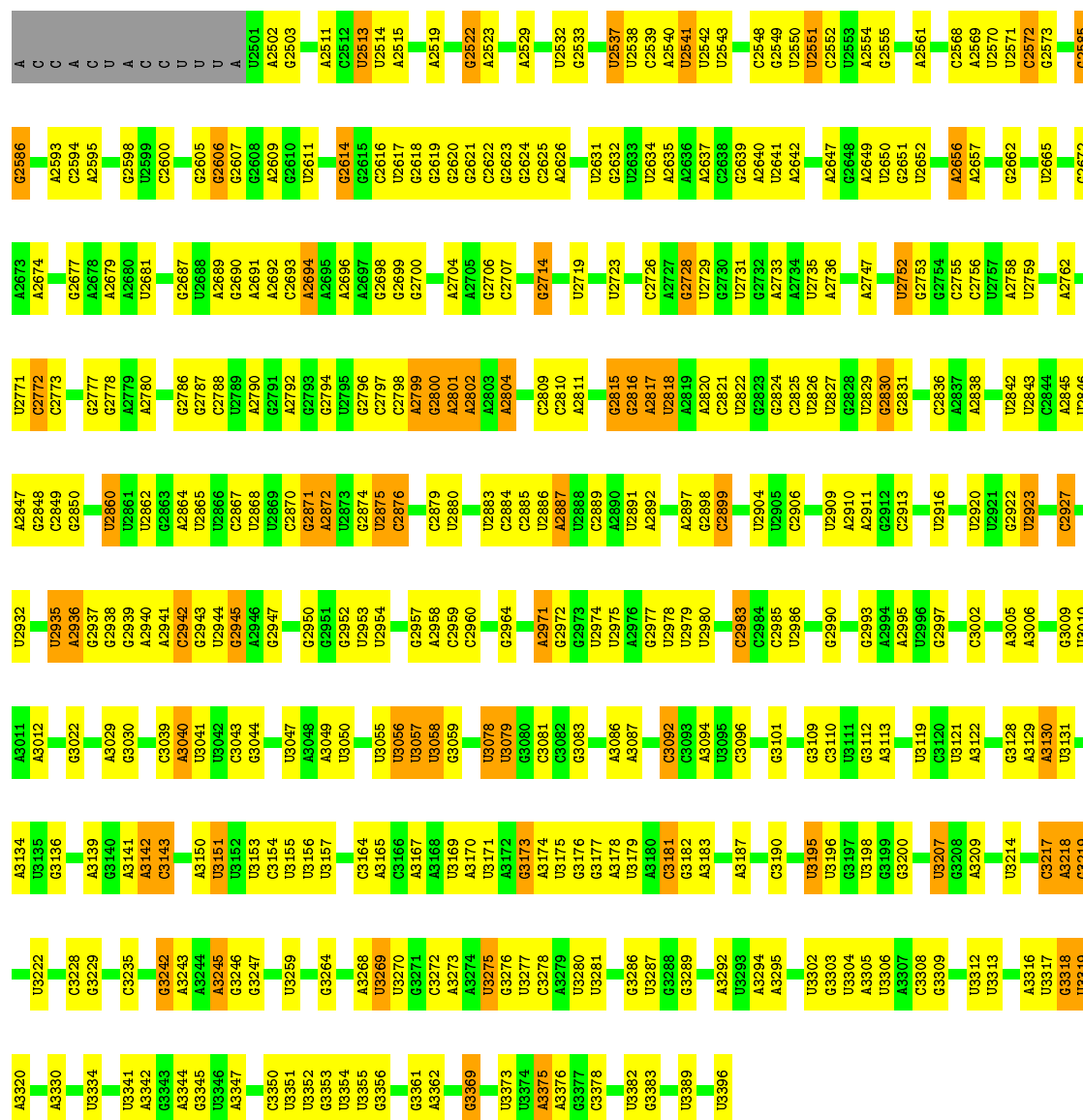


- Molecule 36: 25S ribosomal RNA

Chain 1: 54% 32% 6% 7%

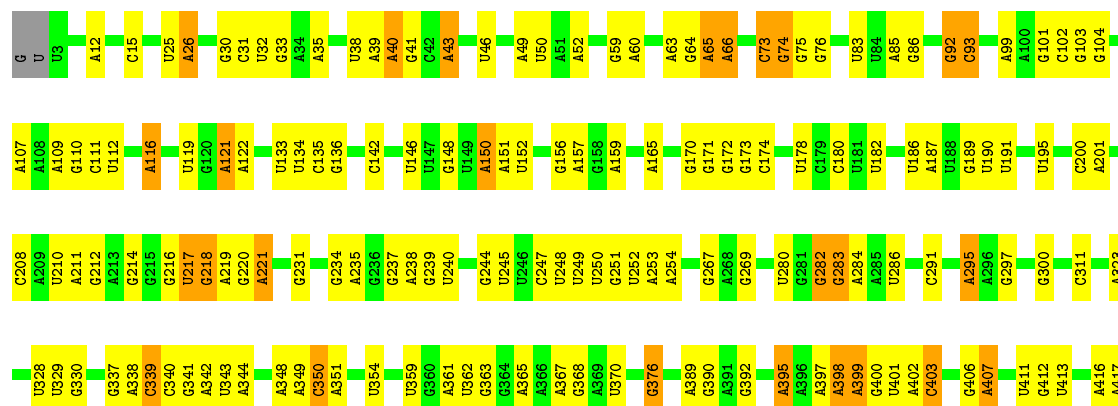


C2415	C2335	A2144	U	G1929	G1925	C1644	C1527	U1436	U1356	A1271	A1182	G1115
U2416	U2336	A2147	C	A1930	U1831	U1645	G1528	C1437	G1357	C1272	C1183	G1116
U2417	U2340	U2148	U	U1931	G	C1657	A1529	G1440	G1362	A1274	A1184	G1117
G2418	A2242	A2149	C	G1935	U	G1660	U1530	G1444	A1363	A1278	C1189	C1119
A2419	A2343	G2150	U	G1935	U1834	C1685	G1533	U1445	A1364	A1279	A1190	A1120
C2422	U2349	C2151	G	G1948	G1838	U1695	U1538	U1446	G1365	C1279	U1191	U1121
U2423	C2350	A2152	U	C1951	A1839	C1685	G1538	G1447	A1366	G1285	C1192	U1122
A2424	G2246	U2153	A	G1952	U1840	A1683	G1547	G1450	G1371	A1286	C1196	U1123
U2434	G2247	G2154	G	G1953	A1841	U1695	U1554	C1481	U1124	A1287	U1125	U1124
G2435	G2249	C2155	A	G1954	A1842	U1715	U1555	A1452	G1376	A1287	G1126	G1127
U2436	G2250	U2156	C	U1955	C1845	U1716	C1556	A1453	G1377	C1282	A1201	A1130
G2437	G2253	A2158	G	A	A1847	U1717	U1560	U1454	G1380	U1293	A1202	G1131
C2444	U2254	G2165	C	G	G1848	U1717	G1561	U1455	A1381	A1294	A1203	C1132
A2445	A2255	A2166	U	U	U1849	G1761	C1562	U1458	A1386	C1296	A1204	G1133
U	C2257	A2167	C	G	G1850	C1725	C1563	U1467	G1389	C1297	G1209	
A	G2257	G2168	G	G	U1851	U1724	U1564	A1468	A1390	U1305	A1212	A1136
G	G2272	U2170	U	G	U1855	G1733	G1576	A1468	A1399	G1306	G1213	G1140
A	G2273	U2175	C	C	A1858	A1741	U1567	A1477	A1394	G1307	C1216	C1141
A	U2176	U2176	G	C	A1859	G1748	U1568	U1477	A1395	A1308	U1217	G1142
G	G2177	A2178	A	U	G1863	A1749	U1569	G1480	G1396	U1309	U1218	A1143
U	C2179	C2179	C	U	G1868	U1750	U1570	A1481	A1399	G1313		U1144
G	A2181	U2184	U	G	G1879	G1751	G1576	A1482	A1400	C1314	G1222	G1145
A	G2185	G2185	A	U	U1880	A1760	C1579	G1483	G1403	U1315	G1226	C1146
A	C2188	U2188	C	C	A1881	C1761	U1580	U1484	G1404	C1316	C1227	G1147
A	U2093	C2094	C	G	A1886	C1762	C1582	A1489	U1405	A1318	G1232	G1149
A	C2094	C2094	C	C	A1887	U1765	A1583	A1490	A1406	C1320	G1233	A1150
A	U2101	U2102	G	G	U1888	G1766	U1584	G1493	A1407	G1323	U1235	G1152
A	U2102	U2102	U	C	G1889	C1767	G1586	U1494	G1409	A1326	G1236	A1153
U	G2111	U2112	C	G	U1890	G1770	A1587	U1495	H410	A1326	G1237	C1155
U	U2112	C2113	U	C	A1891	U1770	A1588	C1496	C1411	U1329	U1241	C1156
U	C2113	C2114	G	G	G1892	G1780	A1589	C1499	G1412	A1330	G1242	G1157
U	G2115	U2115	G	U	U1893	C1781	G1590	U1509	G1413	U1331	A1158	A1159
U	G2116	G2116	U	C	A1894	U1784	G1592	U1511	G1414	A1332	A1244	C1160
U	G2131	G2131	U	G	A1895	G1784	A1593	G1503	U1415	C1333	A1245	G1161
U	G2132	G2132	A	G	G1898	G1789	U1594	C1507	A1419	U1334	G1246	U1162
U	G2133	G2133	C	C	U1901	A1797	U1595	C1508	A1420	C1335	U1247	A1163
U	G2134	G2134	C	U	G1902	U1809	C1596	A1509	G1421	U1336	G1248	A1164
U	G2135	G2135	G	U	C1904	A1810	A1605	U1511	G1422	A1342	G1249	A1165
U	G2136	G2136	C	U	G1905	U1810	A1605	G1514	C1423	A1343	G1250	G1166
U	G2137	G2137	C	G	G1906	A1814	G1610	A1515	U1424	G1346	U1167	U1168
U	U2137	A2138	C	A	C1907	U1815	G1611	C1516	U1425	U1347	U1258	A1169
U	A2139	A2139	U	U	A1908	A1816	C1615	U1517	A1428	G1348	G1262	U1173
U	U2140	U2140	G	C	A1911	G1817	U1620	U1519	A1429	G1349	A1263	G1174
U	U2141	U2141	U	C	G1918	U1818	U1620	G1520	U1430	A1350	U1265	C1175
U	C2227	U2142	A	U	C1919	U1819	U1629	U1523	C1432	A1352	G1266	G1178
U	A2143	A2143	G	U	U1920	U1820	U1643	U1526	A1433	U1353	U1269	A1180
U			G	G	U1920	U1821			A1435	A1355	A1270	U1181



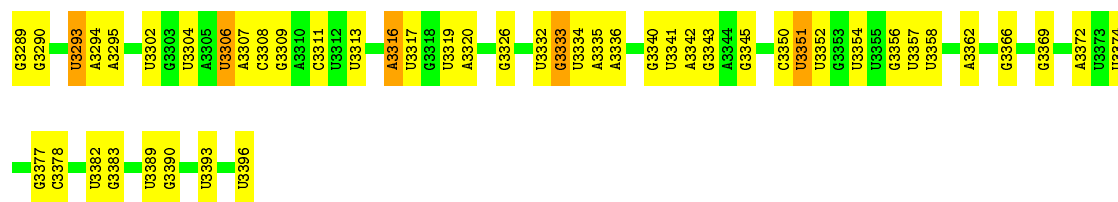
• Molecule 36: 25S ribosomal RNA

Chain 5: 54% 32% 6% 7%





G3202	U8119	A3016	A2936	U2860	C2772	C2664	G2574	U	U2434	C2362	C2287	C2181	C
U3203	C3120	A3017	G2937	U2861	C2773	U2665	G2584	A	G2435	A2363	G2288	A2182	U
C3204	A3123	C3018	G2938	U2865	G2777	C2666	G2585	C	U2436	G2364	U2289	A	A
U3207	A3124	U3019	G2939	U2866	G2778	U2667	G2589	C	G2437	C2365	C2290	U	U
G3208	U3125	U3020	A2940	U2867	G2779	A2674	G2593	U	A2438	C2366	G2293	U2189	U
A3209	C3126	A3033	C2942	C2870	U2794	G2677	A2593	U	U2439	U2367	U2994	U2190	G
C3210	A3130	C3034	G2943	A2872	U2795	A2678	G2598	U	A2440	U2368	A2295	U2191	C
G3211	U3131	A3035	U2944	U2873	G2796	A2679	G2599	A	G2441	G2369	A2296	C2192	G
C3212	U3132	U3036	G2945	U2874	C2797	C2682	G2600	U	U2442	G2370	A2297	U2192	U
A3213	C3133	C3039	A2946	U2875	C2798	U2683	G2601	U	G2443	G2371	G2300	G2201	G
U3214	U3134	A3040	G2947	U2876	C2799	A2684	G2614	U	U2444	A2372	G2301	C2202	C
A3215	C3135	U3041	C2948	G2877	G2800	A2685	G2615	U	A	C2373	U2302	U2203	C
G3216	U3138	U3042	U2949	G2878	A2801	A2686	G2616	U	U2445	C2374	U2303	U2204	U
C3217	C3139	C3043	G2950	U2879	A2802	G2689	G2617	U	U2446	G2375	G2304	C2205	U
A3218	G3140	U3047	U2953	C2881	A2803	G2690	G2618	U	U2447	U2376	A2305	U2206	G
G3219	A3142	A3048	U2954	U2882	A2804	A2691	G2619	U	U2448	G2377	G2306	A2207	G
C3220	C3143	A3049	U2955	U2883	G2805	C2692	G2620	U	U2449	C2378	C2307	G2208	U
U3221	G3144	U3050	A2956	U2884	G2806	A2693	G2621	U	U2450	G2379	U2308	U2209	U
G3222	C3145	G3051	G2957	U2885	G2807	A2694	G2622	U	U2451	U2380	A2309	U2210	G
C3223	A3150	U3055	U2964	A2887	C2810	A2695	G2623	U	U2452	A2381	U2310	G2211	A
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G3225	C3154	U3057	G2968	U2889	C2812	G2698	G2625	U	U2454	U2383	A2312	G2213	A
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C3227	U3156	G3059	G2970	A2891	A2814	G2700	G2627	U	U2456	G2385	U2314	U2134	G
U3228	C3157	U3060	A2971	U2892	G2815	U2701	G2628	U	U2457	U2386	U2315	G2222	C
G3229	U3158	G3061	G2972	A2893	G2816	A2702	G2629	U	U2458	C2387	G2316	A2223	G
C3230	C3159	G3062	U2975	U2894	G2817	A2703	G2630	U	U2459	U2388	G2317	U2135	C
U3231	U3164	G3069	U2976	A2902	U2818	U2704	G2631	U	U2460	C2389	A2318	U2136	U
G3232	C3165	G3075	U2977	U2903	A2819	A2705	G2632	U	U2461	G2390	U2319	G2224	G
U3233	A3168	C3076	U2978	U2904	U2820	A2706	G2633	U	U2462	A2391	G2320	U2137	C
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U3235	G3173	U3079	U2988	U2909	C2822	U2708	G2635	U	U2464	U2401	G2322	G2234	U
G3236	A3174	U3080	U2989	A2910	G2823	A2709	G2636	U	U2465	A2402	U2323	G2235	C
C3237	U3175	A3086	G2990	A2911	A2833	G2710	G2637	U	U2466	G2403	C2338	G2236	U
U3238	C3176	C3092	U2991	A2912	G2834	U2711	G2638	U	U2467	U2404	U2339	U2148	U
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A3240	U3178	U3094	U2993	U2914	C2836	G2713	G2640	U	U2469	U2406	A2341	U2150	C
U3241	C3179	C3095	G2994	U2915	C2837	U2714	A2643	U	U2470	U2411	U2342	U2151	A
G3242	U3180	U3096	A2995	U2916	A2838	U2715	G2644	U	U2471	U2412	U2343	A2152	G
C3243	C3181	C3097	U2996	G2917	U2839	U2716	G2645	U	U2472	G2413	A2344	U2153	C
U3244	U3185	G3098	G2997	G2918	G2840	U2717	G2646	U	U2473	U2414	U2345	U2154	U
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G3251	U3192	C3106	U3010	U2929	G2847	U2724	U2653	U	U2480	C2421	U2352	U2170	G
A3252	C3193	U3107	A3011	A2930	C2848	U2725	G2654	U	U2481	U2422	U2353	G2171	C
U3253	U3194	G3108	A3012	U2931	G2849	U2726	G2655	U	U2482	U2423	C2354	A2158	U
C3254	C3195	U3109	U3013	U2932	C2850	U2727	G2656	U	U2483	U2424	G2355	U2176	G
U3255	U3196	U3110	A3014	U2933	U2851	U2728	G2657	U	U2484	U2425	U2356	G2177	C
G3256	C3197	C3111	U3015	U2934	A2852	U2729	G2658	U	U2485	U2426	U2357	A2178	U
U3257	U3198	U3112	A3016	U2935	C2853	U2730	G2659	U	U2486	U2427	C2358	C2285	C
C3258	C3199	G3113	U3017	U2936	U2854	U2731	G2660	U	U2487	U2428	U2359	C2286	G
U3259	U3200	U3114	A3018	U2937	G2855	U2732	G2661	U	U2488	U2429	A2361	U2287	A
G3260	C3201	C3115	U3019	U2938	U2856	U2733	G2662	U	U2489	U2430	U2362	U2288	C



• Molecule 37: 5S ribosomal RNA

Chain 3: 76% 23%



• Molecule 37: 5S ribosomal RNA

Chain 7: 60% 34% 7%



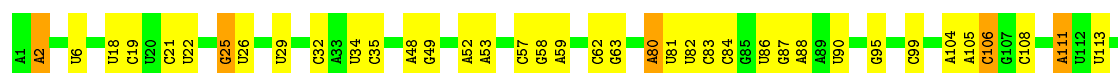
• Molecule 38: 5.8S ribosomal RNA

Chain 4: 64% 30% 6%



• Molecule 38: 5.8S ribosomal RNA

Chain 8: 70% 27%



• Molecule 39: 60S ribosomal protein L2-A

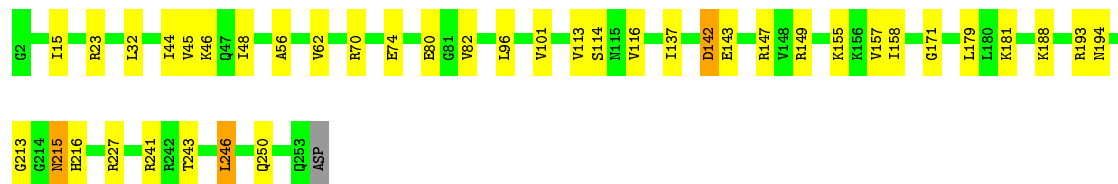
Chain L2: 83% 16%





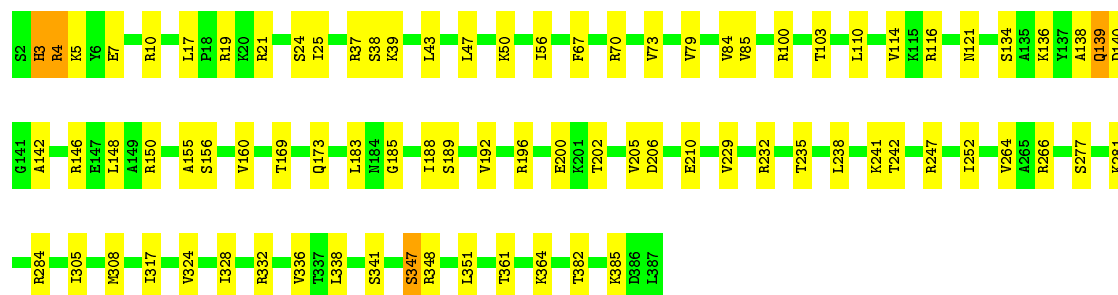
• Molecule 39: 60S ribosomal protein L2-A

Chain l2: 84% 15%



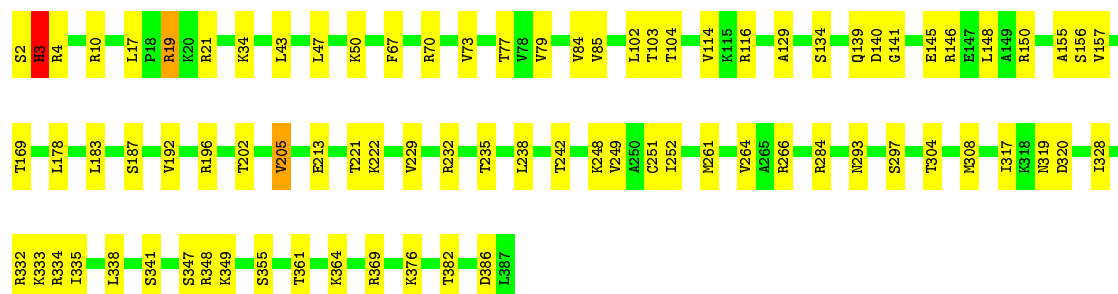
• Molecule 40: 60S ribosomal protein L3

Chain L3: 78% 20%



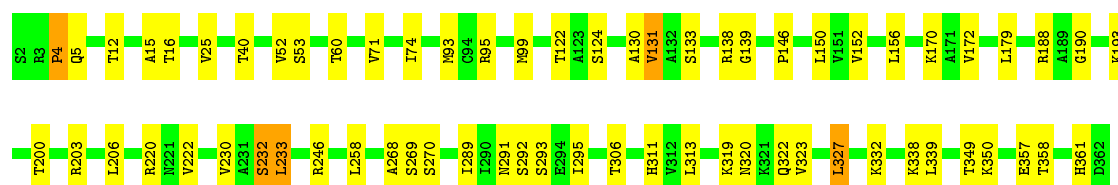
• Molecule 40: 60S ribosomal protein L3

Chain l3: 78% 21%




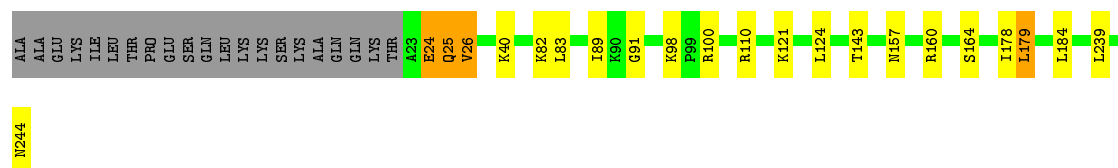
• Molecule 41: 60S ribosomal protein L4-A

Chain L4: 82% 17%




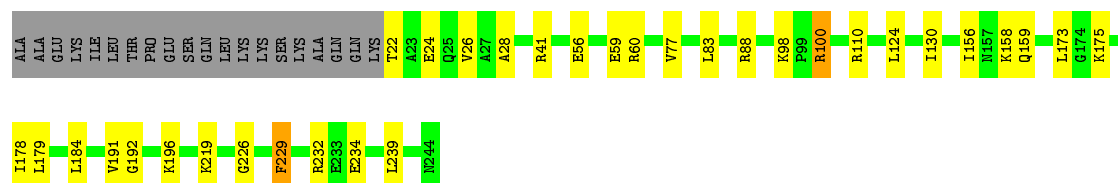
- Molecule 44: 60S ribosomal protein L7-A

Chain L7:  82% 7% 9%




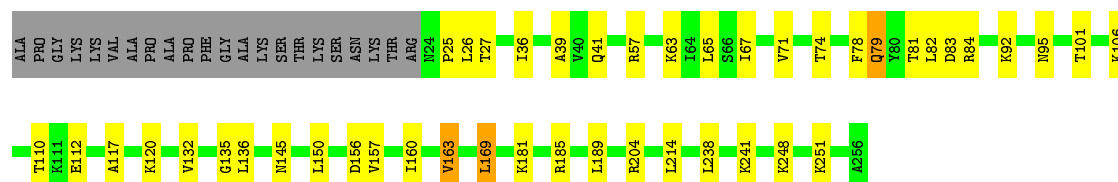
- Molecule 44: 60S ribosomal protein L7-A

Chain L7:  78% 13% 8%



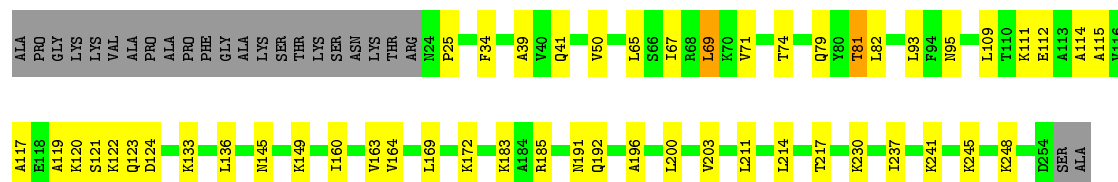
- Molecule 45: 60S ribosomal protein L8-A

Chain L8:  74% 16% 9%




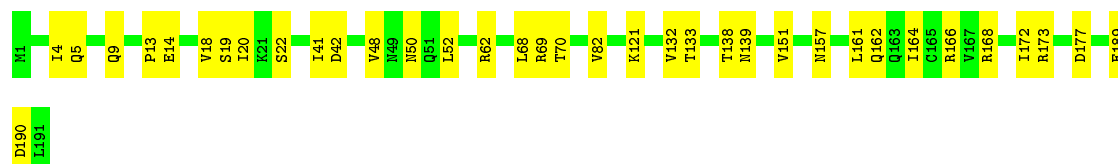
- Molecule 45: 60S ribosomal protein L8-A

Chain L8:  71% 19% 9%

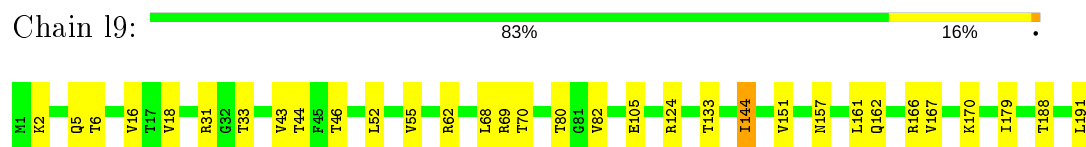


- Molecule 46: 60S ribosomal protein L9-A

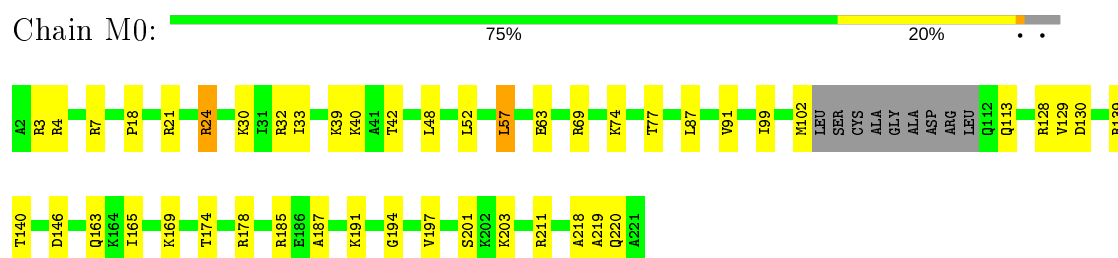
Chain L9:  81% 19%



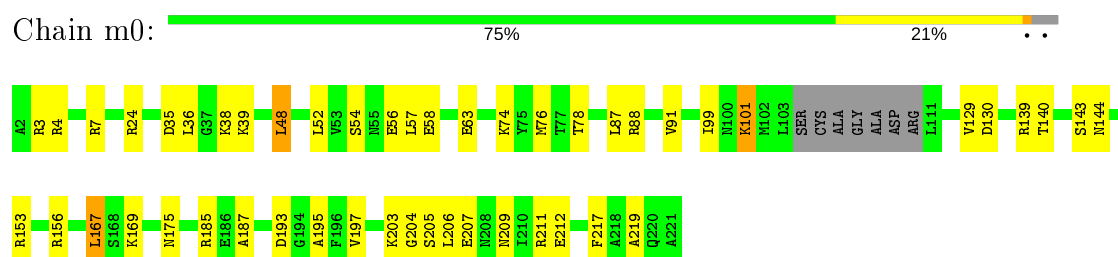
- Molecule 46: 60S ribosomal protein L9-A



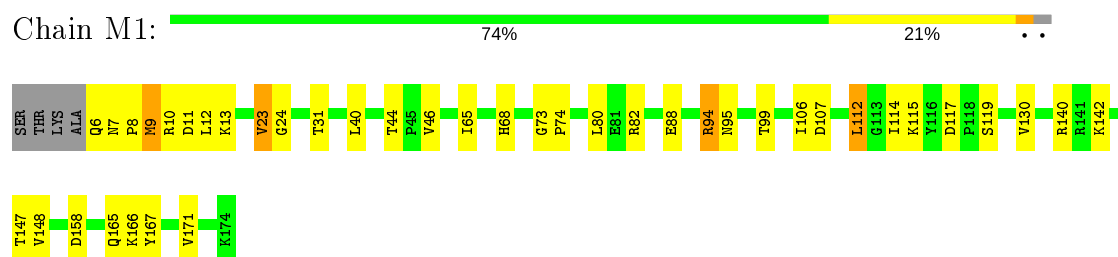
- Molecule 47: 60S ribosomal protein L10



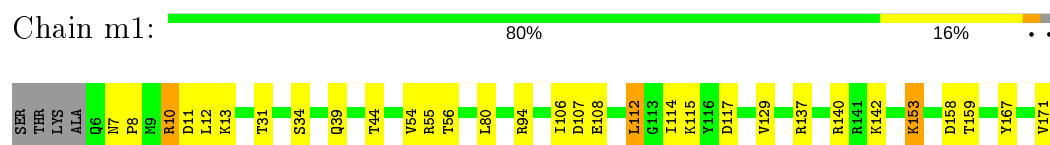
- Molecule 47: 60S ribosomal protein L10



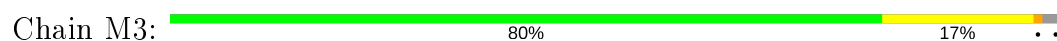
- Molecule 48: 60S ribosomal protein L11-B



- Molecule 48: 60S ribosomal protein L11-B



- Molecule 49: 60S ribosomal protein L13-A





- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 80% 17% ..



- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 82% 15% ...



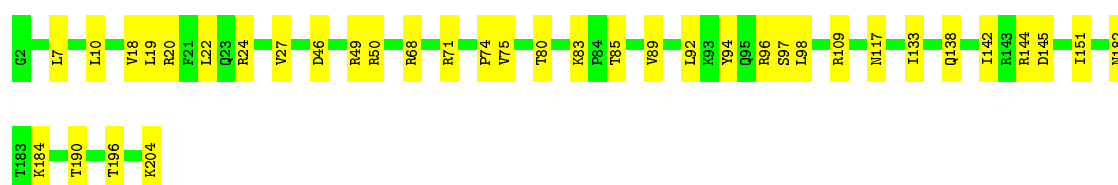
- Molecule 50: 60S ribosomal protein L14-A

Chain m4: 85% 14% .



- Molecule 51: 60S ribosomal protein L15-A

Chain M5: 82% 18%



- Molecule 51: 60S ribosomal protein L15-A

Chain m5: 84% 14% .



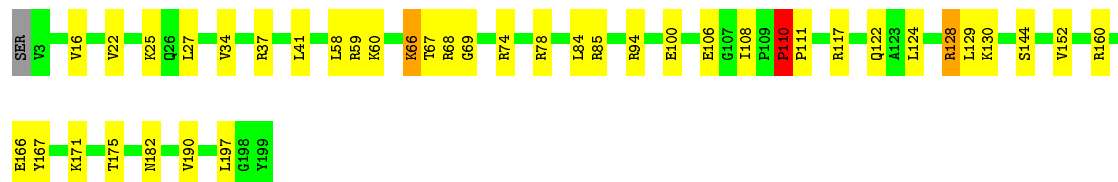
- Molecule 52: 60S ribosomal protein L16-A

Chain M6: 86% 12% ...



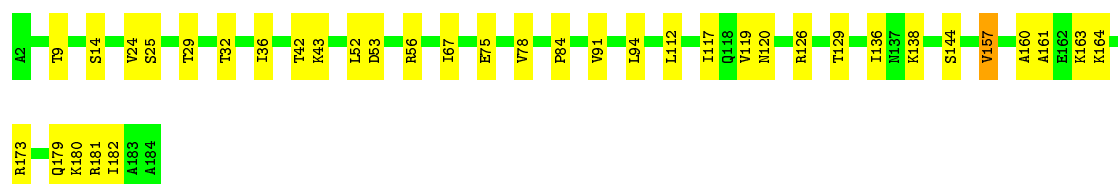
- Molecule 52: 60S ribosomal protein L16-A

Chain m6: 79% 19%



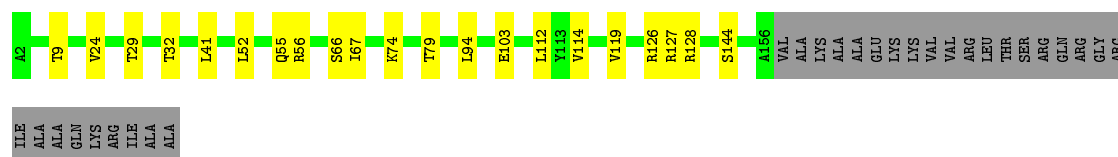
- Molecule 53: 60S ribosomal protein L17-A

Chain M7: 80% 20%



- Molecule 53: 60S ribosomal protein L17-A

Chain m7: 73% 11% 15%



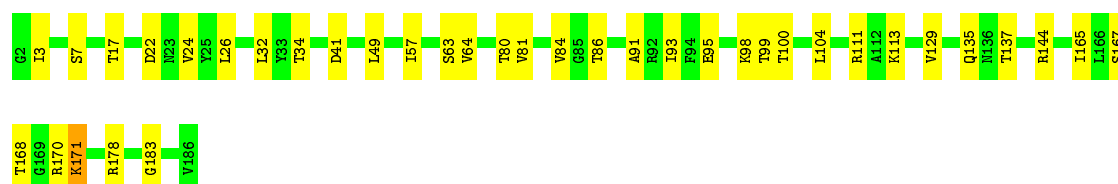
- Molecule 54: 60S ribosomal protein L18-A

Chain M8: 84% 15%



- Molecule 54: 60S ribosomal protein L18-A

Chain m8: 80% 19%




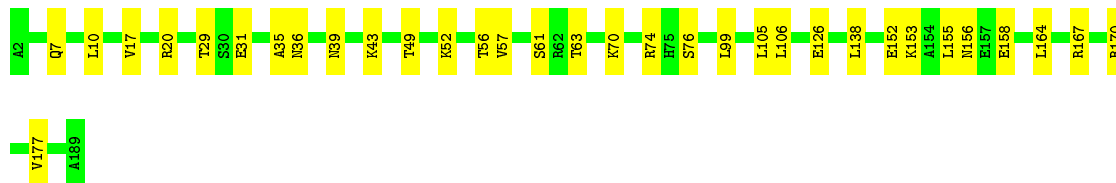
- Molecule 55: 60S ribosomal protein L19-A

Chain M9:  86% 14%




- Molecule 55: 60S ribosomal protein L19-A

Chain m9:  82% 18%




- Molecule 56: 60S ribosomal protein L20-A

Chain N0:  81% 16%




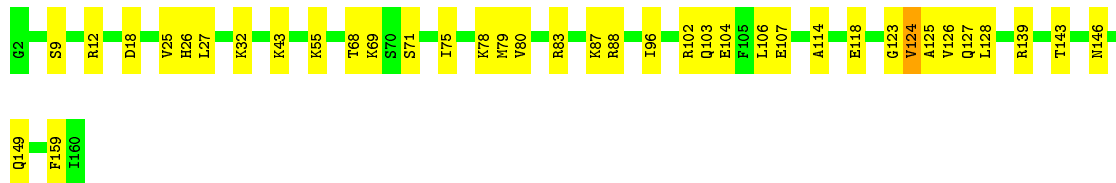
- Molecule 56: 60S ribosomal protein L20-A

Chain n0:  81% 19%




- Molecule 57: 60S ribosomal protein L21-A

Chain N1:  76% 23%



- Molecule 57: 60S ribosomal protein L21-A

Chain n1:  82% 16%



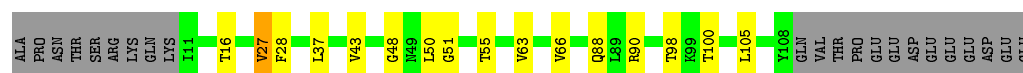
- Molecule 58: 60S ribosomal protein L22-A

Chain N2: 



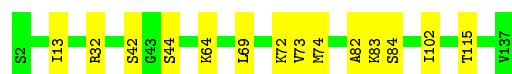
- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 



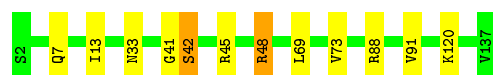
- Molecule 59: 60S ribosomal protein L23-A

Chain N3: 



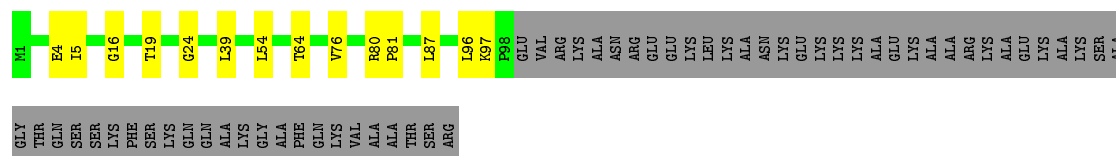
- Molecule 59: 60S ribosomal protein L23-A

Chain n3: 



- Molecule 60: 60S ribosomal protein L24-A

Chain N4: 



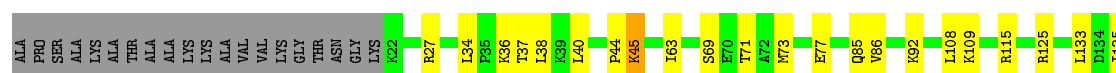
- Molecule 60: 60S ribosomal protein L24-A

Chain n4: 



- Molecule 61: 60S ribosomal protein L25

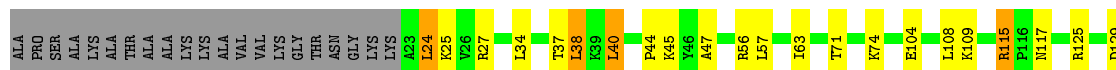
Chain N5: 





- Molecule 61: 60S ribosomal protein L25

Chain n5: 67% 15% 15%



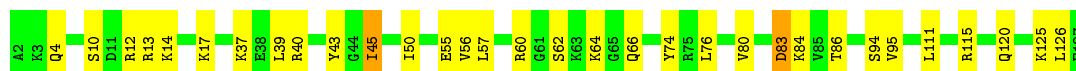
- Molecule 62: 60S ribosomal protein L26-A

Chain N6: 77% 21%



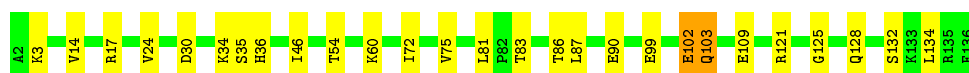
- Molecule 62: 60S ribosomal protein L26-A

Chain n6: 75% 24%



- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 80% 19%



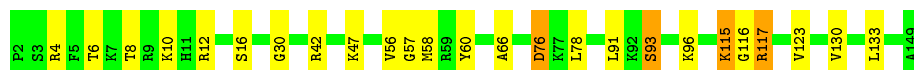
- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 78% 21%




- Molecule 64: 60S ribosomal protein L28

Chain N8: 83% 14%




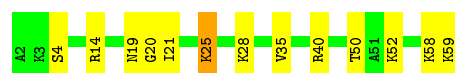
- Molecule 64: 60S ribosomal protein L28

Chain n8:  82% 18%




- Molecule 65: 60S ribosomal protein L29

Chain N9:  78% 21%




- Molecule 65: 60S ribosomal protein L29

Chain n9:  78% 21%




- Molecule 66: 60S ribosomal protein L30

Chain O0:  82% 11% 7%




- Molecule 66: 60S ribosomal protein L30

Chain o0:  80% 15%



- Molecule 67: 60S ribosomal protein L31-A

Chain O1:  79% 18%




- Molecule 67: 60S ribosomal protein L31-A

Chain o1:  71% 27%




- Molecule 68: 60S ribosomal protein L32

Chain O2:  84% 14% ..



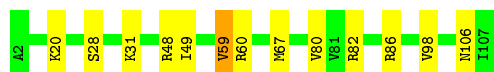
- Molecule 68: 60S ribosomal protein L32

Chain o2:  78% 19% ..




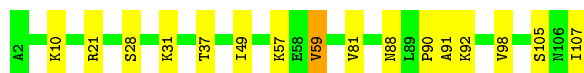
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:  88% 11% .




- Molecule 69: 60S ribosomal protein L33-A

Chain o3:  85% 14% .




- Molecule 70: 60S ribosomal protein L34-A

Chain O4:  76% 17% • 6%




- Molecule 70: 60S ribosomal protein L34-A

Chain o4:  81% 13% • 6%




- Molecule 71: 60S ribosomal protein L35-A

Chain O5:  80% 18% .




- Molecule 71: 60S ribosomal protein L35-A

Chain o5:  82% 18%



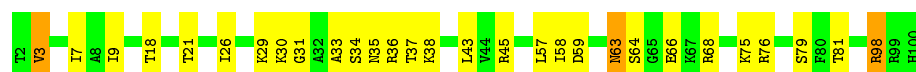
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:  78% 19%




- Molecule 72: 60S ribosomal protein L36-A

Chain o6:  71% 26%




- Molecule 73: 60S ribosomal protein L37-A

Chain O7:  85% 13%




- Molecule 73: 60S ribosomal protein L37-A

Chain o7:  80% 20%




- Molecule 74: 60S ribosomal protein L38

Chain O8:  79% 19%




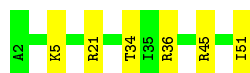
- Molecule 74: 60S ribosomal protein L38

Chain o8:  83% 16%




- Molecule 75: 60S ribosomal protein L39

Chain O9:  88% 12%




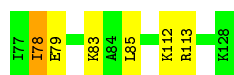
- Molecule 75: 60S ribosomal protein L39

Chain o9:  84% 16%




- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:  88% 10%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  81% 19%



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  68% 32%




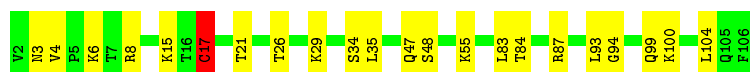
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  76% 20%




- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  79% 20%




- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  81% 18%




- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  82% 18%




- Molecule 79: 60S ribosomal protein L43-A

Chain q3:  81% 18%



- Molecule 80: 40S ribosomal protein S30-A

Chain e0:  76% 24%



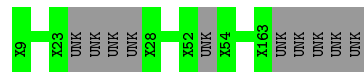
- Molecule 81: Ubiquitin-40S ribosomal protein S31

Chain e1:  58% 34% 7%




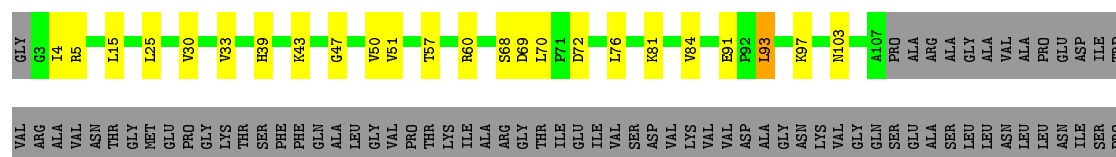
- Molecule 82: UNKNOWN PROTEIN m2

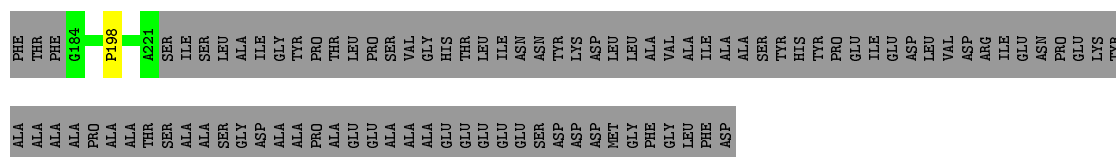
Chain m2:  94% 6%



- Molecule 83: 60S acidic ribosomal protein P0

Chain p0:  38% 8% 54%





- Molecule 84: UNKNOWN PROTEIN p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

- Molecule 85: UNKNOWN PROTEIN p2

Chain p2: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.43Å 288.22Å 305.08Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	267.37 – 2.90	Depositor
% Data completeness (in resolution range)	100.0 (267.37-2.90)	Depositor
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.204 , 0.245	Depositor
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.213	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411205	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OHX, MG, 3HE

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	0.69	3/41698 (0.0%)	1.25	259/64972 (0.4%)
1	6	0.83	9/42765 (0.0%)	1.36	416/66634 (0.6%)
2	S0	0.45	0/1617	0.63	0/2215
2	s0	0.50	0/1623	0.70	0/2222
3	S1	0.35	0/1735	0.63	2/2335 (0.1%)
3	s1	0.49	0/1748	0.68	0/2352
4	S2	0.49	0/1665	0.66	1/2263 (0.0%)
4	s2	0.60	0/1665	0.76	2/2263 (0.1%)
5	S3	0.49	0/1759	0.62	0/2368
5	s3	0.47	0/1759	0.60	0/2368
6	S4	0.48	0/2109	0.71	1/2839 (0.0%)
6	s4	0.57	0/2109	0.77	1/2839 (0.0%)
7	S5	0.39	0/1629	0.58	0/2202
7	s5	0.45	0/1629	0.63	0/2202
8	S6	0.45	0/1823	0.64	0/2439
8	s6	0.55	0/1779	0.69	0/2379
9	S7	0.43	0/1506	0.63	0/2028
9	s7	0.49	0/1516	0.68	0/2043
10	S8	0.53	0/1514	0.74	1/2021 (0.0%)
10	s8	0.62	0/1514	0.76	1/2021 (0.0%)
11	S9	0.46	0/1519	0.64	0/2035
11	s9	0.56	0/1519	0.72	1/2035 (0.0%)
12	C0	0.42	0/790	0.67	1/1069 (0.1%)
12	c0	0.39	0/777	0.63	3/1049 (0.3%)
13	C1	0.61	0/1240	0.80	1/1675 (0.1%)
13	c1	0.63	0/1194	0.78	0/1610
14	C2	0.36	0/900	0.63	0/1224
14	c2	0.30	0/900	0.56	0/1224
15	C3	0.46	0/1215	0.66	3/1638 (0.2%)
15	c3	0.56	0/1215	0.73	1/1638 (0.1%)
16	C4	0.36	0/901	0.63	0/1217
16	c4	0.51	0/960	0.72	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.46	0/998	0.65	0/1341
17	c5	0.51	0/1060	0.66	1/1426 (0.1%)
18	C6	0.45	0/1125	0.66	2/1510 (0.1%)
18	c6	0.49	0/1131	0.71	0/1518
19	C7	0.43	0/935	0.63	0/1254
19	c7	0.51	0/914	0.73	0/1224
20	C8	0.46	0/1211	0.64	0/1628
20	c8	0.49	0/1211	0.71	2/1628 (0.1%)
21	C9	0.46	0/1130	0.67	1/1517 (0.1%)
21	c9	0.51	0/1130	0.74	2/1517 (0.1%)
22	D0	0.46	0/865	0.65	0/1169
22	d0	0.51	0/892	0.68	0/1205
23	D1	0.43	0/693	0.60	0/935
23	d1	0.54	0/693	0.71	0/935
24	D2	0.53	0/1038	0.73	3/1395 (0.2%)
24	d2	0.62	0/1038	0.74	0/1395
25	D3	0.60	0/1139	0.81	3/1518 (0.2%)
25	d3	0.70	0/1139	0.79	1/1518 (0.1%)
26	D4	0.45	0/1087	0.59	0/1449
26	d4	0.51	0/1087	0.68	0/1449
27	D5	0.40	0/571	0.71	1/768 (0.1%)
27	d5	0.44	0/566	0.63	0/761
28	D6	0.44	0/782	0.67	0/1047
28	d6	0.54	0/782	0.72	0/1047
29	D7	0.43	0/620	0.67	1/838 (0.1%)
29	d7	0.49	0/620	0.68	0/838
30	D8	0.34	0/499	0.55	0/670
30	d8	0.42	0/499	0.66	0/670
31	D9	0.52	0/452	0.73	1/600 (0.2%)
31	d9	0.54	0/452	0.67	0/600
32	E0	0.46	0/483	0.61	0/643
33	E1	0.45	0/577	0.73	0/770
34	SR	0.89	2/2494 (0.1%)	1.42	4/3393 (0.1%)
34	sR	0.41	0/2495	0.58	0/3395
35	SM	0.52	0/1113	0.68	2/1502 (0.1%)
35	sM	0.50	0/683	0.66	1/923 (0.1%)
36	1	1.08	69/75394 (0.1%)	1.60	1618/117545 (1.4%)
36	5	1.10	113/75414 (0.1%)	1.60	1498/117575 (1.3%)
37	3	0.87	1/2883 (0.0%)	1.39	30/4491 (0.7%)
37	7	1.10	5/2883 (0.2%)	1.61	64/4491 (1.4%)
38	4	1.01	0/3746	1.51	61/5832 (1.0%)
38	8	0.87	0/3746	1.37	23/5832 (0.4%)
39	L2	0.72	0/1948	0.87	4/2617 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	l2	0.72	1/1946 (0.1%)	0.86	2/2614 (0.1%)
40	L3	0.73	0/3146	0.83	3/4228 (0.1%)
40	l3	0.82	2/3146 (0.1%)	0.89	7/4228 (0.2%)
41	L4	0.79	0/2800	0.94	6/3790 (0.2%)
41	l4	0.73	0/2800	0.88	3/3790 (0.1%)
42	L5	0.58	0/2425	0.70	0/3271
42	l5	0.71	0/2408	0.76	0/3248
43	L6	0.77	0/1260	0.84	1/1694 (0.1%)
43	l6	0.72	0/1269	0.82	1/1705 (0.1%)
44	L7	0.79	0/1821	0.85	1/2451 (0.0%)
44	l7	0.82	0/1828	0.86	3/2461 (0.1%)
45	L8	0.55	0/1836	0.67	1/2481 (0.0%)
45	l8	0.52	0/1796	0.69	1/2431 (0.0%)
46	L9	0.64	0/1539	0.76	1/2073 (0.0%)
46	l9	0.78	0/1539	0.82	0/2073
47	M0	0.72	0/1741	0.83	3/2335 (0.1%)
47	m0	0.77	1/1758 (0.1%)	0.85	3/2358 (0.1%)
48	M1	0.52	0/1374	0.71	1/1842 (0.1%)
48	m1	0.64	0/1374	0.79	1/1842 (0.1%)
49	M3	0.73	0/1568	0.84	3/2106 (0.1%)
49	m3	0.66	0/1573	0.82	3/2113 (0.1%)
50	M4	0.70	0/1068	0.80	1/1438 (0.1%)
50	m4	0.77	0/1074	0.81	1/1446 (0.1%)
51	M5	0.76	0/1757	0.82	0/2354
51	m5	0.65	0/1757	0.78	1/2354 (0.0%)
52	M6	0.83	1/1585 (0.1%)	0.92	3/2128 (0.1%)
52	m6	0.98	1/1585 (0.1%)	0.98	8/2128 (0.4%)
53	M7	0.78	1/1443 (0.1%)	0.83	0/1944
53	m7	0.84	0/1250	0.81	0/1683
54	M8	0.76	0/1465	0.91	4/1965 (0.2%)
54	m8	0.71	0/1465	0.87	1/1965 (0.1%)
55	M9	0.54	0/1538	0.66	0/2050
55	m9	0.59	0/1538	0.66	0/2050
56	N0	0.76	0/1481	0.83	1/1990 (0.1%)
56	n0	0.86	0/1481	0.83	0/1990
57	N1	0.78	1/1300 (0.1%)	0.81	0/1743
57	n1	0.82	1/1300 (0.1%)	0.81	0/1743
58	N2	0.44	0/812	0.61	0/1099
58	n2	0.51	0/794	0.67	0/1076
59	N3	0.72	0/1018	0.80	0/1369
59	n3	0.83	0/1018	0.94	3/1369 (0.2%)
60	N4	0.60	0/712	0.66	0/958
60	n4	0.66	0/1052	0.75	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	N5	0.61	0/979	0.77	1/1321 (0.1%)
61	n5	0.62	0/974	0.75	1/1314 (0.1%)
62	N6	0.70	0/1004	0.88	3/1341 (0.2%)
62	n6	0.63	0/1004	0.80	1/1341 (0.1%)
63	N7	0.50	0/1118	0.65	0/1497
63	n7	0.45	0/1118	0.61	0/1497
64	N8	0.82	0/1204	0.92	2/1612 (0.1%)
64	n8	0.76	0/1204	0.95	3/1612 (0.2%)
65	N9	0.73	0/473	0.80	1/629 (0.2%)
65	n9	0.81	0/473	1.00	1/629 (0.2%)
66	O0	0.45	0/751	0.63	0/1008
66	o0	0.49	0/775	0.66	0/1040
67	O1	0.61	0/890	0.72	0/1196
67	o1	0.77	0/897	0.82	0/1205
68	O2	0.83	0/1041	0.92	2/1394 (0.1%)
68	o2	0.82	0/1041	0.92	3/1394 (0.2%)
69	O3	0.89	0/868	0.88	1/1168 (0.1%)
69	o3	0.89	0/868	0.84	0/1168
70	O4	0.59	0/890	0.75	1/1189 (0.1%)
70	o4	0.61	1/890 (0.1%)	0.73	0/1189
71	O5	0.67	0/978	0.78	0/1301
71	o5	0.58	0/974	0.66	0/1297
72	O6	0.63	0/778	0.82	1/1034 (0.1%)
72	o6	0.52	0/777	0.68	0/1033
73	O7	0.81	1/696 (0.1%)	0.95	2/923 (0.2%)
73	o7	0.70	0/696	0.79	0/923
74	O8	0.51	0/618	0.63	0/826
74	o8	0.44	0/614	0.61	0/822
75	O9	0.77	0/443	0.89	0/588
75	o9	0.69	0/443	0.76	1/588 (0.2%)
76	Q0	0.67	0/423	0.76	0/562
76	q0	0.81	0/423	0.90	0/562
77	Q1	0.68	0/234	1.04	0/300
77	q1	0.83	0/234	0.94	1/300 (0.3%)
78	Q2	0.93	1/860 (0.1%)	0.87	2/1136 (0.2%)
78	q2	0.86	1/860 (0.1%)	0.81	0/1136
79	Q3	0.77	0/701	0.82	0/934
79	q3	0.70	0/701	0.85	2/934 (0.2%)
80	e0	0.52	0/499	0.72	0/665
81	e1	0.39	0/619	0.73	1/822 (0.1%)
83	p0	0.43	0/1092	0.60	0/1474
All	All	0.85	215/430075 (0.0%)	1.27	4114/631366 (0.7%)

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
3	s1	0	1
6	s4	0	1
7	s5	0	1
9	S7	0	1
9	s7	0	1
10	S8	0	1
13	C1	0	1
16	C4	0	2
17	c5	0	1
19	C7	0	2
19	c7	0	1
20	c8	0	1
22	d0	0	1
25	d3	0	1
27	D5	0	3
28	D6	0	3
34	SR	0	2
39	L2	0	1
39	l2	0	2
42	l5	0	1
43	L6	0	1
44	L7	0	1
44	l7	0	2
52	M6	0	1
52	m6	0	1
53	M7	0	1
53	m7	0	1
56	n0	0	1
59	n3	0	1
62	n6	0	1
64	N8	0	2
64	n8	0	1
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	1
75	o9	0	1
78	Q2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
81	e1	0	1
All	All	0	50

All (215) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	SR	160	GLU	C-N	-30.25	0.64	1.34
34	SR	161	LYS	C-N	-24.97	0.76	1.34
78	Q2	17	CYS	CB-SG	16.00	2.09	1.82
36	5	1152	G	N9-C4	-13.57	1.27	1.38
78	q2	17	CYS	CB-SG	12.94	2.04	1.82
52	m6	66	LYS	CE-NZ	8.92	1.71	1.49
36	5	1152	G	C2-N3	-8.88	1.25	1.32
36	5	1152	G	N9-C8	8.55	1.43	1.37
36	1	2726	C	N3-C4	-8.17	1.28	1.33
36	1	3181	C	N3-C4	-7.93	1.28	1.33
36	5	2726	C	N3-C4	-7.92	1.28	1.33
36	5	2873	U	C2-N3	7.89	1.43	1.37
36	5	1152	G	N1-C2	7.49	1.43	1.37
36	5	2943	G	N7-C5	-7.42	1.34	1.39
39	l2	213	GLY	C-O	7.37	1.35	1.23
36	1	1153	A	N7-C5	-7.33	1.34	1.39
1	6	163	G	N9-C4	-7.25	1.32	1.38
36	5	2954	U	C4-O4	7.20	1.29	1.23
36	1	644	G	N7-C5	-7.16	1.34	1.39
36	1	2910	A	N9-C4	-7.04	1.33	1.37
36	5	2971	A	N9-C4	7.04	1.42	1.37
36	1	2799	A	N7-C5	-6.97	1.35	1.39
36	5	1152	G	N3-C4	-6.97	1.30	1.35
36	1	2412	G	N7-C5	-6.93	1.35	1.39
36	1	1103	A	N9-C4	6.91	1.42	1.37
36	5	631	U	C2-N3	-6.84	1.32	1.37
36	5	2335	G	N3-C4	-6.84	1.30	1.35
36	1	659	G	N7-C5	-6.81	1.35	1.39
57	n1	104	GLU	CB-CG	6.81	1.65	1.52
36	5	2375	G	C6-N1	-6.76	1.34	1.39
36	5	953	G	C5-C4	-6.75	1.33	1.38
36	5	2314	U	N3-C4	6.69	1.44	1.38
36	1	895	A	N9-C8	6.68	1.43	1.37
36	1	2714	G	N9-C4	-6.47	1.32	1.38
36	5	877	C	C4-N4	-6.47	1.28	1.33
36	1	61	A	C5-C6	-6.47	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	970	A	N9-C4	-6.44	1.33	1.37
36	1	1133	A	N9-C4	-6.42	1.33	1.37
36	5	2341	A	N9-C8	-6.31	1.32	1.37
36	1	1416	C	N3-C4	-6.30	1.29	1.33
36	5	2899	C	N3-C4	-6.27	1.29	1.33
36	1	2836	C	N3-C4	-6.23	1.29	1.33
36	1	2404	A	N9-C4	6.22	1.41	1.37
36	5	3218	A	C5-C6	-6.21	1.35	1.41
36	1	317	A	N7-C5	-6.20	1.35	1.39
36	5	2401	A	N3-C4	6.15	1.38	1.34
36	1	2983	C	N3-C4	-6.14	1.29	1.33
36	5	2872	A	C6-N1	6.14	1.39	1.35
37	7	95	A	N9-C4	-6.13	1.34	1.37
36	1	426	G	N1-C2	-6.10	1.32	1.37
36	1	2815	G	N3-C4	-6.09	1.31	1.35
36	1	2640	A	C6-N1	-6.04	1.31	1.35
36	5	1113	G	C6-N1	-6.03	1.35	1.39
36	1	1429	G	N9-C8	-6.01	1.33	1.37
36	5	1115	G	N7-C5	-6.00	1.35	1.39
36	1	2714	G	N9-C8	5.98	1.42	1.37
36	5	1849	C	N1-C6	-5.95	1.33	1.37
36	5	2954	U	C2-N3	5.91	1.41	1.37
36	5	3107	U	C2-N3	-5.91	1.33	1.37
73	O7	37	CYS	CB-SG	-5.90	1.72	1.81
36	5	2147	A	C5-C6	-5.90	1.35	1.41
36	5	426	G	C5-C4	-5.89	1.34	1.38
1	2	992	A	N9-C4	-5.87	1.34	1.37
36	5	2138	A	N7-C5	-5.86	1.35	1.39
36	5	1148	G	C5-C4	-5.86	1.34	1.38
36	5	2814	G	N7-C5	-5.85	1.35	1.39
36	1	1127	G	C5-C6	-5.83	1.36	1.42
36	5	420	G	N9-C8	-5.80	1.33	1.37
36	5	1152	G	C5-C6	-5.80	1.36	1.42
37	7	85	G	N1-C2	-5.79	1.33	1.37
36	1	200	C	N1-C6	-5.77	1.33	1.37
36	1	980	A	N9-C4	5.77	1.41	1.37
36	5	2303	A	N7-C5	-5.76	1.35	1.39
36	5	3209	A	C5-C4	5.76	1.42	1.38
36	5	1133	A	N7-C5	-5.75	1.35	1.39
36	1	1399	A	N9-C4	-5.74	1.34	1.37
36	5	2698	G	N9-C8	-5.73	1.33	1.37
36	5	2147	A	N7-C5	-5.73	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2617	U	N3-C4	-5.72	1.33	1.38
36	5	2635	A	N3-C4	-5.72	1.31	1.34
36	5	2640	A	N3-C4	-5.71	1.31	1.34
36	1	2404	A	N3-C4	5.70	1.38	1.34
36	1	402	A	N3-C4	-5.70	1.31	1.34
36	1	659	G	N1-C2	-5.70	1.33	1.37
36	1	317	A	C5-C6	-5.69	1.35	1.41
36	5	2858	U	C2-N3	-5.69	1.33	1.37
36	5	2954	U	N3-C4	5.69	1.43	1.38
36	5	719	U	N1-C2	5.69	1.43	1.38
36	5	1891	A	N9-C4	-5.69	1.34	1.37
36	1	48	A	N9-C8	-5.67	1.33	1.37
36	5	895	A	N9-C4	-5.66	1.34	1.37
36	1	2138	A	N7-C5	-5.66	1.35	1.39
36	1	2406	C	N1-C6	-5.65	1.33	1.37
36	1	296	A	N9-C4	5.65	1.41	1.37
36	5	1113	G	N3-C4	-5.65	1.31	1.35
36	5	2894	C	C4-C5	-5.64	1.38	1.43
36	5	2941	A	N9-C4	-5.64	1.34	1.37
1	6	623	A	N9-C4	-5.63	1.34	1.37
36	5	1328	C	N1-C6	-5.63	1.33	1.37
36	1	361	A	N9-C4	-5.62	1.34	1.37
36	1	2657	A	N7-C5	-5.62	1.35	1.39
36	1	3209	A	C6-N1	5.59	1.39	1.35
36	5	1115	G	N1-C2	-5.58	1.33	1.37
36	1	2147	A	N7-C5	-5.57	1.35	1.39
36	5	2417	U	C4-O4	5.57	1.28	1.23
1	6	538	A	N9-C4	5.57	1.41	1.37
36	1	667	C	N3-C4	-5.57	1.30	1.33
1	2	1291	G	N3-C4	-5.53	1.31	1.35
36	5	924	G	C2-N3	-5.53	1.28	1.32
36	5	1307	G	P-O5'	-5.53	1.54	1.59
36	5	3308	C	N3-C4	-5.53	1.30	1.33
36	5	2376	G	N9-C8	-5.51	1.33	1.37
36	5	1173	U	C2-N3	-5.51	1.33	1.37
36	5	2957	G	C5-C4	-5.51	1.34	1.38
36	1	2679	A	N9-C4	-5.50	1.34	1.37
36	1	962	A	N7-C5	-5.50	1.35	1.39
36	5	367	A	N9-C4	-5.50	1.34	1.37
1	6	1744	A	N9-C4	-5.49	1.34	1.37
36	1	1132	C	N3-C4	-5.48	1.30	1.33
36	5	1177	G	N3-C4	-5.46	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1149	G	N9-C8	-5.46	1.34	1.37
1	6	1781	A	N9-C4	5.46	1.41	1.37
36	1	584	G	N7-C5	-5.45	1.35	1.39
37	3	88	G	C6-N1	-5.45	1.35	1.39
70	o4	84	CYS	CB-SG	5.45	1.91	1.82
36	1	1103	A	C6-N1	5.43	1.39	1.35
36	5	971	G	C5-C4	-5.43	1.34	1.38
36	5	661	G	N7-C5	-5.42	1.35	1.39
37	7	91	G	N7-C5	-5.42	1.35	1.39
36	5	2762	A	N9-C4	-5.42	1.34	1.37
36	5	719	U	C2-O2	5.40	1.27	1.22
36	1	2409	G	N3-C4	-5.39	1.31	1.35
36	5	40	A	N7-C5	-5.38	1.36	1.39
36	5	960	U	N1-C2	5.37	1.43	1.38
36	1	2143	A	N3-C4	-5.37	1.31	1.34
36	5	2401	A	N9-C4	5.36	1.41	1.37
36	5	917	A	N3-C4	-5.36	1.31	1.34
36	5	2646	C	N1-C6	-5.35	1.33	1.37
36	5	1134	G	N1-C2	-5.35	1.33	1.37
36	5	2419	A	P-O5'	5.35	1.65	1.59
36	1	1112	A	N9-C4	-5.34	1.34	1.37
36	5	2937	G	N7-C5	-5.33	1.36	1.39
36	1	2800	G	C5-C4	-5.32	1.34	1.38
36	5	2627	C	N3-C4	-5.31	1.30	1.33
36	1	2409	G	N7-C5	-5.30	1.36	1.39
36	5	2755	C	N1-C6	-5.30	1.33	1.37
36	1	2874	G	C5-C4	5.28	1.42	1.38
36	5	1207	G	N1-C2	-5.28	1.33	1.37
52	M6	4	GLU	CD-OE1	5.28	1.31	1.25
36	1	1002	A	N9-C4	-5.27	1.34	1.37
36	5	2911	A	N7-C5	-5.27	1.36	1.39
36	5	2632	G	C6-N1	-5.27	1.35	1.39
1	2	1599	C	N1-C6	-5.26	1.33	1.37
36	1	1507	G	N9-C8	-5.26	1.34	1.37
36	5	3245	A	N9-C4	-5.26	1.34	1.37
36	1	947	G	C6-N1	-5.26	1.35	1.39
36	5	1152	G	C8-N7	5.24	1.34	1.30
36	5	2300	G	N1-C2	-5.23	1.33	1.37
36	1	2867	C	N3-C4	-5.23	1.30	1.33
36	1	2822	U	N1-C2	-5.22	1.33	1.38
57	N1	107	GLU	CG-CD	5.22	1.59	1.51
36	5	2940	A	N7-C5	-5.22	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	1773	C	C4-N4	5.21	1.38	1.33
36	5	1902	G	C5-C4	-5.20	1.34	1.38
36	5	2246	G	N1-C2	-5.19	1.33	1.37
36	5	2280	A	N9-C4	-5.19	1.34	1.37
36	5	1299	U	C4-O4	-5.19	1.19	1.23
36	5	859	G	N1-C2	-5.18	1.33	1.37
36	5	1192	C	N3-C4	5.18	1.37	1.33
36	5	3216	G	N7-C5	-5.18	1.36	1.39
36	5	872	U	C4-O4	-5.18	1.19	1.23
36	5	1902	G	N7-C5	-5.18	1.36	1.39
36	5	2814	G	C5-C6	-5.16	1.37	1.42
36	5	3008	A	N9-C4	-5.16	1.34	1.37
53	M7	129	THR	CB-CG2	-5.16	1.35	1.52
36	5	2942	C	N1-C6	-5.16	1.34	1.37
36	1	931	C	C2-N3	-5.15	1.31	1.35
36	5	1370	G	C6-N1	-5.15	1.35	1.39
36	5	2365	C	N3-C4	-5.15	1.30	1.33
1	6	337	G	C2-N2	5.15	1.39	1.34
1	6	163	G	N3-C4	-5.14	1.31	1.35
36	5	3374	U	C4-O4	-5.13	1.19	1.23
36	1	2975	U	C4-O4	-5.12	1.19	1.23
36	1	1430	U	N1-C2	-5.12	1.33	1.38
36	5	2955	U	C2-N3	-5.11	1.34	1.37
36	5	1908	A	C5-C4	-5.11	1.35	1.38
36	5	342	A	N3-C4	-5.10	1.31	1.34
36	5	2971	A	C5-C4	5.10	1.42	1.38
37	7	93	C	N3-C4	-5.09	1.30	1.33
36	1	3130	A	C6-N1	-5.09	1.31	1.35
36	1	2958	A	C6-N6	-5.08	1.29	1.33
36	5	1138	U	C4-O4	-5.08	1.19	1.23
40	l3	73	VAL	CB-CG1	-5.08	1.42	1.52
36	1	1660	C	N1-C6	-5.08	1.34	1.37
36	1	279	U	C4-O4	-5.07	1.19	1.23
36	1	421	G	N1-C2	-5.07	1.33	1.37
36	1	1103	A	N3-C4	5.06	1.37	1.34
36	5	3062	G	N7-C5	-5.06	1.36	1.39
36	5	3124	G	N3-C4	-5.06	1.31	1.35
36	1	343	U	N3-C4	-5.05	1.33	1.38
36	5	2762	A	N3-C4	-5.05	1.31	1.34
36	5	1103	A	N9-C4	5.05	1.40	1.37
36	5	1338	C	N3-C4	-5.05	1.30	1.33
1	6	1537	C	C2-N3	5.05	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	m0	56	GLU	CG-CD	5.04	1.59	1.51
36	5	802	C	N1-C6	-5.04	1.34	1.37
36	5	1330	A	C5-C6	-5.04	1.36	1.41
36	5	2385	G	N9-C4	-5.04	1.33	1.38
36	1	576	C	N1-C6	-5.03	1.34	1.37
36	5	2287	C	N1-C6	5.03	1.40	1.37
37	7	94	C	C2-N3	-5.02	1.31	1.35
36	5	2873	U	C2-O2	5.01	1.26	1.22
36	5	2314	U	C2-N3	5.01	1.41	1.37
36	1	420	G	N9-C8	-5.01	1.34	1.37
40	l3	251	CYS	CB-SG	-5.00	1.73	1.81

All (4114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	SR	161	LYS	O-C-N	-44.54	51.44	122.70
34	SR	160	GLU	C-N-CA	-39.83	22.12	121.70
34	SR	160	GLU	CA-C-N	-34.85	40.53	117.20
36	5	1152	G	N3-C4-C5	27.52	142.36	128.60
36	5	1152	G	N3-C4-N9	-27.23	109.66	126.00
34	SR	160	GLU	O-C-N	-26.99	79.52	122.70
36	5	1152	G	N3-C2-N2	-21.11	105.12	119.90
36	5	1152	G	C2-N3-C4	-19.93	101.93	111.90
36	5	2334	U	O5'-P-OP2	-16.83	90.50	110.70
36	1	1308	A	O5'-P-OP2	-16.07	91.23	105.70
36	5	1152	G	C8-N9-C1'	16.00	147.81	127.00
1	2	553	G	N1-C6-O6	15.36	129.12	119.90
36	5	1152	G	C4-N9-C1'	-14.55	107.58	126.50
36	5	1152	G	C5-N7-C8	-14.40	97.10	104.30
36	1	2373	A	O5'-P-OP1	-14.34	92.79	105.70
36	1	2714	G	N3-C4-C5	14.10	135.65	128.60
36	5	1152	G	N1-C6-O6	13.77	128.16	119.90
36	5	2899	C	N3-C2-O2	-13.71	112.30	121.90
36	1	2923	U	O5'-P-OP1	-13.68	93.39	105.70
36	1	2617	U	C5-C4-O4	13.50	134.00	125.90
1	6	163	G	N3-C4-N9	-13.11	118.14	126.00
36	1	2714	G	N3-C4-N9	-12.98	118.21	126.00
36	5	1152	G	N1-C2-N2	12.92	127.83	116.20
36	5	2945	G	O5'-P-OP2	-12.90	94.09	105.70
1	6	1773	C	N3-C4-C5	-12.76	116.80	121.90
36	1	1495	U	C5-C6-N1	-12.71	116.34	122.70
36	5	1116	G	O5'-P-OP1	-12.65	94.31	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2726	C	C5-C4-N4	12.60	129.02	120.20
36	5	2373	A	O5'-P-OP1	-12.53	94.42	105.70
36	1	1495	U	N1-C2-N3	12.47	122.38	114.90
36	5	922	U	N1-C2-N3	12.42	122.35	114.90
36	1	406	G	O4'-C1'-N9	12.35	118.08	108.20
36	5	877	C	N3-C4-C5	12.33	126.83	121.90
36	5	922	U	N3-C2-O2	-12.22	113.64	122.20
36	5	2639	G	C5-C6-O6	-12.21	121.28	128.60
36	1	1495	U	C4-C5-C6	12.16	127.00	119.70
1	2	1200	G	N1-C6-O6	12.02	127.11	119.90
1	6	352	A	O5'-P-OP1	-11.98	94.92	105.70
36	5	1307	G	P-O3'-C3'	11.93	134.01	119.70
36	1	1117	G	O5'-P-OP1	-11.88	95.01	105.70
36	5	2341	A	C8-N9-C4	11.73	110.49	105.80
36	1	979	U	C6-N1-C2	-11.67	114.00	121.00
36	1	817	A	O5'-P-OP1	-11.56	95.29	105.70
36	5	1371	G	N1-C6-O6	-11.55	112.97	119.90
36	5	1313	G	O5'-P-OP2	-11.46	95.39	105.70
36	1	1396	C	C6-N1-C2	11.44	124.88	120.30
36	1	3181	C	N3-C2-O2	-11.36	113.95	121.90
36	1	776	U	C4-C5-C6	11.35	126.51	119.70
36	5	2121	G	O5'-P-OP2	-11.33	95.50	105.70
36	1	2945	G	O5'-P-OP2	-11.28	95.55	105.70
1	6	1537	C	C6-N1-C2	-11.24	115.81	120.30
36	5	1513	G	C8-N9-C4	-11.23	101.91	106.40
36	5	3245	A	C5-N7-C8	-11.19	98.30	103.90
36	1	3305	A	O5'-P-OP2	-11.13	95.68	105.70
36	5	2315	G	O5'-P-OP1	-11.12	95.69	105.70
36	5	3140	G	C5-C6-O6	-11.01	122.00	128.60
36	1	2726	C	N3-C4-N4	-11.00	110.30	118.00
36	5	2726	C	C6-N1-C2	-10.92	115.93	120.30
36	1	968	G	C8-N9-C4	-10.89	102.05	106.40
36	1	3375	A	O5'-P-OP2	-10.71	96.06	105.70
36	1	2983	C	C5-C6-N1	-10.70	115.65	121.00
36	5	3245	A	C2-N3-C4	-10.70	105.25	110.60
36	1	2617	U	N1-C2-N3	10.64	121.29	114.90
36	5	2726	C	N3-C2-O2	-10.64	114.45	121.90
36	1	1216	C	C6-N1-C2	-10.46	116.12	120.30
1	2	1773	C	C6-N1-C2	-10.44	116.12	120.30
36	1	2983	C	C4-C5-C6	10.43	122.61	117.40
1	6	163	G	N3-C4-C5	10.43	133.81	128.60
36	5	2818	U	O5'-P-OP1	-10.28	96.45	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2860	U	C5-C6-N1	10.28	127.84	122.70
36	1	2726	C	N3-C2-O2	-10.26	114.72	121.90
1	6	337	G	C6-C5-N7	-10.24	124.26	130.40
1	6	542	A	N7-C8-N9	10.16	118.88	113.80
36	1	3362	A	C2-N3-C4	-10.13	105.53	110.60
1	6	1473	U	N3-C2-O2	-10.13	115.11	122.20
36	5	50	U	O5'-P-OP1	-10.12	96.59	105.70
36	1	709	A	C8-N9-C4	10.11	109.85	105.80
36	1	2983	C	C5-C4-N4	10.09	127.27	120.20
36	1	979	U	N3-C2-O2	-10.09	115.14	122.20
36	5	2899	C	C6-N1-C2	-10.08	116.27	120.30
36	5	3245	A	N7-C8-N9	10.05	118.83	113.80
36	5	1152	G	C5-C6-O6	-10.04	122.57	128.60
1	2	639	U	N3-C2-O2	-10.03	115.18	122.20
36	1	2393	G	C5-C6-O6	-10.02	122.59	128.60
1	6	609	U	C5-C4-O4	10.02	131.91	125.90
1	6	1537	C	N3-C4-C5	-10.02	117.89	121.90
36	1	2617	U	C4-C5-C6	10.01	125.71	119.70
1	2	553	G	C6-C5-N7	-10.01	124.39	130.40
36	5	437	G	C8-N9-C4	-9.99	102.41	106.40
36	5	776	U	N3-C2-O2	-9.97	115.22	122.20
36	1	818	C	C6-N1-C2	-9.96	116.31	120.30
36	1	2726	C	C5-C4-N4	9.96	127.17	120.20
1	2	1560	U	N3-C2-O2	-9.96	115.23	122.20
36	5	2634	U	C2-N3-C4	-9.95	121.03	127.00
36	5	2954	U	N3-C4-O4	9.94	126.36	119.40
36	5	835	G	O4'-C1'-N9	9.92	116.14	108.20
36	5	922	U	C5-C4-O4	9.92	131.85	125.90
36	1	3344	A	N7-C8-N9	9.90	118.75	113.80
36	1	2936	A	O5'-P-OP1	-9.89	96.80	105.70
36	1	895	A	C5-N7-C8	-9.88	98.96	103.90
36	1	2983	C	N3-C4-N4	-9.86	111.10	118.00
1	2	1200	G	C5-C6-O6	-9.82	122.71	128.60
36	1	2846	U	N3-C2-O2	-9.81	115.33	122.20
36	1	960	U	N3-C4-O4	-9.80	112.54	119.40
36	5	3012	A	C8-N9-C4	9.74	109.70	105.80
1	2	1783	C	O5'-P-OP2	-9.73	96.94	105.70
36	5	2899	C	N1-C2-N3	9.72	126.01	119.20
37	7	120	C	C6-N1-C2	9.72	124.19	120.30
36	1	2617	U	C5-C6-N1	-9.71	117.84	122.70
36	5	1165	A	O5'-P-OP2	-9.70	96.97	105.70
36	5	1419	A	O5'-P-OP2	-9.70	96.97	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	553	G	C5-C6-O6	-9.69	122.79	128.60
36	1	942	U	OP1-P-OP2	-9.69	105.07	119.60
1	6	144	U	N3-C2-O2	-9.68	115.42	122.20
36	5	776	U	N1-C2-N3	9.67	120.70	114.90
36	1	67	A	O5'-P-OP1	-9.65	97.01	105.70
36	1	792	G	O5'-P-OP1	-9.65	97.01	105.70
37	3	86	U	C5-C4-O4	-9.64	120.11	125.90
36	5	2941	A	O4'-C1'-N9	-9.63	100.50	108.20
1	6	337	G	C4-C5-N7	9.60	114.64	110.80
36	1	439	C	C2-N1-C1'	9.53	129.28	118.80
36	1	639	G	N1-C6-O6	9.51	125.61	119.90
36	1	2621	G	N3-C2-N2	-9.50	113.25	119.90
36	5	2833	A	N1-C6-N6	-9.50	112.90	118.60
36	5	1117	G	O5'-P-OP1	-9.49	97.16	105.70
36	1	1495	U	N3-C2-O2	-9.47	115.57	122.20
36	1	801	A	O5'-P-OP2	-9.47	97.18	105.70
1	2	453	U	N3-C2-O2	-9.45	115.59	122.20
36	5	719	U	N1-C2-O2	9.45	129.41	122.80
36	5	2954	U	C2-N1-C1'	9.44	129.02	117.70
36	5	1879	A	O5'-P-OP1	9.42	122.00	110.70
1	6	1773	C	N3-C4-N4	9.41	124.59	118.00
36	1	521	A	N1-C6-N6	9.41	124.24	118.60
36	1	960	U	N3-C4-C5	9.40	120.24	114.60
36	5	1847	A	O5'-P-OP2	-9.39	97.25	105.70
1	6	453	U	N3-C2-O2	-9.38	115.64	122.20
36	1	2827	U	C5-C4-O4	9.37	131.52	125.90
1	2	1773	C	N3-C4-C5	-9.36	118.16	121.90
36	5	2619	G	C5-C6-O6	-9.32	123.01	128.60
36	5	1461	A	C8-N9-C4	9.31	109.52	105.80
36	1	980	A	C8-N9-C4	-9.31	102.08	105.80
36	5	960	U	C5-C6-N1	-9.30	118.05	122.70
36	1	3209	A	N1-C6-N6	9.30	124.18	118.60
36	5	2988	C	C2-N3-C4	-9.30	115.25	119.90
1	6	973	A	O5'-P-OP2	-9.30	97.33	105.70
36	1	2412	G	C8-N9-C4	-9.29	102.68	106.40
37	3	88	G	N1-C6-O6	-9.29	114.32	119.90
36	1	406	G	O5'-P-OP2	-9.28	97.35	105.70
36	5	955	U	C5-C4-O4	-9.27	120.33	125.90
36	5	2290	C	C5-C6-N1	-9.26	116.37	121.00
36	1	2375	G	C8-N9-C4	9.25	110.10	106.40
36	1	979	U	N1-C2-N3	9.24	120.44	114.90
36	5	1115	G	C8-N9-C4	-9.23	102.71	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2341	A	N7-C8-N9	-9.23	109.18	113.80
36	5	519	A	N1-C6-N6	9.23	124.14	118.60
1	2	453	U	N1-C2-O2	9.22	129.25	122.80
36	5	864	G	O5'-P-OP2	-9.22	97.40	105.70
36	5	2136	C	C2-N3-C4	-9.22	115.29	119.90
36	1	2306	C	N1-C2-O2	9.21	124.43	118.90
1	6	434	G	O5'-P-OP2	-9.17	97.44	105.70
36	1	2600	C	N1-C2-O2	9.17	124.40	118.90
36	1	2343	C	N3-C4-C5	9.16	125.56	121.90
1	6	308	C	C2-N3-C4	-9.15	115.33	119.90
36	5	2634	U	N1-C2-N3	9.13	120.38	114.90
1	2	1596	C	N3-C2-O2	-9.11	115.52	121.90
36	1	591	G	C5-C6-O6	-9.11	123.13	128.60
36	1	3181	C	C5-C4-N4	9.11	126.58	120.20
36	5	2327	U	C5-C6-N1	-9.11	118.15	122.70
36	1	776	U	N1-C2-N3	9.10	120.36	114.90
36	5	2572	C	N1-C2-O2	9.09	124.36	118.90
36	5	1419	A	O5'-P-OP1	9.08	121.60	110.70
36	5	2375	G	N1-C6-O6	-9.07	114.46	119.90
36	1	2983	C	N3-C2-O2	-9.04	115.57	121.90
36	1	919	U	O5'-P-OP1	9.04	121.55	110.70
36	5	2392	C	C2-N3-C4	-9.04	115.38	119.90
36	5	922	U	N3-C4-O4	-9.03	113.08	119.40
36	1	2891	U	C5-C4-O4	-9.03	120.48	125.90
36	1	1296	C	C6-N1-C2	-9.02	116.69	120.30
36	1	53	G	C8-N9-C4	9.01	110.00	106.40
36	1	1168	U	N1-C2-O2	9.01	129.11	122.80
36	1	960	U	C2-N1-C1'	-9.00	106.90	117.70
36	5	965	A	O5'-P-OP2	-9.00	97.60	105.70
36	5	945	C	C6-N1-C2	8.99	123.90	120.30
36	5	1301	A	N1-C6-N6	8.98	123.99	118.60
36	1	2572	C	N1-C2-O2	8.97	124.28	118.90
36	1	1316	C	N1-C2-O2	-8.97	113.52	118.90
36	5	406	G	O4'-C1'-N9	8.96	115.37	108.20
36	1	3306	U	N3-C2-O2	-8.95	115.94	122.20
36	5	960	U	C2-N3-C4	-8.94	121.63	127.00
36	1	776	U	C5-C6-N1	-8.94	118.23	122.70
52	M6	110	PRO	C-N-CD	-8.93	100.95	120.60
36	5	776	U	C4-C5-C6	8.92	125.05	119.70
36	5	2965	U	N1-C2-O2	-8.92	116.56	122.80
36	1	3214	U	C5-C4-O4	8.90	131.24	125.90
1	6	44	U	N1-C2-O2	-8.90	116.57	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1189	C	N1-C2-O2	-8.89	113.56	118.90
36	1	1400	G	O5'-P-OP2	-8.88	97.70	105.70
36	5	3093	C	C6-N1-C2	8.88	123.85	120.30
36	1	3181	C	C6-N1-C2	-8.87	116.75	120.30
36	1	2846	U	C5-C4-O4	8.87	131.22	125.90
36	5	3140	G	N1-C6-O6	8.87	125.22	119.90
37	7	98	C	O5'-P-OP2	-8.86	97.72	105.70
36	5	1307	G	O5'-P-OP1	-8.86	97.73	105.70
36	1	1405	U	C5-C6-N1	-8.85	118.28	122.70
1	6	647	G	N3-C4-N9	-8.85	120.69	126.00
40	l3	19	ARG	NE-CZ-NH2	-8.85	115.88	120.30
36	5	2953	U	C5-C4-O4	-8.82	120.61	125.90
36	1	1904	C	C6-N1-C2	-8.79	116.78	120.30
36	1	2400	G	C6-C5-N7	-8.78	125.14	130.40
36	1	2897	A	C8-N9-C4	8.77	109.31	105.80
36	1	3344	A	C8-N9-C4	-8.77	102.29	105.80
36	5	2870	C	N3-C4-C5	8.76	125.40	121.90
36	1	2617	U	N3-C2-O2	-8.73	116.09	122.20
36	1	639	G	C5-C6-O6	-8.72	123.37	128.60
36	5	1152	G	C4-C5-N7	8.72	114.29	110.80
36	1	835	G	O4'-C1'-N9	8.71	115.17	108.20
36	1	960	U	C6-N1-C2	8.71	126.22	121.00
1	6	1100	G	N3-C4-N9	8.70	131.22	126.00
36	1	1405	U	C2-N3-C4	-8.70	121.78	127.00
36	5	1305	U	C5-C4-O4	-8.70	120.68	125.90
1	6	542	A	C8-N9-C4	-8.68	102.33	105.80
36	1	1396	C	N3-C4-C5	8.68	125.37	121.90
36	5	2827	U	O4'-C1'-N1	8.67	115.14	108.20
36	1	3362	A	C5-N7-C8	-8.67	99.56	103.90
36	5	2923	U	O5'-P-OP1	-8.67	97.90	105.70
36	1	1494	U	C5-C6-N1	-8.66	118.37	122.70
36	1	885	U	C5-C6-N1	-8.65	118.37	122.70
36	5	2393	G	N1-C6-O6	8.65	125.09	119.90
65	n9	23	LYS	C-N-CD	8.65	146.56	128.40
36	1	1127	G	N1-C6-O6	8.64	125.09	119.90
1	2	1291	G	N7-C8-N9	8.64	117.42	113.10
36	5	2639	G	N1-C6-O6	8.63	125.08	119.90
36	1	2714	G	C2-N3-C4	-8.63	107.59	111.90
36	1	2884	C	N3-C4-C5	8.63	125.35	121.90
12	C0	88	PRO	N-CA-CB	8.61	113.63	103.30
36	5	947	G	N3-C4-C5	-8.60	124.30	128.60
36	5	2634	U	C5-C4-O4	-8.60	120.74	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3217	C	C2-N1-C1'	8.60	128.26	118.80
36	1	2797	C	O5'-P-OP1	-8.59	97.97	105.70
36	1	2391	G	N1-C6-O6	-8.59	114.75	119.90
36	1	2617	U	N3-C4-O4	-8.59	113.39	119.40
1	6	402	C	O5'-P-OP2	-8.58	97.98	105.70
36	1	1838	G	C5-C6-O6	-8.57	123.46	128.60
36	1	280	U	C5-C4-O4	-8.57	120.76	125.90
36	5	1879	A	N1-C6-N6	8.56	123.74	118.60
1	6	163	G	C2-N3-C4	-8.56	107.62	111.90
36	5	1482	A	O5'-P-OP2	-8.55	98.00	105.70
36	5	1879	A	C5-N7-C8	-8.55	99.63	103.90
36	5	2726	C	N3-C4-C5	-8.55	118.48	121.90
36	5	1159	A	O5'-P-OP1	-8.54	98.01	105.70
36	5	2797	C	N1-C2-O2	-8.54	113.77	118.90
36	5	2244	A	O5'-P-OP1	8.54	120.94	110.70
36	1	2222	A	C8-N9-C4	-8.53	102.39	105.80
36	5	636	C	C2-N3-C4	-8.53	115.64	119.90
36	1	776	U	C5-C4-O4	8.51	131.01	125.90
36	5	420	G	N3-C4-C5	-8.51	124.35	128.60
36	5	1192	C	N3-C4-N4	8.51	123.95	118.00
36	5	922	U	C5-C6-N1	-8.50	118.45	122.70
36	5	3154	C	N1-C2-O2	8.50	124.00	118.90
36	1	3092	C	C6-N1-C2	8.49	123.69	120.30
36	1	196	G	C5-C6-O6	-8.48	123.51	128.60
36	1	2400	G	N9-C4-C5	-8.48	102.01	105.40
36	1	1049	C	O5'-P-OP2	-8.48	98.07	105.70
36	1	635	G	C5-C6-O6	-8.48	123.51	128.60
36	1	65	A	P-O3'-C3'	8.48	129.87	119.70
36	1	2836	C	C5-C4-N4	8.47	126.13	120.20
36	1	2983	C	C2-N3-C4	-8.47	115.66	119.90
36	5	776	U	C5-C6-N1	-8.47	118.46	122.70
36	5	216	G	N1-C6-O6	8.46	124.98	119.90
36	5	3218	A	N1-C6-N6	8.46	123.68	118.60
36	5	2392	C	N1-C2-O2	-8.46	113.82	118.90
36	1	1446	A	O5'-P-OP1	-8.45	98.10	105.70
36	1	3278	C	N3-C2-O2	-8.45	115.99	121.90
36	1	966	U	N3-C2-O2	-8.44	116.29	122.20
36	5	2272	G	O4'-C1'-N9	8.44	114.95	108.20
36	1	3181	C	N3-C4-N4	-8.44	112.09	118.00
1	6	543	C	C5-C6-N1	8.43	125.22	121.00
36	5	437	G	N9-C4-C5	8.43	108.77	105.40
36	5	1879	A	C4-C5-N7	8.42	114.91	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2340	U	N3-C4-C5	8.42	119.65	114.60
36	5	2136	C	C5-C6-N1	-8.42	116.79	121.00
38	8	32	C	N1-C2-O2	-8.42	113.85	118.90
36	1	970	A	C8-N9-C4	-8.40	102.44	105.80
36	5	907	G	O5'-P-OP1	-8.40	98.14	105.70
37	7	49	G	N1-C6-O6	8.40	124.94	119.90
36	1	2679	A	C2-N3-C4	-8.39	106.40	110.60
36	1	706	A	O5'-P-OP1	-8.39	98.15	105.70
36	5	644	G	C2-N3-C4	8.39	116.09	111.90
36	5	2933	A	O5'-P-OP2	-8.37	98.17	105.70
36	1	2572	C	C2-N1-C1'	8.37	128.00	118.80
1	2	402	C	O5'-P-OP1	-8.36	98.18	105.70
36	1	2614	G	N7-C8-N9	-8.36	108.92	113.10
36	5	1192	C	C5-C4-N4	-8.35	114.36	120.20
36	5	3140	G	O5'-P-OP2	-8.35	98.19	105.70
36	1	895	A	N7-C8-N9	8.35	117.97	113.80
36	1	1405	U	N3-C4-C5	8.33	119.60	114.60
36	1	2790	A	O5'-P-OP2	-8.31	98.22	105.70
36	1	2887	A	O5'-P-OP2	-8.30	98.23	105.70
36	1	2393	G	O5'-P-OP2	-8.30	98.23	105.70
36	5	2383	C	N1-C2-O2	-8.30	113.92	118.90
36	1	1127	G	C5-C6-O6	-8.30	123.62	128.60
1	6	543	C	C6-N1-C2	-8.28	116.99	120.30
36	5	2314	U	C5-C4-O4	-8.27	120.94	125.90
36	1	2836	C	C4-C5-C6	8.27	121.53	117.40
36	1	1405	U	C6-N1-C2	8.27	125.96	121.00
36	1	1904	C	C5-C6-N1	8.26	125.13	121.00
36	1	3214	U	N3-C2-O2	-8.26	116.42	122.20
36	1	3344	A	C5-N7-C8	-8.25	99.77	103.90
36	5	1308	A	O5'-P-OP2	8.25	120.60	110.70
36	1	3275	U	C5-C6-N1	8.24	126.82	122.70
36	5	41	G	N1-C6-O6	8.24	124.84	119.90
36	5	2393	G	N9-C4-C5	-8.23	102.11	105.40
36	1	398	A	N1-C6-N6	8.23	123.54	118.60
36	1	1838	G	N1-C6-O6	8.23	124.84	119.90
36	1	3362	A	O4'-C1'-N9	8.22	114.77	108.20
41	L4	327	LEU	CA-CB-CG	8.21	134.19	115.30
36	5	420	G	N3-C4-N9	8.21	130.93	126.00
36	5	3013	U	O5'-P-OP2	-8.22	98.31	105.70
36	5	2704	A	O5'-P-OP1	-8.21	98.31	105.70
36	5	2323	G	C8-N9-C4	-8.21	103.12	106.40
36	5	282	G	P-O3'-C3'	8.20	129.53	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2279	A	N9-C4-C5	-8.19	102.52	105.80
36	1	3362	A	N7-C8-N9	8.19	117.89	113.80
36	1	2614	G	C8-N9-C4	8.18	109.67	106.40
36	5	922	U	C2-N3-C4	-8.17	122.10	127.00
36	1	1196	C	C6-N1-C2	8.16	123.57	120.30
36	1	709	A	N9-C4-C5	-8.16	102.53	105.80
36	1	2816	G	C5-C6-N1	8.16	115.58	111.50
36	5	2278	C	C6-N1-C2	-8.16	117.03	120.30
36	5	2142	A	O5'-P-OP2	8.16	120.50	110.70
36	1	1433	A	C5-C6-N1	8.16	121.78	117.70
36	1	2818	U	O5'-P-OP2	-8.16	98.36	105.70
36	1	1891	A	C8-N9-C4	8.15	109.06	105.80
36	1	2864	A	O5'-P-OP1	-8.14	98.37	105.70
36	5	2988	C	C5-C6-N1	-8.14	116.93	121.00
36	1	1902	G	C5-C6-O6	-8.13	123.72	128.60
38	4	113	U	N1-C2-N3	8.14	119.78	114.90
1	6	542	A	O5'-P-OP1	-8.12	98.40	105.70
36	1	334	A	C8-N9-C4	-8.11	102.56	105.80
36	1	2726	C	N1-C2-N3	8.11	124.88	119.20
36	5	966	U	N3-C2-O2	-8.11	116.52	122.20
36	5	883	A	C8-N9-C4	8.11	109.04	105.80
36	5	3140	G	C6-C5-N7	-8.10	125.54	130.40
1	6	1634	C	N1-C2-O2	8.08	123.75	118.90
36	5	92	G	N1-C6-O6	-8.08	115.05	119.90
36	5	890	C	O5'-P-OP2	-8.08	98.43	105.70
36	5	955	U	C2-N3-C4	-8.07	122.16	127.00
36	5	1181	U	C5-C6-N1	-8.07	118.67	122.70
36	5	3245	A	C4-C5-N7	8.07	114.73	110.70
36	5	2728	G	O5'-P-OP2	-8.06	98.44	105.70
1	6	1773	C	N1-C2-O2	-8.06	114.06	118.90
36	5	2572	C	C2-N1-C1'	8.06	127.67	118.80
36	5	2701	U	C5-C4-O4	-8.06	121.06	125.90
1	6	1773	C	C4-C5-C6	8.06	121.43	117.40
36	1	3306	U	N3-C4-O4	-8.04	113.77	119.40
36	5	283	G	C5-C6-O6	-8.04	123.78	128.60
36	5	631	U	N3-C2-O2	-8.04	116.57	122.20
36	1	345	G	O5'-P-OP2	-8.02	98.49	105.70
36	1	421	G	N3-C4-N9	8.01	130.81	126.00
36	5	339	C	N1-C2-O2	-8.01	114.09	118.90
36	1	650	C	N1-C2-O2	-8.00	114.10	118.90
36	5	417	A	N1-C6-N6	-8.00	113.80	118.60
36	5	960	U	N3-C2-O2	-8.00	116.60	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	881	C	C5-C6-N1	8.00	125.00	121.00
36	5	2945	G	O5'-P-OP1	7.99	120.29	110.70
36	5	838	G	N1-C6-O6	-7.99	115.11	119.90
39	12	246	LEU	CA-CB-CG	7.98	133.66	115.30
37	7	44	C	N1-C2-O2	-7.98	114.11	118.90
36	1	2614	G	C5-N7-C8	7.97	108.29	104.30
36	5	2372	A	C8-N9-C4	-7.97	102.61	105.80
36	1	1881	A	C8-N9-C4	7.96	108.99	105.80
36	1	112	U	C2-N1-C1'	7.95	127.25	117.70
36	5	3140	G	N9-C4-C5	-7.95	102.22	105.40
36	1	645	A	C6-N1-C2	-7.95	113.83	118.60
36	1	2298	U	C5-C6-N1	-7.95	118.73	122.70
36	5	3362	A	N7-C8-N9	7.94	117.77	113.80
36	1	1434	G	O5'-P-OP1	-7.93	98.56	105.70
36	1	2411	U	N3-C4-C5	7.92	119.36	114.60
36	5	1152	G	C4-C5-C6	-7.92	114.05	118.80
36	1	2400	G	N1-C6-O6	7.92	124.65	119.90
36	1	218	G	O5'-P-OP2	-7.91	98.58	105.70
36	1	1381	A	O5'-P-OP2	7.91	120.19	110.70
36	5	585	A	O5'-P-OP2	-7.91	98.58	105.70
36	1	1313	G	C4-C5-N7	7.91	113.96	110.80
37	7	101	G	N1-C6-O6	7.90	124.64	119.90
36	5	2290	C	C6-N1-C2	7.90	123.46	120.30
36	5	3308	C	N1-C2-O2	-7.89	114.16	118.90
36	1	968	G	N7-C8-N9	7.89	117.05	113.10
36	5	1848	G	C5-C6-O6	-7.89	123.87	128.60
36	5	3144	G	C8-N9-C4	-7.89	103.24	106.40
36	5	2882	U	O5'-P-OP2	-7.89	98.60	105.70
36	1	645	A	C2-N3-C4	7.89	114.54	110.60
36	1	1307	G	N1-C6-O6	-7.89	115.17	119.90
36	1	2606	G	N3-C4-N9	7.88	130.73	126.00
36	1	2723	U	N1-C2-O2	-7.88	117.28	122.80
36	1	2809	C	N1-C2-O2	7.87	123.62	118.90
36	5	974	G	N3-C4-C5	-7.87	124.66	128.60
36	5	3362	A	O4'-C1'-N9	7.87	114.50	108.20
36	5	2726	C	N3-C4-N4	-7.86	112.50	118.00
36	1	2809	C	N3-C2-O2	-7.86	116.40	121.90
1	6	337	G	C8-N9-C1'	-7.86	116.78	127.00
36	1	1902	G	C4-C5-N7	7.86	113.94	110.80
36	1	2362	C	O5'-P-OP2	-7.86	98.63	105.70
36	1	2938	G	O5'-P-OP1	-7.86	98.63	105.70
36	1	2824	G	O5'-P-OP2	-7.85	98.64	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2392	C	C5-C4-N4	-7.85	114.71	120.20
36	5	1390	A	C8-N9-C4	-7.83	102.67	105.80
36	1	903	U	N3-C2-O2	-7.83	116.72	122.20
36	1	3057	U	C5-C4-O4	7.82	130.59	125.90
36	5	938	C	N3-C4-C5	7.82	125.03	121.90
31	D9	36	LEU	CA-CB-CG	7.81	133.27	115.30
36	5	3362	A	C5-N7-C8	-7.81	100.00	103.90
1	6	308	C	C5-C6-N1	-7.80	117.10	121.00
1	6	1039	A	O4'-C1'-N9	7.80	114.44	108.20
1	6	314	C	O5'-P-OP1	-7.80	98.68	105.70
36	1	716	A	N1-C6-N6	7.80	123.28	118.60
36	1	2192	C	O5'-P-OP2	-7.80	98.68	105.70
36	1	1495	U	C5-C4-O4	7.79	130.58	125.90
36	1	641	C	N3-C4-C5	7.79	125.02	121.90
36	1	1495	U	C2-N3-C4	-7.79	122.33	127.00
36	1	3057	U	N3-C4-O4	-7.78	113.95	119.40
36	1	806	A	O5'-P-OP1	-7.77	98.71	105.70
1	6	25	C	C6-N1-C2	-7.76	117.20	120.30
36	5	2953	U	N3-C4-O4	7.76	124.83	119.40
10	S8	29	LEU	CA-CB-CG	7.75	133.13	115.30
36	1	3217	C	C6-N1-C1'	-7.75	111.50	120.80
36	1	3218	A	C8-N9-C4	-7.75	102.70	105.80
36	5	1004	U	N1-C2-O2	7.75	128.22	122.80
36	1	988	U	C5-C6-N1	-7.75	118.83	122.70
36	5	1902	G	C5-C6-O6	-7.74	123.96	128.60
37	7	85	G	N1-C6-O6	-7.74	115.26	119.90
36	5	2634	U	N1-C2-O2	-7.73	117.39	122.80
36	1	346	C	C5-C6-N1	-7.73	117.13	121.00
36	1	3181	C	N1-C2-N3	7.73	124.61	119.20
36	5	3218	A	C4-C5-N7	7.73	114.56	110.70
36	1	1918	C	C6-N1-C2	-7.73	117.21	120.30
38	4	94	C	C6-N1-C2	7.72	123.39	120.30
37	7	85	G	O5'-P-OP2	7.72	119.97	110.70
36	1	521	A	C5-C6-N6	-7.72	117.52	123.70
1	6	17	C	C6-N1-C2	-7.72	117.21	120.30
36	5	2572	C	N3-C2-O2	-7.72	116.50	121.90
36	5	3306	U	N3-C4-C5	7.71	119.23	114.60
36	5	1115	G	C4-N9-C1'	7.71	136.52	126.50
36	5	2315	G	C8-N9-C4	7.71	109.48	106.40
1	6	1596	C	N3-C2-O2	-7.70	116.51	121.90
36	5	2211	U	N1-C2-N3	7.70	119.52	114.90
36	5	283	G	OP1-P-OP2	-7.70	108.05	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1600	A	C2-N3-C4	-7.70	106.75	110.60
1	6	609	U	C5-C6-N1	-7.70	118.85	122.70
36	5	2393	G	O5'-P-OP2	-7.69	98.78	105.70
36	5	2874	G	C5-C6-O6	7.69	133.22	128.60
36	1	1556	C	N3-C2-O2	-7.69	116.52	121.90
38	4	113	U	N3-C2-O2	-7.68	116.82	122.20
36	5	3140	G	C4-C5-N7	7.68	113.87	110.80
36	1	3109	G	N1-C6-O6	-7.68	115.29	119.90
1	6	158	U	P-O3'-C3'	7.68	128.91	119.70
1	2	1339	C	P-O3'-C3'	7.67	128.91	119.70
1	6	1537	C	N1-C2-O2	-7.67	114.30	118.90
36	1	1847	A	OP1-P-OP2	7.66	131.10	119.60
36	1	958	C	C2-N3-C4	-7.66	116.07	119.90
36	5	1337	A	C8-N9-C4	-7.66	102.73	105.80
36	5	3154	C	C5-C6-N1	7.66	124.83	121.00
1	6	453	U	N1-C2-O2	7.66	128.16	122.80
36	1	2600	C	N3-C2-O2	-7.65	116.54	121.90
36	1	2870	C	C2-N1-C1'	-7.65	110.38	118.80
36	5	2211	U	C4-C5-C6	7.65	124.29	119.70
36	1	922	U	N1-C2-O2	7.65	128.16	122.80
1	2	830	U	N3-C2-O2	-7.64	116.85	122.20
36	1	2983	C	N1-C2-N3	7.64	124.55	119.20
36	1	2513	U	O4'-C1'-N1	7.64	114.31	108.20
36	1	908	G	O4'-C1'-N9	-7.64	102.09	108.20
36	1	2372	A	C2-N3-C4	7.64	114.42	110.60
1	6	194	U	C2-N1-C1'	7.64	126.86	117.70
36	1	2139	A	N1-C6-N6	-7.63	114.02	118.60
1	6	1634	C	C2-N1-C1'	7.63	127.19	118.80
36	1	895	A	C4-C5-N7	7.63	114.51	110.70
36	1	2621	G	N1-C6-O6	7.62	124.47	119.90
36	5	2340	U	N3-C4-O4	-7.62	114.06	119.40
36	1	3209	A	N9-C4-C5	-7.62	102.75	105.80
36	5	1513	G	N7-C8-N9	7.62	116.91	113.10
36	5	283	G	C4-C5-N7	7.62	113.85	110.80
36	1	2975	U	N3-C4-C5	7.61	119.17	114.60
36	5	580	C	C6-N1-C2	-7.61	117.25	120.30
36	5	1390	A	N9-C4-C5	7.61	108.84	105.80
1	6	337	G	C4-N9-C1'	7.61	136.39	126.50
36	5	1370	G	N1-C6-O6	-7.61	115.33	119.90
36	5	2955	U	N3-C2-O2	-7.61	116.88	122.20
36	5	2393	G	C5-C6-O6	-7.61	124.04	128.60
36	5	2405	C	C2-N3-C4	-7.61	116.10	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1493	G	O4'-C1'-N9	7.60	114.28	108.20
36	5	2290	C	C2-N3-C4	-7.60	116.10	119.90
36	1	1144	U	C2-N3-C4	-7.59	122.44	127.00
36	1	2404	A	C2-N3-C4	7.59	114.39	110.60
36	1	2978	U	O5'-P-OP2	-7.59	98.87	105.70
1	2	75	U	N1-C2-O2	7.58	128.11	122.80
36	1	2816	G	C5-C6-O6	-7.58	124.05	128.60
1	2	1291	G	C8-N9-C4	-7.57	103.37	106.40
36	5	2858	U	N3-C2-O2	-7.57	116.90	122.20
36	5	1308	A	O5'-P-OP1	-7.57	98.89	105.70
36	1	2687	G	N1-C6-O6	-7.56	115.36	119.90
36	1	609	G	O5'-P-OP2	-7.56	98.90	105.70
36	1	2827	U	C6-N1-C1'	7.56	131.78	121.20
36	5	3336	A	N1-C6-N6	7.56	123.14	118.60
38	4	30	C	O5'-P-OP1	-7.56	98.90	105.70
36	5	838	G	C5-C6-O6	7.56	133.13	128.60
36	1	847	A	N1-C6-N6	7.55	123.13	118.60
36	5	1057	A	N1-C6-N6	7.55	123.13	118.60
36	1	2222	A	N9-C4-C5	7.55	108.82	105.80
36	5	1307	G	OP1-P-O3'	-7.55	88.59	105.20
36	5	3154	C	C2-N1-C1'	7.55	127.10	118.80
36	1	646	A	O5'-P-OP2	-7.54	98.91	105.70
36	5	2393	G	C8-N9-C4	7.54	109.42	106.40
36	1	1212	A	O5'-P-OP2	-7.54	98.92	105.70
1	2	453	U	C2-N1-C1'	7.54	126.74	117.70
36	1	1342	C	N3-C4-C5	7.54	124.92	121.90
36	5	2343	C	N3-C4-C5	7.54	124.92	121.90
36	1	3092	C	O5'-P-OP1	-7.54	98.92	105.70
36	1	1007	U	C5-C4-O4	-7.53	121.38	125.90
36	5	2352	A	N1-C2-N3	7.53	133.07	129.30
1	6	448	C	C6-N1-C2	-7.53	117.29	120.30
36	1	2130	G	C5-C6-O6	7.53	133.12	128.60
36	1	3143	C	C6-N1-C2	7.53	123.31	120.30
36	5	2821	C	N1-C2-O2	-7.53	114.38	118.90
36	5	993	G	O5'-P-OP2	-7.52	98.93	105.70
36	5	2812	C	O5'-P-OP1	-7.52	98.93	105.70
1	2	1560	U	C5-C4-O4	7.52	130.41	125.90
36	1	2114	C	O5'-P-OP2	-7.52	98.93	105.70
36	5	2797	C	N3-C2-O2	7.52	127.16	121.90
36	1	805	G	OP1-P-OP2	-7.52	108.33	119.60
36	1	1153	A	N1-C6-N6	7.52	123.11	118.60
36	1	1349	G	N3-C4-N9	7.51	130.51	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2424	A	N1-C6-N6	7.51	123.11	118.60
36	1	2409	G	C8-N9-C4	-7.51	103.39	106.40
36	1	2884	C	C6-N1-C2	7.50	123.30	120.30
36	1	1117	G	C5-C6-O6	-7.50	124.10	128.60
36	1	1484	U	P-O3'-C3'	7.50	128.70	119.70
1	6	358	U	O5'-P-OP1	-7.50	98.95	105.70
36	5	971	G	C5-N7-C8	7.49	108.05	104.30
1	2	1291	G	N1-C2-N3	7.48	128.39	123.90
36	1	931	C	N3-C4-C5	7.48	124.89	121.90
36	5	2620	G	C5-C6-N1	7.48	115.24	111.50
36	1	867	G	N3-C2-N2	-7.48	114.67	119.90
36	5	362	U	N1-C2-N3	7.48	119.39	114.90
36	1	2370	G	O5'-P-OP2	-7.48	98.97	105.70
36	1	645	A	N3-C4-C5	-7.47	121.57	126.80
36	5	1113	G	C2-N3-C4	-7.46	108.17	111.90
1	6	163	G	N3-C2-N2	-7.46	114.68	119.90
1	6	1537	C	C6-N1-C1'	7.46	129.75	120.80
10	s8	29	LEU	CA-CB-CG	7.46	132.45	115.30
36	1	347	G	C5-C6-N1	7.45	115.23	111.50
36	5	1848	G	N1-C6-O6	7.45	124.37	119.90
36	1	200	C	N1-C2-O2	7.45	123.37	118.90
36	1	2522	G	C4-N9-C1'	7.45	136.18	126.50
36	1	2384	A	N1-C6-N6	7.44	123.07	118.60
1	6	609	U	N3-C2-O2	-7.44	116.99	122.20
1	2	553	G	N3-C2-N2	-7.44	114.69	119.90
36	1	718	G	N3-C4-C5	7.44	132.32	128.60
36	1	591	G	C5-C6-N1	7.43	115.22	111.50
36	5	35	A	N9-C4-C5	-7.43	102.83	105.80
1	2	402	C	C6-N1-C2	7.43	123.27	120.30
36	1	2283	G	N3-C2-N2	-7.43	114.70	119.90
36	5	675	C	N1-C2-O2	-7.43	114.44	118.90
36	5	2726	C	N1-C2-N3	7.43	124.40	119.20
36	1	716	A	N9-C4-C5	-7.42	102.83	105.80
36	1	648	C	O5'-P-OP1	-7.42	99.02	105.70
36	5	65	A	O5'-P-OP2	-7.42	99.02	105.70
36	1	1082	U	C5-C6-N1	7.42	126.41	122.70
36	1	2944	U	N1-C2-O2	7.42	127.99	122.80
36	5	2814	G	C4-C5-N7	7.42	113.77	110.80
36	5	2314	U	N3-C4-O4	7.41	124.59	119.40
36	5	1888	U	C4-C5-C6	7.41	124.15	119.70
36	1	2952	G	N1-C6-O6	7.40	124.34	119.90
36	1	1433	A	C6-N1-C2	-7.40	114.16	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	348	A	O5'-P-OP1	-7.39	99.05	105.70
36	5	65	A	P-O3'-C3'	7.39	128.57	119.70
36	1	2179	C	N3-C4-C5	7.39	124.86	121.90
36	5	3309	G	N3-C4-C5	-7.38	124.91	128.60
36	1	369	A	C2-N3-C4	7.38	114.29	110.60
38	4	55	U	N3-C2-O2	-7.37	117.04	122.20
1	6	337	G	N9-C4-C5	-7.37	102.45	105.40
36	1	2409	G	C5-C6-O6	7.37	133.02	128.60
36	1	3278	C	N1-C2-O2	7.37	123.32	118.90
36	5	2938	G	O5'-P-OP1	-7.37	99.07	105.70
36	1	659	G	N3-C4-N9	7.37	130.42	126.00
1	6	1100	G	N3-C4-C5	-7.37	124.92	128.60
36	5	2821	C	N3-C2-O2	7.37	127.06	121.90
36	5	2860	U	N3-C2-O2	7.37	127.36	122.20
36	1	1556	C	C6-N1-C2	-7.37	117.35	120.30
36	5	1881	A	N1-C6-N6	7.36	123.02	118.60
40	13	19	ARG	NE-CZ-NH1	7.36	123.98	120.30
37	3	10	C	O5'-P-OP2	-7.36	99.08	105.70
38	4	79	A	C8-N9-C4	-7.36	102.86	105.80
36	1	2384	A	N9-C4-C5	-7.35	102.86	105.80
36	1	2411	U	N3-C4-O4	-7.35	114.25	119.40
1	6	901	G	C4-C5-N7	7.35	113.74	110.80
36	5	2930	A	N1-C6-N6	-7.35	114.19	118.60
36	1	1148	G	C8-N9-C4	7.34	109.34	106.40
1	6	1535	U	N3-C2-O2	-7.34	117.06	122.20
36	1	2960	C	C5-C6-N1	-7.33	117.33	121.00
1	2	1096	C	C2-N1-C1'	7.33	126.86	118.80
36	5	915	A	C2-N3-C4	7.33	114.27	110.60
36	5	2135	U	C6-N1-C2	7.33	125.40	121.00
1	6	1145	U	O5'-P-OP2	-7.32	99.11	105.70
1	6	630	A	O5'-P-OP2	-7.32	99.11	105.70
36	1	2614	G	N1-C6-O6	-7.31	115.51	119.90
36	1	1124	U	C4-C5-C6	-7.30	115.32	119.70
36	1	1517	G	O5'-P-OP2	-7.30	99.13	105.70
36	5	3173	G	C5-C6-O6	-7.30	124.22	128.60
36	1	960	U	C5-C6-N1	-7.30	119.05	122.70
1	6	364	G	C8-N9-C4	7.30	109.32	106.40
36	5	423	A	C2-N3-C4	7.30	114.25	110.60
36	1	1329	U	N1-C1'-C2'	-7.30	103.97	112.00
1	6	542	A	C5-N7-C8	-7.30	100.25	103.90
36	5	2375	G	C5-C6-O6	7.29	132.97	128.60
36	5	3306	U	C6-N1-C2	7.29	125.38	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	M0	57	LEU	CA-CB-CG	7.29	132.07	115.30
36	5	2872	A	C8-N9-C4	7.28	108.71	105.80
36	5	1846	C	C2-N3-C4	-7.28	116.26	119.90
36	1	3050	U	N3-C2-O2	-7.28	117.11	122.20
36	5	1882	G	N1-C6-O6	-7.28	115.53	119.90
36	1	950	G	N9-C4-C5	-7.28	102.49	105.40
36	1	1841	A	C2-N3-C4	7.28	114.24	110.60
36	1	2400	G	C4-C5-N7	7.28	113.71	110.80
36	5	1506	A	C8-N9-C4	-7.28	102.89	105.80
36	5	297	G	O4'-C1'-N9	7.27	114.02	108.20
36	5	2814	G	C6-C5-N7	-7.27	126.04	130.40
36	5	2354	C	N1-C2-O2	-7.27	114.54	118.90
36	1	938	C	N3-C4-C5	7.27	124.81	121.90
36	5	2257	C	C6-N1-C2	-7.27	117.39	120.30
36	5	2954	U	C6-N1-C1'	-7.26	111.03	121.20
36	5	2288	G	C5-C6-N1	7.26	115.13	111.50
36	5	2300	G	N1-C6-O6	-7.26	115.54	119.90
36	5	2878	G	C5-C6-N1	7.25	115.12	111.50
36	1	909	G	C8-N9-C4	7.24	109.30	106.40
1	2	1432	U	C6-N1-C2	7.24	125.34	121.00
36	5	2353	G	N1-C6-O6	7.24	124.25	119.90
36	5	1083	G	O5'-P-OP1	-7.24	99.19	105.70
36	5	2643	A	N1-C2-N3	-7.24	125.68	129.30
36	1	2215	A	C8-N9-C4	7.23	108.69	105.80
36	5	1846	C	C5-C6-N1	-7.23	117.39	121.00
1	6	1560	U	N3-C2-O2	-7.22	117.14	122.20
1	2	1773	C	N3-C4-N4	7.22	123.06	118.00
36	1	439	C	C6-N1-C1'	-7.22	112.13	120.80
36	1	1319	G	N1-C6-O6	-7.22	115.57	119.90
36	5	644	G	N1-C2-N3	-7.22	119.57	123.90
36	1	806	A	N9-C4-C5	-7.21	102.91	105.80
36	1	1902	G	N9-C4-C5	-7.21	102.51	105.40
1	6	93	A	N1-C6-N6	7.21	122.93	118.60
36	5	776	U	C5-C4-O4	7.21	130.23	125.90
1	2	1560	U	N1-C2-N3	7.21	119.22	114.90
36	1	890	C	C6-N1-C2	-7.21	117.42	120.30
36	5	3245	A	C6-C5-N7	-7.21	127.26	132.30
36	5	3334	U	N3-C2-O2	-7.21	117.16	122.20
36	1	966	U	N1-C2-O2	7.20	127.84	122.80
36	1	1428	A	C8-N9-C4	-7.20	102.92	105.80
36	5	3060	C	N1-C2-O2	-7.20	114.58	118.90
36	1	1168	U	N3-C2-O2	-7.20	117.16	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2341	A	C5-N7-C8	7.19	107.50	103.90
36	1	1556	C	C2-N1-C1'	7.19	126.71	118.80
41	14	327	LEU	CA-CB-CG	7.19	131.84	115.30
36	1	1308	A	C8-N9-C4	-7.18	102.93	105.80
1	2	830	U	N1-C2-O2	7.18	127.83	122.80
36	1	517	G	C8-N9-C4	-7.18	103.53	106.40
36	1	946	U	N1-C2-N3	7.18	119.21	114.90
36	1	2735	U	N3-C4-C5	7.18	118.91	114.60
36	5	1513	G	N3-C4-C5	-7.18	125.01	128.60
36	5	3218	A	C5-N7-C8	-7.18	100.31	103.90
36	1	505	G	N9-C4-C5	7.18	108.27	105.40
36	1	421	G	O5'-P-OP1	-7.18	99.24	105.70
36	1	2798	C	N3-C4-C5	-7.18	119.03	121.90
36	1	324	A	C6-N1-C2	-7.17	114.30	118.60
36	5	2524	A	O4'-C1'-N9	7.17	113.94	108.20
36	5	3140	G	N3-C4-N9	7.17	130.30	126.00
36	1	716	A	C2-N3-C4	-7.17	107.02	110.60
36	1	777	U	O5'-P-OP2	-7.17	99.25	105.70
54	M8	138	LEU	CA-CB-CG	7.17	131.79	115.30
36	1	1316	C	C2-N3-C4	-7.17	116.32	119.90
1	6	163	G	C5-N7-C8	-7.17	100.72	104.30
1	2	1389	C	N1-C2-O2	7.16	123.20	118.90
36	1	2572	C	N3-C2-O2	-7.16	116.89	121.90
36	5	971	G	N7-C8-N9	-7.16	109.52	113.10
37	3	102	A	O5'-P-OP1	-7.16	99.25	105.70
36	5	952	A	N1-C6-N6	7.16	122.90	118.60
36	5	412	G	C8-N9-C4	-7.16	103.54	106.40
1	2	287	G	O4'-C1'-N9	7.15	113.92	108.20
36	1	24	G	C5-C6-O6	-7.15	124.31	128.60
36	1	3308	C	O5'-P-OP1	-7.15	99.27	105.70
36	1	770	G	O4'-C1'-N9	7.15	113.92	108.20
36	5	1437	C	C5-C6-N1	7.15	124.57	121.00
36	1	2679	A	O4'-C1'-N9	7.14	113.91	108.20
36	5	73	C	C6-N1-C2	7.14	123.16	120.30
36	5	343	U	C5-C6-N1	-7.14	119.13	122.70
36	5	3362	A	C8-N9-C4	-7.14	102.94	105.80
36	1	2138	A	C8-N9-C4	-7.14	102.94	105.80
36	1	2144	A	O4'-C1'-N9	7.14	113.91	108.20
36	5	645	A	C6-N1-C2	-7.14	114.32	118.60
36	1	76	G	N3-C4-C5	-7.14	125.03	128.60
1	2	1200	G	N3-C2-N2	-7.14	114.90	119.90
36	1	1082	U	C6-N1-C2	-7.14	116.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	818	C	C2-N3-C4	-7.13	116.33	119.90
36	5	1879	A	N7-C8-N9	7.13	117.37	113.80
36	5	2367	A	O5'-P-OP2	7.13	119.26	110.70
36	1	2827	U	C2-N1-C1'	-7.13	109.15	117.70
1	6	1124	A	C8-N9-C4	7.13	108.65	105.80
36	5	3185	U	C5-C6-N1	-7.13	119.14	122.70
36	5	1197	A	N1-C6-N6	7.12	122.88	118.60
36	1	2726	C	C5-C6-N1	-7.12	117.44	121.00
1	6	609	U	N3-C4-O4	-7.12	114.42	119.40
36	1	612	U	O5'-P-OP1	-7.11	99.30	105.70
36	1	945	C	N3-C4-N4	-7.11	113.02	118.00
1	2	1291	G	C5-N7-C8	-7.11	100.75	104.30
1	6	1150	G	N3-C4-C5	7.11	132.16	128.60
37	3	86	U	C2-N3-C4	-7.11	122.73	127.00
36	1	1409	G	N1-C6-O6	-7.11	115.64	119.90
1	6	1745	G	C5-C6-O6	-7.11	124.33	128.60
39	12	216	HIS	N-CA-C	-7.11	91.81	111.00
36	1	1581	C	N1-C2-O2	7.11	123.16	118.90
36	1	895	A	C2-N3-C4	-7.10	107.05	110.60
38	4	125	U	C2-N1-C1'	7.10	126.22	117.70
36	5	1208	U	C5-C4-O4	7.10	130.16	125.90
36	5	2817	A	O5'-P-OP1	7.10	119.22	110.70
36	1	810	A	N1-C6-N6	-7.10	114.34	118.60
36	5	637	C	N1-C2-O2	-7.10	114.64	118.90
1	6	272	U	P-O3'-C3'	7.09	128.21	119.70
1	6	453	U	C2-N1-C1'	7.09	126.21	117.70
36	1	2168	A	C8-N9-C4	7.09	108.64	105.80
1	2	1486	G	N7-C8-N9	7.09	116.64	113.10
36	1	874	U	N3-C4-C5	7.09	118.85	114.60
36	1	2958	A	O5'-P-OP2	-7.09	99.32	105.70
1	6	1651	A	O5'-P-OP2	-7.09	99.32	105.70
1	2	507	U	C2-N1-C1'	7.08	126.20	117.70
36	1	970	A	N9-C4-C5	7.08	108.63	105.80
36	1	659	G	N3-C4-C5	-7.08	125.06	128.60
1	2	639	U	N1-C2-O2	7.08	127.75	122.80
36	1	1437	C	C6-N1-C2	-7.08	117.47	120.30
36	1	2960	C	C2-N3-C4	-7.07	116.36	119.90
36	5	1841	A	O5'-P-OP2	-7.07	99.34	105.70
36	1	2298	U	C2-N3-C4	-7.07	122.76	127.00
36	5	882	A	O5'-P-OP2	-7.07	99.34	105.70
36	1	2385	G	N3-C4-C5	7.07	132.13	128.60
36	1	941	G	OP1-P-O3'	7.06	120.73	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3055	U	C5-C4-O4	-7.06	121.67	125.90
36	5	971	G	C4-C5-N7	-7.06	107.98	110.80
36	5	1461	A	N7-C8-N9	-7.06	110.27	113.80
36	5	3048	A	O5'-P-OP2	-7.06	99.35	105.70
36	1	2639	G	C8-N9-C4	7.05	109.22	106.40
36	5	3133	C	C6-N1-C2	-7.05	117.48	120.30
38	8	111	A	O5'-P-OP2	-7.04	99.36	105.70
36	1	2977	G	C8-N9-C4	7.04	109.22	106.40
36	5	2293	C	C5-C4-N4	-7.04	115.27	120.20
36	1	2952	G	C4-C5-N7	7.04	113.61	110.80
36	1	3214	U	C6-N1-C2	-7.03	116.78	121.00
36	1	340	C	N3-C4-C5	7.03	124.71	121.90
36	5	2211	U	N3-C2-O2	-7.03	117.28	122.20
36	1	2694	A	O5'-P-OP2	-7.03	99.37	105.70
36	1	939	U	N1-C2-O2	-7.03	117.88	122.80
1	6	1634	C	N3-C2-O2	-7.03	116.98	121.90
36	1	2624	G	C8-N9-C4	-7.02	103.59	106.40
36	1	359	U	C4-C5-C6	7.02	123.91	119.70
36	5	1666	G	N1-C6-O6	-7.02	115.69	119.90
70	O4	51	LEU	CA-CB-CG	7.02	131.45	115.30
36	5	1392	G	C8-N9-C4	7.02	109.21	106.40
36	5	2359	C	N3-C4-C5	7.02	124.71	121.90
36	5	883	A	N7-C8-N9	-7.02	110.29	113.80
39	L2	191	LEU	CA-CB-CG	-7.02	99.16	115.30
36	5	938	C	C6-N1-C2	7.02	123.11	120.30
36	1	999	G	OP2-P-O3'	7.01	120.63	105.20
36	5	1390	A	N1-C6-N6	-7.01	114.39	118.60
36	1	1377	G	C5-C6-N1	7.01	115.01	111.50
36	5	1834	U	N3-C4-C5	-7.01	110.39	114.60
36	5	2246	G	O5'-P-OP2	7.01	119.11	110.70
36	5	2392	C	C5-C6-N1	-7.01	117.50	121.00
44	17	232	ARG	NE-CZ-NH1	-7.01	116.80	120.30
36	1	1216	C	C5-C6-N1	7.01	124.50	121.00
36	1	521	A	N9-C4-C5	-7.00	103.00	105.80
36	1	1450	G	O5'-P-OP1	-7.00	99.40	105.70
36	1	2870	C	C6-N1-C1'	7.00	129.20	120.80
1	2	1789	G	C8-N9-C4	7.00	109.20	106.40
36	1	2278	C	C4-C5-C6	-7.00	113.90	117.40
36	1	1331	U	O4'-C1'-N1	-7.00	102.60	108.20
36	1	2651	G	N3-C2-N2	-7.00	115.00	119.90
36	5	66	A	C8-N9-C4	6.99	108.60	105.80
36	5	2385	G	N3-C4-C5	6.99	132.10	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1905	G	C5-C6-O6	-6.99	124.41	128.60
36	5	3154	C	C6-N1-C2	-6.99	117.50	120.30
36	1	502	U	N3-C2-O2	-6.99	117.31	122.20
36	5	2632	G	N3-C2-N2	6.99	124.79	119.90
36	5	2636	A	O5'-P-OP2	6.99	119.08	110.70
41	14	339	LEU	CA-CB-CG	6.99	131.37	115.30
36	1	895	A	C8-N9-C4	-6.99	103.01	105.80
1	6	603	U	N1-C2-O2	-6.99	117.91	122.80
36	5	2814	G	N1-C6-O6	6.99	124.09	119.90
36	5	1112	A	N1-C6-N6	6.98	122.79	118.60
36	1	2606	G	N3-C2-N2	6.98	124.79	119.90
36	5	116	A	O4'-C1'-N9	6.98	113.79	108.20
36	5	1452	A	C5-C6-N6	-6.98	118.11	123.70
36	5	881	C	C2-N3-C4	6.98	123.39	119.90
36	5	2600	C	O5'-P-OP1	-6.98	99.42	105.70
36	5	3005	A	O5'-P-OP2	-6.98	99.42	105.70
36	5	1845	G	C5-C6-N1	6.98	114.99	111.50
36	5	2913	C	N1-C2-O2	-6.98	114.71	118.90
36	5	1313	G	O5'-P-OP1	6.98	119.07	110.70
36	1	1316	C	C5-C6-N1	-6.97	117.51	121.00
36	5	3245	A	N1-C6-N6	6.97	122.78	118.60
36	5	1115	G	N1-C2-N2	-6.97	109.93	116.20
36	5	3309	G	N3-C4-N9	6.97	130.18	126.00
36	5	2993	G	C5-C6-O6	-6.97	124.42	128.60
37	7	49	G	C5-C6-O6	-6.97	124.42	128.60
36	1	2704	A	O5'-P-OP1	-6.96	99.43	105.70
1	6	647	G	N3-C4-C5	6.96	132.08	128.60
36	5	39	A	N1-C6-N6	6.96	122.78	118.60
36	5	1305	U	N3-C4-O4	6.96	124.27	119.40
36	5	2400	G	C8-N9-C4	6.96	109.19	106.40
36	5	2639	G	C6-N1-C2	-6.96	120.92	125.10
36	1	958	C	N3-C4-C5	6.96	124.68	121.90
36	5	3195	U	OP1-P-O3'	6.96	120.51	105.20
36	5	1371	G	C5-C6-O6	6.96	132.78	128.60
1	6	163	G	C8-N9-C1'	6.96	136.04	127.00
1	6	542	A	C4-N9-C1'	6.96	138.82	126.30
36	1	1184	A	O5'-P-OP2	-6.95	99.44	105.70
36	5	2392	C	N3-C4-C5	6.95	124.68	121.90
36	1	196	G	C4-C5-N7	6.95	113.58	110.80
47	M0	24	ARG	NE-CZ-NH1	6.95	123.78	120.30
36	5	2968	G	C5-N7-C8	6.95	107.77	104.30
1	6	542	A	C6-C5-N7	-6.95	127.44	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3012	A	N9-C4-C5	-6.94	103.02	105.80
36	1	2622	C	C6-N1-C2	-6.94	117.52	120.30
36	1	217	U	OP1-P-O3'	6.94	120.46	105.20
36	5	2870	C	C2-N3-C4	-6.94	116.43	119.90
36	5	426	G	N1-C6-O6	-6.94	115.74	119.90
36	1	2384	A	C5-C6-N6	-6.93	118.16	123.70
1	2	581	U	C2-N1-C1'	6.93	126.02	117.70
36	1	2366	C	C5-C6-N1	6.93	124.47	121.00
1	6	425	A	O5'-P-OP2	-6.93	99.46	105.70
1	6	1767	G	C8-N9-C4	6.93	109.17	106.40
1	6	1106	U	O5'-P-OP1	-6.93	99.47	105.70
1	6	272	U	N3-C2-O2	-6.92	117.35	122.20
36	5	691	A	O5'-P-OP1	-6.92	99.47	105.70
36	5	1124	U	N3-C4-C5	6.92	118.75	114.60
1	6	453	U	C5-C4-O4	6.92	130.05	125.90
36	1	2130	G	N1-C6-O6	-6.92	115.75	119.90
17	c5	36	LEU	CA-CB-CG	6.92	131.21	115.30
36	5	2989	U	C5-C6-N1	-6.92	119.24	122.70
36	5	3209	A	O4'-C1'-N9	6.92	113.74	108.20
1	2	758	U	N3-C2-O2	-6.92	117.36	122.20
36	1	1365	G	C8-N9-C4	-6.92	103.63	106.40
36	5	2719	U	C2-N1-C1'	-6.92	109.40	117.70
36	1	2216	G	N1-C6-O6	-6.91	115.75	119.90
36	5	1938	U	C5-C6-N1	-6.91	119.25	122.70
36	1	404	G	O5'-P-OP2	-6.91	99.48	105.70
36	1	979	U	P-O3'-C3'	6.91	127.99	119.70
37	3	88	G	C5-C6-O6	6.91	132.74	128.60
36	5	2624	G	C8-N9-C4	-6.91	103.64	106.40
36	5	1331	U	C5-C6-N1	-6.90	119.25	122.70
36	5	2353	G	C5-C6-O6	-6.90	124.46	128.60
36	1	351	A	OP1-P-OP2	6.89	129.94	119.60
36	1	972	A	C8-N9-C4	6.89	108.56	105.80
1	6	399	A	C8-N9-C4	6.89	108.55	105.80
1	6	864	U	N3-C2-O2	-6.89	117.38	122.20
36	5	960	U	N3-C4-C5	6.88	118.73	114.60
36	1	1157	G	OP2-P-O3'	6.88	120.34	105.20
36	1	53	G	N7-C8-N9	-6.88	109.66	113.10
36	5	1150	A	C2-N3-C4	-6.88	107.16	110.60
59	n3	48	ARG	NE-CZ-NH1	6.88	123.74	120.30
36	5	3362	A	C2-N3-C4	-6.88	107.16	110.60
36	1	2393	G	N1-C6-O6	6.87	124.02	119.90
36	1	2899	C	N3-C2-O2	-6.87	117.09	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3212	C	N1-C2-O2	-6.87	114.78	118.90
36	5	41	G	C5-C6-O6	-6.87	124.48	128.60
1	2	75	U	N3-C2-O2	-6.86	117.40	122.20
36	5	2189	U	O5'-P-OP1	-6.86	99.52	105.70
36	5	982	C	OP2-P-O3'	6.86	120.30	105.20
36	5	1878	G	C4-N9-C1'	6.86	135.42	126.50
36	5	1881	A	C5-C6-N6	-6.86	118.21	123.70
1	6	1029	U	O5'-P-OP2	-6.86	99.53	105.70
36	1	111	C	C6-N1-C2	6.86	123.04	120.30
36	1	1902	G	C6-C5-N7	-6.86	126.29	130.40
36	1	2152	A	N1-C6-N6	-6.85	114.49	118.60
36	5	2323	G	N7-C8-N9	6.85	116.53	113.10
1	2	320	U	C5-C4-O4	-6.85	121.79	125.90
36	1	1313	G	C5-C6-O6	-6.84	124.49	128.60
36	5	1330	A	N1-C6-N6	6.84	122.71	118.60
36	5	3214	U	N3-C2-O2	-6.84	117.41	122.20
36	1	3092	C	C5-C6-N1	-6.84	117.58	121.00
62	N6	13	ARG	NE-CZ-NH2	-6.84	116.88	120.30
36	1	582	G	C8-N9-C4	-6.84	103.67	106.40
36	5	1421	G	O5'-P-OP2	-6.84	99.55	105.70
36	5	1437	C	C6-N1-C2	-6.84	117.57	120.30
36	1	1141	C	C4-C5-C6	6.83	120.82	117.40
36	5	2550	U	C5-C4-O4	6.83	130.00	125.90
36	5	2643	A	C2-N3-C4	6.83	114.02	110.60
36	1	980	A	N7-C8-N9	6.83	117.22	113.80
36	1	192	C	O5'-P-OP1	-6.83	99.55	105.70
36	1	2157	G	O5'-P-OP1	-6.83	99.56	105.70
36	5	2434	U	C5-C6-N1	-6.83	119.29	122.70
36	5	871	U	N3-C4-O4	-6.82	114.62	119.40
38	8	99	C	C6-N1-C2	6.82	123.03	120.30
36	1	2920	U	C2-N3-C4	-6.82	122.91	127.00
1	2	553	G	C5-C6-N1	-6.82	108.09	111.50
36	5	2703	A	C8-N9-C4	-6.82	103.07	105.80
1	6	542	A	O4'-C1'-N9	6.81	113.65	108.20
1	2	942	G	N1-C6-O6	-6.81	115.81	119.90
36	1	945	C	N3-C4-C5	6.81	124.62	121.90
36	1	1496	C	C2-N1-C1'	6.81	126.29	118.80
36	1	3344	A	C6-C5-N7	-6.81	127.53	132.30
38	4	140	G	C8-N9-C4	-6.81	103.68	106.40
1	2	359	A	C4-C5-C6	-6.81	113.60	117.00
1	2	973	A	O5'-P-OP2	-6.81	99.57	105.70
36	5	1208	U	N3-C2-O2	-6.81	117.44	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	25	G	C5-C6-O6	-6.81	124.52	128.60
36	5	2993	G	C4-C5-N7	6.80	113.52	110.80
36	1	2614	G	C5-C6-O6	6.80	132.68	128.60
36	5	2400	G	C5-C6-O6	-6.80	124.52	128.60
38	4	23	U	C5-C4-O4	-6.80	121.82	125.90
1	6	542	A	P-O3'-C3'	6.80	127.86	119.70
36	5	3039	C	O5'-P-OP2	-6.80	99.58	105.70
36	1	196	G	O5'-P-OP2	-6.80	99.58	105.70
36	1	645	A	N3-C4-N9	6.80	132.84	127.40
36	1	1851	G	N3-C4-C5	-6.80	125.20	128.60
36	1	2417	U	C2-N3-C4	-6.80	122.92	127.00
36	5	1473	G	C8-N9-C4	6.80	109.12	106.40
36	1	1394	A	OP2-P-O3'	6.79	120.15	105.20
36	5	825	U	N1-C2-O2	6.79	127.56	122.80
36	1	116	A	O4'-C1'-N9	6.79	113.63	108.20
36	1	2874	G	C5-C6-O6	6.79	132.67	128.60
36	5	2899	C	C5-C4-N4	6.79	124.95	120.20
36	5	2801	A	C2-N3-C4	6.78	113.99	110.60
36	1	1581	C	N3-C2-O2	-6.78	117.15	121.90
36	1	1582	C	O5'-P-OP1	-6.78	99.60	105.70
36	1	2306	C	N3-C2-O2	-6.78	117.15	121.90
36	1	421	G	N9-C4-C5	-6.78	102.69	105.40
1	6	362	G	N3-C4-N9	6.78	130.07	126.00
36	5	1445	U	C5-C4-O4	-6.78	121.83	125.90
36	1	196	G	N9-C4-C5	-6.78	102.69	105.40
36	5	2865	U	C4-C5-C6	-6.77	115.64	119.70
36	5	437	G	N7-C8-N9	6.77	116.48	113.10
36	1	804	C	N1-C2-O2	-6.77	114.84	118.90
36	1	2798	C	N1-C2-O2	-6.77	114.84	118.90
36	5	1430	U	C5-C6-N1	-6.77	119.31	122.70
36	5	2231	C	O4'-C1'-N1	6.77	113.62	108.20
36	1	2169	G	N1-C6-O6	-6.77	115.84	119.90
36	5	2831	G	N1-C6-O6	-6.77	115.84	119.90
1	6	1596	C	C6-N1-C2	-6.76	117.59	120.30
36	5	2834	G	O5'-P-OP1	-6.76	99.61	105.70
36	5	2660	G	C8-N9-C4	6.76	109.11	106.40
1	6	755	A	O4'-C1'-N9	6.76	113.61	108.20
1	2	1761	U	C5-C4-O4	6.76	129.96	125.90
36	1	1308	A	N7-C8-N9	6.76	117.18	113.80
36	1	2719	U	N1-C2-O2	-6.76	118.07	122.80
36	5	966	U	N1-C2-O2	6.76	127.53	122.80
36	1	664	U	C5-C6-N1	-6.75	119.32	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	959	C	C6-N1-C2	6.75	123.00	120.30
36	5	1207	G	N1-C6-O6	-6.75	115.85	119.90
36	1	282	G	C8-N9-C4	-6.75	103.70	106.40
1	2	359	A	C8-N9-C4	6.75	108.50	105.80
1	2	542	A	O4'-C1'-N9	6.75	113.60	108.20
36	5	2913	C	C6-N1-C2	-6.75	117.60	120.30
36	1	765	C	N1-C2-O2	6.74	122.95	118.90
36	1	2243	A	C8-N9-C4	6.74	108.50	105.80
36	5	2956	A	C8-N9-C4	-6.74	103.10	105.80
36	5	3143	C	N1-C2-O2	-6.74	114.86	118.90
36	1	887	G	O5'-P-OP2	-6.74	99.64	105.70
36	5	426	G	N7-C8-N9	-6.74	109.73	113.10
36	5	612	U	O5'-P-OP1	-6.74	99.64	105.70
36	5	3164	C	O4'-C1'-N1	6.74	113.59	108.20
64	n8	28	HIS	N-CA-C	6.74	129.19	111.00
36	1	2726	C	C2-N3-C4	-6.73	116.53	119.90
36	1	429	U	O5'-P-OP1	-6.73	99.64	105.70
36	5	2816	G	O4'-C1'-N9	6.73	113.58	108.20
36	1	3178	A	O5'-P-OP1	-6.73	99.65	105.70
36	1	99	A	O5'-P-OP2	-6.72	99.65	105.70
36	1	1297	C	C5-C6-N1	-6.72	117.64	121.00
36	5	2524	A	C5-N7-C8	-6.72	100.54	103.90
36	1	1555	U	C2-N1-C1'	-6.72	109.63	117.70
36	5	889	U	N3-C4-C5	6.72	118.63	114.60
36	1	3217	C	N1-C2-O2	6.72	122.93	118.90
1	6	351	C	C4-C5-C6	6.72	120.76	117.40
36	5	2831	G	C2-N3-C4	6.72	115.26	111.90
36	1	2249	G	N1-C6-O6	-6.72	115.87	119.90
36	5	1112	A	C5-C6-N6	-6.72	118.33	123.70
36	5	437	G	N3-C2-N2	-6.72	115.20	119.90
36	5	497	C	O5'-P-OP1	-6.72	99.66	105.70
1	6	1473	U	C6-N1-C2	-6.71	116.97	121.00
36	1	1419	A	O5'-P-OP2	-6.71	99.66	105.70
36	1	2870	C	C4-C5-C6	-6.71	114.04	117.40
36	1	919	U	C5-C4-O4	-6.71	121.87	125.90
36	1	1296	C	N3-C4-C5	-6.71	119.22	121.90
36	5	2192	C	O5'-P-OP2	-6.71	99.66	105.70
36	5	1148	G	C5-C6-O6	-6.71	124.58	128.60
36	1	650	C	C2-N3-C4	-6.70	116.55	119.90
36	1	2283	G	N1-C6-O6	6.70	123.92	119.90
36	5	3115	C	N1-C2-O2	-6.70	114.88	118.90
36	1	1376	C	N3-C4-C5	-6.70	119.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	112	U	C6-N1-C1'	-6.70	111.82	121.20
36	1	2892	A	N1-C6-N6	-6.70	114.58	118.60
36	5	777	U	O5'-P-OP2	-6.69	99.67	105.70
36	5	283	G	C6-C5-N7	-6.69	126.39	130.40
36	1	936	A	N1-C6-N6	6.69	122.61	118.60
36	1	1858	A	C2-N3-C4	6.69	113.94	110.60
1	2	577	G	C4-C5-N7	6.68	113.47	110.80
3	S1	218	LEU	CA-CB-CG	6.68	130.68	115.30
36	1	170	G	O5'-P-OP1	-6.68	99.69	105.70
36	1	2836	C	C6-N1-C2	-6.68	117.63	120.30
36	5	1907	C	N1-C2-O2	-6.68	114.89	118.90
36	5	2278	C	C5-C6-N1	6.68	124.34	121.00
36	1	1890	U	C5-C6-N1	-6.68	119.36	122.70
36	1	2944	U	OP1-P-O3'	6.68	119.89	105.20
36	5	3138	U	N1-C2-N3	6.68	118.91	114.90
52	m6	69	GLY	N-CA-C	-6.68	96.41	113.10
1	2	1432	U	C5-C6-N1	-6.67	119.36	122.70
38	4	138	A	N1-C6-N6	-6.67	114.59	118.60
36	1	1902	G	N1-C6-O6	6.67	123.90	119.90
36	5	2996	U	O5'-P-OP1	6.67	118.70	110.70
36	1	42	C	N1-C2-O2	-6.66	114.90	118.90
36	5	2302	G	C5-C6-O6	6.66	132.60	128.60
36	5	2693	C	N3-C2-O2	-6.66	117.24	121.90
36	1	369	A	O5'-P-OP2	-6.66	99.71	105.70
36	1	3362	A	N1-C2-N3	6.65	132.63	129.30
36	5	340	C	C2-N3-C4	-6.65	116.57	119.90
36	1	950	G	C4-C5-N7	6.65	113.46	110.80
36	1	3143	C	C5-C6-N1	-6.65	117.67	121.00
36	5	2872	A	N9-C4-C5	-6.65	103.14	105.80
1	2	811	A	C8-N9-C4	-6.65	103.14	105.80
1	2	1568	C	P-O3'-C3'	6.65	127.68	119.70
36	1	652	G	N1-C2-N2	-6.65	110.22	116.20
36	1	2302	G	C5-C6-O6	6.65	132.59	128.60
36	1	2818	U	C5-C6-N1	6.65	126.02	122.70
1	6	1032	G	C8-N9-C4	6.64	109.06	106.40
15	C3	22	ALA	C-N-CD	-6.64	105.99	120.60
36	1	2631	U	C2-N3-C4	-6.64	123.01	127.00
36	1	2945	G	C8-N9-C4	6.64	109.06	106.40
36	5	2614	G	C8-N9-C4	6.64	109.06	106.40
36	1	1419	A	O5'-P-OP1	6.64	118.67	110.70
25	D3	23	ARG	NE-CZ-NH1	6.64	123.62	120.30
36	5	419	G	N3-C2-N2	6.64	124.55	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	871	U	C5-C4-O4	6.64	129.88	125.90
15	C3	114	ARG	NE-CZ-NH1	6.63	123.62	120.30
36	1	709	A	N7-C8-N9	-6.63	110.48	113.80
36	1	2817	A	C5-C6-N1	6.63	121.02	117.70
36	1	2830	G	N3-C2-N2	-6.63	115.26	119.90
36	5	1592	G	C5-C6-N1	-6.63	108.18	111.50
48	m1	112	LEU	CA-CB-CG	6.63	130.56	115.30
36	5	35	A	C8-N9-C4	6.63	108.45	105.80
36	5	1879	A	C6-C5-N7	-6.63	127.66	132.30
36	1	2364	G	C5-C6-O6	-6.63	124.62	128.60
36	5	1402	C	N3-C2-O2	-6.63	117.26	121.90
36	5	2116	G	C6-C5-N7	-6.63	126.42	130.40
36	1	2747	A	N1-C6-N6	-6.63	114.62	118.60
36	1	3058	U	C2-N1-C1'	6.62	125.65	117.70
36	5	3052	G	C5-C6-O6	6.62	132.57	128.60
36	5	1307	G	OP2-P-O3'	6.62	119.77	105.20
36	5	1481	A	P-O3'-C3'	6.62	127.65	119.70
36	1	414	U	O5'-P-OP2	-6.62	99.74	105.70
36	1	3306	U	N1-C2-N3	6.62	118.87	114.90
1	6	308	C	N1-C2-N3	6.62	123.83	119.20
38	4	53	A	C2-N3-C4	6.62	113.91	110.60
36	5	33	G	C5-C6-O6	-6.62	124.63	128.60
36	1	2409	G	N1-C2-N2	-6.62	110.24	116.20
36	5	3086	A	C8-N9-C4	6.62	108.45	105.80
36	1	51	A	N1-C6-N6	6.62	122.57	118.60
36	1	1414	G	O5'-P-OP2	-6.62	99.75	105.70
38	4	37	A	C8-N9-C4	-6.62	103.15	105.80
36	5	989	A	N1-C6-N6	-6.61	114.63	118.60
36	5	3197	G	N3-C2-N2	-6.60	115.28	119.90
36	1	957	C	N1-C2-O2	-6.60	114.94	118.90
41	L4	95	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	6	350	U	N1-C2-N3	6.60	118.86	114.90
36	1	1157	G	N9-C4-C5	6.60	108.04	105.40
36	1	2714	G	C5-N7-C8	-6.60	101.00	104.30
36	1	2952	G	C5-C6-O6	-6.60	124.64	128.60
1	6	1473	U	C2-N1-C1'	6.60	125.62	117.70
36	1	120	G	C8-N9-C4	6.59	109.04	106.40
36	1	667	C	N3-C4-N4	-6.59	113.38	118.00
1	2	1486	G	C5-N7-C8	-6.59	101.00	104.30
36	5	1931	U	C2-N1-C1'	-6.59	109.79	117.70
1	2	1339	C	C6-N1-C2	-6.59	117.66	120.30
36	1	2372	A	O5'-P-OP1	-6.59	99.77	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2403	G	O4'-C1'-N9	6.59	113.47	108.20
36	1	1153	A	C4-C5-C6	6.59	120.29	117.00
1	6	956	C	C6-N1-C2	6.59	122.94	120.30
1	6	250	C	O5'-P-OP2	-6.58	99.77	105.70
36	1	3119	U	N3-C4-O4	-6.58	114.79	119.40
1	6	696	C	O4'-C1'-N1	6.58	113.47	108.20
36	1	143	G	N3-C4-C5	-6.58	125.31	128.60
36	1	718	G	C5-N7-C8	-6.58	101.01	104.30
36	1	1863	G	O5'-P-OP2	-6.58	99.78	105.70
37	3	86	U	C6-N1-C2	6.58	124.94	121.00
1	6	364	G	N7-C8-N9	-6.58	109.81	113.10
36	5	2142	A	C6-N1-C2	-6.58	114.66	118.60
36	1	2728	G	C2-N3-C4	6.57	115.19	111.90
36	1	2936	A	O5'-P-OP2	6.57	118.59	110.70
36	5	25	U	N1-C2-N3	6.57	118.84	114.90
36	5	2995	A	C8-N9-C4	6.57	108.43	105.80
1	2	1092	A	N9-C4-C5	-6.57	103.17	105.80
1	6	163	G	N9-C4-C5	6.57	108.03	105.40
36	1	2298	U	N3-C4-O4	-6.57	114.80	119.40
36	5	340	C	C5-C6-N1	-6.57	117.72	121.00
36	5	3017	A	C8-N9-C4	-6.57	103.17	105.80
36	1	2679	A	N1-C2-N3	6.56	132.58	129.30
36	5	2188	A	C8-N9-C4	6.56	108.43	105.80
36	5	1172	G	OP2-P-O3'	6.56	119.64	105.20
36	5	426	G	C5-C6-O6	6.56	132.54	128.60
36	5	2913	C	C4-C5-C6	6.56	120.68	117.40
38	4	74	U	O5'-P-OP1	-6.56	99.80	105.70
36	5	64	G	C5-C6-O6	-6.55	124.67	128.60
36	5	2166	A	O5'-P-OP1	-6.55	99.80	105.70
36	1	2375	G	N7-C8-N9	-6.55	109.83	113.10
36	5	1049	C	O5'-P-OP2	-6.55	99.81	105.70
36	1	646	A	C8-N9-C4	-6.55	103.18	105.80
36	1	2641	U	C5-C6-N1	-6.55	119.43	122.70
36	1	3143	C	O5'-P-OP2	-6.55	99.81	105.70
1	6	1514	U	C5-C4-O4	6.54	129.83	125.90
36	5	1660	C	C6-N1-C2	-6.54	117.68	120.30
1	6	957	G	N1-C6-O6	6.54	123.83	119.90
37	7	46	A	C8-N9-C4	-6.54	103.18	105.80
36	1	1381	A	O5'-P-OP1	-6.54	99.81	105.70
36	5	2913	C	N1-C2-N3	6.54	123.78	119.20
1	2	1324	G	N3-C4-N9	-6.54	122.08	126.00
36	1	2417	U	C5-C6-N1	-6.54	119.43	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	38	U	O5'-P-OP2	-6.54	99.82	105.70
36	5	2950	G	C4-C5-N7	6.54	113.42	110.80
36	1	2938	G	OP1-P-OP2	6.54	129.40	119.60
1	6	1473	U	C5-C4-O4	6.54	129.82	125.90
36	1	1160	C	O5'-P-OP1	-6.53	99.82	105.70
36	5	1168	U	N3-C4-C5	6.53	118.52	114.60
36	5	2278	C	N3-C2-O2	-6.53	117.33	121.90
36	1	2121	G	N1-C6-O6	-6.53	115.98	119.90
37	3	12	U	C5-C4-O4	-6.53	121.98	125.90
36	1	421	G	C4-C5-N7	6.53	113.41	110.80
36	1	1530	U	C6-N1-C2	6.53	124.92	121.00
1	6	825	U	N3-C2-O2	6.53	126.77	122.20
36	5	41	G	C5-N7-C8	-6.53	101.04	104.30
36	1	1825	G	O5'-P-OP2	-6.53	99.83	105.70
36	5	1149	G	N1-C6-O6	6.53	123.82	119.90
36	1	1604	G	N3-C4-C5	-6.52	125.34	128.60
49	M3	36	ARG	NE-CZ-NH1	-6.52	117.04	120.30
36	1	582	G	N9-C4-C5	6.52	108.01	105.40
36	5	1006	A	O5'-P-OP2	-6.52	99.83	105.70
1	2	1654	G	O5'-P-OP2	-6.52	99.83	105.70
1	6	1629	G	O5'-P-OP2	-6.52	99.83	105.70
35	sM	167	PRO	N-CA-CB	6.52	111.12	103.30
36	5	3309	G	C4-N9-C1'	6.52	134.97	126.50
1	6	1124	A	N9-C4-C5	-6.52	103.19	105.80
36	1	2153	U	N1-C2-N3	6.51	118.81	114.90
38	4	113	U	C5-C6-N1	-6.51	119.44	122.70
36	5	3018	C	O5'-P-OP2	-6.51	99.84	105.70
35	SM	167	PRO	N-CA-CB	6.51	111.11	103.30
36	1	970	A	N7-C8-N9	6.51	117.06	113.80
36	5	696	C	C5-C4-N4	-6.51	115.64	120.20
36	1	591	G	C6-N1-C2	-6.51	121.19	125.10
36	1	2817	A	C6-N1-C2	-6.51	114.69	118.60
36	5	2370	G	C5-C6-N1	6.51	114.75	111.50
36	5	216	G	C6-C5-N7	-6.50	126.50	130.40
36	5	189	G	N1-C6-O6	-6.50	116.00	119.90
1	6	1498	G	N1-C6-O6	-6.50	116.00	119.90
36	5	2295	A	C8-N9-C4	6.50	108.40	105.80
36	5	2371	G	N3-C4-C5	6.50	131.85	128.60
36	5	1452	A	N1-C6-N6	6.50	122.50	118.60
36	5	2630	C	C2-N3-C4	-6.50	116.65	119.90
36	5	2980	U	N1-C2-N3	6.50	118.80	114.90
36	1	2241	U	O5'-P-OP1	-6.49	99.86	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2231	C	C6-N1-C2	-6.49	117.70	120.30
36	5	1399	A	O5'-P-OP2	-6.49	99.86	105.70
36	1	2758	A	N1-C2-N3	-6.49	126.06	129.30
36	5	2630	C	N3-C4-C5	6.49	124.50	121.90
1	2	553	G	C4-C5-C6	6.49	122.69	118.80
36	1	2297	U	N3-C2-O2	-6.49	117.66	122.20
36	5	2385	G	N1-C6-O6	6.49	123.79	119.90
1	2	1585	U	O5'-P-OP2	-6.49	99.86	105.70
36	5	796	U	N1-C2-O2	6.49	127.34	122.80
38	8	2	A	C8-N9-C4	-6.49	103.21	105.80
1	2	73	U	OP1-P-O3'	6.48	119.46	105.20
36	1	919	U	OP1-P-OP2	-6.48	109.87	119.60
36	5	1483	G	O5'-P-OP1	-6.48	99.86	105.70
1	6	194	U	N1-C2-O2	6.48	127.34	122.80
1	6	1793	G	C4-C5-N7	-6.48	108.21	110.80
36	5	1054	A	C8-N9-C4	6.48	108.39	105.80
1	2	1662	G	O5'-P-OP2	-6.47	99.87	105.70
36	1	1741	A	C2-N3-C4	-6.47	107.36	110.60
36	1	24	G	N1-C6-O6	6.47	123.78	119.90
36	1	97	U	C5-C6-N1	-6.47	119.47	122.70
36	1	3058	U	C6-N1-C1'	-6.47	112.15	121.20
1	6	1081	A	O4'-C1'-N9	6.47	113.37	108.20
36	5	1123	U	C5-C6-N1	-6.47	119.47	122.70
36	1	634	C	N1-C2-O2	6.46	122.78	118.90
36	1	2923	U	N3-C2-O2	6.46	126.72	122.20
36	5	3308	C	C4-C5-C6	6.46	120.63	117.40
36	5	2360	C	C4-C5-C6	6.46	120.63	117.40
36	1	3092	C	C2-N1-C1'	-6.46	111.69	118.80
36	5	3374	U	N3-C4-C5	6.46	118.48	114.60
1	6	1483	A	O5'-P-OP1	-6.46	99.89	105.70
36	5	1910	A	OP2-P-O3'	6.46	119.41	105.20
37	7	94	C	C4-C5-C6	-6.46	114.17	117.40
36	5	1148	G	C8-N9-C4	6.46	108.98	106.40
36	5	2382	G	N1-C6-O6	-6.46	116.03	119.90
37	7	101	G	N9-C4-C5	-6.46	102.82	105.40
36	1	3318	G	C4-N9-C1'	6.45	134.89	126.50
36	5	2630	C	N1-C2-O2	-6.45	115.03	118.90
36	5	2865	U	N1-C2-O2	6.45	127.32	122.80
44	17	229	PHE	CB-CG-CD1	6.45	125.32	120.80
36	1	2642	A	C8-N9-C4	6.45	108.38	105.80
36	1	2958	A	N1-C6-N6	-6.45	114.73	118.60
1	2	142	G	N3-C4-C5	6.45	131.82	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2213	A	C8-N9-C4	6.45	108.38	105.80
1	2	934	C	O5'-P-OP1	-6.45	99.90	105.70
36	1	874	U	C6-N1-C2	6.45	124.87	121.00
36	5	1152	G	N9-C4-C5	6.45	107.98	105.40
36	1	1060	U	C5-C6-N1	-6.44	119.48	122.70
36	1	1589	A	O4'-C1'-N9	-6.44	103.05	108.20
36	1	2550	U	N1-C2-N3	6.44	118.77	114.90
36	5	2136	C	N3-C4-C5	6.44	124.48	121.90
36	1	2281	A	C8-N9-C4	6.44	108.38	105.80
36	1	3275	U	OP1-P-O3'	6.44	119.36	105.20
36	5	208	C	C6-N1-C2	-6.44	117.72	120.30
36	5	3245	A	N1-C2-N3	6.44	132.52	129.30
36	1	921	A	O4'-C1'-N9	-6.44	103.05	108.20
36	1	643	U	N1-C2-O2	-6.43	118.30	122.80
36	5	2181	C	N1-C2-O2	-6.43	115.04	118.90
36	1	86	G	C5-C6-N1	6.43	114.72	111.50
36	1	906	A	C5-C6-N1	6.43	120.92	117.70
1	6	107	C	C6-N1-C2	6.43	122.87	120.30
36	1	1169	A	OP2-P-O3'	6.42	119.34	105.20
36	1	1182	A	C8-N9-C4	6.42	108.37	105.80
36	1	30	G	C5-C6-O6	6.42	132.45	128.60
36	1	2983	C	O5'-P-OP1	-6.42	99.92	105.70
62	N6	126	LEU	CA-CB-CG	6.42	130.07	115.30
36	5	2302	G	N1-C6-O6	-6.42	116.05	119.90
36	5	871	U	N3-C2-O2	-6.42	117.71	122.20
36	1	957	C	O5'-P-OP2	-6.42	99.93	105.70
36	1	1140	G	N3-C4-N9	6.41	129.85	126.00
36	5	970	A	N1-C6-N6	6.41	122.45	118.60
36	5	2147	A	N1-C6-N6	6.41	122.45	118.60
36	1	1142	G	C5-C6-O6	-6.41	124.75	128.60
36	5	1321	G	O5'-P-OP2	-6.41	99.93	105.70
1	6	1782	A	C8-N9-C4	-6.41	103.24	105.80
36	5	1307	G	C2'-C3'-O3'	6.41	123.95	113.70
1	6	1783	C	N1-C2-O2	6.40	122.74	118.90
36	1	1279	C	C6-N1-C2	-6.40	117.74	120.30
38	4	32	C	N1-C2-O2	-6.40	115.06	118.90
38	4	125	U	N1-C2-O2	6.40	127.28	122.80
36	5	26	A	C8-N9-C4	6.40	108.36	105.80
36	5	806	A	C6-N1-C2	6.40	122.44	118.60
36	5	2234	G	C5-C6-O6	-6.40	124.76	128.60
36	5	2969	A	C8-N9-C4	6.40	108.36	105.80
36	5	2993	G	N9-C4-C5	-6.40	102.84	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1513	G	C2-N3-C4	6.40	115.10	111.90
36	5	1162	U	N1-C2-O2	-6.40	118.32	122.80
36	5	519	A	C5-C6-N6	-6.40	118.58	123.70
36	1	2952	G	C6-C5-N7	-6.39	126.56	130.40
36	1	1429	G	N3-C4-C5	-6.39	125.40	128.60
37	3	96	U	C5-C6-N1	-6.39	119.50	122.70
36	1	3057	U	N3-C2-O2	-6.39	117.73	122.20
36	5	2378	C	O5'-P-OP2	-6.39	99.95	105.70
36	1	2551	U	N3-C2-O2	-6.39	117.73	122.20
36	5	2386	A	C8-N9-C4	-6.39	103.24	105.80
1	6	65	A	C2-N3-C4	-6.39	107.41	110.60
36	5	3101	G	O5'-P-OP1	-6.39	99.95	105.70
36	1	1144	U	C5-C6-N1	-6.39	119.51	122.70
36	1	2651	G	N3-C4-N9	-6.39	122.17	126.00
36	1	868	C	N1-C2-O2	6.38	122.73	118.90
1	6	858	G	O4'-C1'-N9	6.38	113.31	108.20
36	5	1064	A	N1-C6-N6	6.38	122.43	118.60
36	5	1284	C	C6-N1-C2	-6.38	117.75	120.30
36	5	2954	U	N3-C4-C5	-6.38	110.77	114.60
36	5	1116	G	N3-C4-C5	-6.38	125.41	128.60
36	5	3214	U	C5-C4-O4	6.38	129.73	125.90
36	1	339	C	O5'-P-OP1	-6.38	99.96	105.70
36	5	2352	A	C4-C5-C6	6.38	120.19	117.00
1	2	1486	G	C8-N9-C4	-6.38	103.85	106.40
38	4	114	G	O5'-P-OP1	-6.37	99.96	105.70
38	4	148	G	N1-C6-O6	-6.37	116.08	119.90
36	5	3011	A	OP1-P-O3'	6.37	119.22	105.20
1	2	610	G	C8-N9-C1'	-6.37	118.72	127.00
36	1	957	C	C5-C4-N4	-6.37	115.74	120.20
1	6	1620	C	C6-N1-C2	-6.37	117.75	120.30
36	5	3218	A	C6-C5-N7	-6.37	127.84	132.30
1	2	554	C	N1-C2-O2	6.37	122.72	118.90
1	6	272	U	C2-N1-C1'	6.37	125.34	117.70
36	1	41	G	C5-C6-O6	6.37	132.42	128.60
36	1	2298	U	N1-C2-N3	6.37	118.72	114.90
36	5	981	U	C5-C6-N1	6.37	125.88	122.70
36	5	3215	A	N1-C6-N6	6.37	122.42	118.60
36	1	1911	A	N1-C6-N6	6.36	122.42	118.60
1	6	1787	C	N1-C2-O2	-6.36	115.08	118.90
36	5	1048	A	OP1-P-O3'	6.36	119.20	105.20
36	1	2142	A	C6-N1-C2	-6.36	114.78	118.60
36	5	2899	C	N3-C4-N4	-6.36	113.55	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3012	A	N7-C8-N9	-6.36	110.62	113.80
36	1	1408	G	N1-C6-O6	-6.36	116.09	119.90
36	5	520	U	N1-C2-N3	6.36	118.72	114.90
36	5	2965	U	N3-C2-O2	6.36	126.65	122.20
36	5	3195	U	P-O3'-C3'	6.36	127.33	119.70
1	2	144	U	N3-C2-O2	-6.36	117.75	122.20
1	2	1654	G	C5-C6-O6	-6.36	124.79	128.60
36	1	635	G	C4-C5-N7	6.35	113.34	110.80
38	4	113	U	C4-C5-C6	6.35	123.51	119.70
36	5	2231	C	C2-N1-C1'	6.35	125.79	118.80
36	5	3197	G	N3-C4-N9	-6.35	122.19	126.00
36	1	698	U	N1-C2-N3	6.35	118.71	114.90
38	4	21	C	C2-N1-C1'	-6.35	111.82	118.80
36	5	1371	G	C6-C5-N7	6.35	134.21	130.40
36	5	2249	G	C8-N9-C4	-6.35	103.86	106.40
36	1	913	A	O5'-P-OP1	-6.34	99.99	105.70
36	1	917	A	N1-C6-N6	-6.34	114.79	118.60
36	5	818	C	C5-C6-N1	-6.34	117.83	121.00
1	2	607	G	N1-C6-O6	6.34	123.71	119.90
36	1	1294	A	O4'-C1'-N9	6.34	113.27	108.20
36	1	2836	C	N3-C2-O2	-6.34	117.46	121.90
36	5	2342	U	C2-N3-C4	-6.34	123.19	127.00
36	1	718	G	C4-C5-N7	6.34	113.34	110.80
1	6	402	C	C5-C4-N4	-6.34	115.76	120.20
36	5	2614	G	N7-C8-N9	-6.34	109.93	113.10
36	5	2700	G	C5-C6-O6	-6.34	124.80	128.60
36	1	874	U	N3-C4-O4	-6.34	114.97	119.40
36	1	2385	G	O5'-P-OP1	-6.34	100.00	105.70
36	5	2112	U	C6-N1-C2	-6.34	117.20	121.00
47	m0	48	LEU	CA-CB-CG	6.34	129.88	115.30
36	5	1302	A	N9-C4-C5	6.33	108.33	105.80
36	5	2327	U	C2-N3-C4	-6.33	123.20	127.00
36	1	339	C	O5'-P-OP2	6.33	118.30	110.70
36	1	1893	A	N9-C4-C5	6.33	108.33	105.80
36	5	282	G	C2'-C3'-O3'	6.33	123.83	113.70
36	5	874	U	O5'-P-OP1	-6.33	100.00	105.70
36	5	945	C	N3-C4-C5	6.33	124.43	121.90
1	2	1662	G	C5-C6-N1	6.33	114.67	111.50
36	5	1481	A	C8-N9-C4	-6.33	103.27	105.80
36	1	439	C	N1-C2-O2	6.33	122.70	118.90
36	5	2388	U	N1-C2-O2	-6.33	118.37	122.80
36	5	3041	U	N3-C4-C5	6.33	118.40	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1141	C	N3-C4-C5	-6.33	119.37	121.90
36	5	970	A	C5-C6-N6	-6.33	118.64	123.70
36	5	1322	U	N3-C4-C5	6.33	118.39	114.60
1	6	767	U	N3-C2-O2	-6.32	117.77	122.20
36	1	806	A	N1-C6-N6	6.32	122.39	118.60
36	1	2401	A	N1-C2-N3	-6.32	126.14	129.30
36	1	291	C	OP2-P-O3'	6.32	119.10	105.20
36	1	1507	G	N3-C4-C5	-6.32	125.44	128.60
36	5	952	A	N9-C4-C5	-6.32	103.27	105.80
1	2	1761	U	C6-N1-C2	-6.32	117.21	121.00
1	6	1114	G	N3-C4-C5	-6.32	125.44	128.60
36	5	1859	A	O5'-P-OP2	-6.31	100.02	105.70
36	5	2948	C	N3-C4-N4	-6.31	113.58	118.00
36	5	3008	A	OP2-P-O3'	6.31	119.09	105.20
36	1	1164	G	N1-C6-O6	-6.31	116.11	119.90
36	1	2647	A	C6-N1-C2	-6.31	114.81	118.60
36	5	634	C	C2-N3-C4	-6.31	116.74	119.90
36	1	2941	A	O4'-C1'-N9	-6.31	103.15	108.20
36	5	2980	U	C6-N1-C2	-6.31	117.21	121.00
36	1	1748	G	N1-C6-O6	-6.31	116.11	119.90
36	1	660	A	N1-C6-N6	-6.31	114.82	118.60
36	1	3242	G	C8-N9-C4	6.30	108.92	106.40
1	6	1755	A	N1-C6-N6	6.30	122.38	118.60
36	5	1301	A	N9-C4-C5	-6.30	103.28	105.80
37	7	41	G	C4-C5-N7	6.30	113.32	110.80
36	1	53	G	N9-C4-C5	-6.30	102.88	105.40
65	N9	20	GLY	N-CA-C	6.30	128.86	113.10
36	5	1480	G	O4'-C1'-N9	6.30	113.24	108.20
36	5	3177	G	O5'-P-OP1	6.30	118.26	110.70
36	1	2393	G	O4'-C1'-N9	6.30	113.24	108.20
36	5	2891	U	C5-C6-N1	-6.30	119.55	122.70
36	1	939	U	C5-C4-O4	-6.30	122.12	125.90
36	1	2860	U	N3-C4-O4	6.30	123.81	119.40
36	5	947	G	C2-N3-C4	6.30	115.05	111.90
36	1	212	G	O4'-C1'-N9	6.30	113.24	108.20
1	6	964	U	O5'-P-OP2	-6.29	100.03	105.70
36	1	1789	G	N3-C2-N2	6.29	124.31	119.90
36	5	669	U	C5-C6-N1	-6.29	119.55	122.70
36	5	2211	U	C5-C4-O4	6.29	129.67	125.90
1	2	973	A	C2-N3-C4	-6.29	107.46	110.60
36	1	324	A	C4-C5-C6	6.29	120.14	117.00
36	5	189	G	N9-C4-C5	6.29	107.91	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	90	U	C6-N1-C2	6.28	124.77	121.00
36	1	2897	A	N7-C8-N9	-6.28	110.66	113.80
36	1	426	G	N3-C4-N9	6.28	129.77	126.00
36	1	1389	G	C5-C6-O6	-6.28	124.83	128.60
36	5	1301	A	C5-C6-N6	-6.28	118.68	123.70
37	3	83	U	N3-C4-C5	6.28	118.36	114.60
36	5	2632	G	N1-C6-O6	-6.28	116.13	119.90
36	1	1114	U	C6-N1-C2	6.27	124.76	121.00
36	1	1888	U	C5-C6-N1	-6.27	119.56	122.70
36	5	2397	A	O5'-P-OP2	-6.27	100.06	105.70
36	5	2694	A	O5'-P-OP1	-6.27	100.05	105.70
36	5	2910	A	OP2-P-O3'	6.27	119.00	105.20
36	5	3118	C	C5-C6-N1	6.27	124.14	121.00
36	1	806	A	C8-N9-C4	6.27	108.31	105.80
36	1	3141	A	OP2-P-O3'	6.27	119.00	105.20
36	1	1419	A	C5'-C4'-O4'	6.27	116.62	109.10
36	1	2279	A	C8-N9-C4	6.27	108.31	105.80
36	1	2306	C	N3-C4-N4	-6.27	113.61	118.00
36	5	1189	C	N1-C2-O2	-6.27	115.14	118.90
36	1	339	C	C2-N3-C4	-6.27	116.77	119.90
1	6	795	U	N3-C2-O2	-6.27	117.81	122.20
36	5	2618	G	C4-C5-N7	6.27	113.31	110.80
1	6	913	G	O5'-P-OP1	-6.27	100.06	105.70
1	2	1448	G	O5'-P-OP1	-6.26	100.06	105.70
36	1	3362	A	C4-C5-N7	6.26	113.83	110.70
36	5	1152	G	N7-C8-N9	6.26	116.23	113.10
36	1	2616	C	O5'-P-OP1	-6.26	100.06	105.70
36	5	1886	A	O5'-P-OP2	-6.26	100.06	105.70
36	5	994	G	N3-C2-N2	6.26	124.28	119.90
36	5	2389	C	N3-C4-C5	6.26	124.40	121.90
36	1	2152	A	C2-N3-C4	6.26	113.73	110.60
36	1	666	A	N7-C8-N9	-6.26	110.67	113.80
36	1	709	A	N1-C6-N6	6.26	122.35	118.60
36	1	2618	G	N1-C6-O6	-6.26	116.15	119.90
36	5	1010	G	O5'-P-OP2	-6.26	100.07	105.70
36	5	2135	U	N3-C4-C5	6.26	118.35	114.60
36	1	1133	A	C8-N9-C4	6.25	108.30	105.80
36	1	2714	G	O5'-P-OP2	6.25	118.20	110.70
11	s9	149	ARG	NE-CZ-NH1	6.25	123.43	120.30
36	1	1422	G	O5'-P-OP1	-6.25	100.08	105.70
36	1	2550	U	C5-C4-O4	6.25	129.65	125.90
36	5	2639	G	C6-C5-N7	-6.25	126.65	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1399	C	C5-C6-N1	6.25	124.12	121.00
36	5	428	A	OP2-P-O3'	6.25	118.95	105.20
36	5	1469	C	N3-C4-C5	-6.25	119.40	121.90
36	5	3078	U	C2-N1-C1'	6.25	125.19	117.70
1	6	647	G	N3-C2-N2	-6.24	115.53	119.90
64	n8	42	ARG	NE-CZ-NH1	6.24	123.42	120.30
36	5	3093	C	C5-C6-N1	-6.24	117.88	121.00
36	5	2371	G	C2-N3-C4	-6.24	108.78	111.90
36	5	2664	C	C5-C6-N1	6.24	124.12	121.00
37	7	88	G	C5-C6-O6	6.24	132.34	128.60
36	1	1881	A	N1-C6-N6	6.23	122.34	118.60
36	1	3022	G	O4'-C1'-N9	6.23	113.18	108.20
36	1	1489	A	N1-C6-N6	6.22	122.33	118.60
36	1	1891	A	C2-N3-C4	-6.22	107.49	110.60
36	1	1116	G	OP2-P-O3'	6.22	118.89	105.20
36	5	2849	C	N1-C2-O2	-6.22	115.17	118.90
1	2	1749	A	N1-C6-N6	6.22	122.33	118.60
36	5	770	G	O4'-C1'-N9	6.22	113.17	108.20
36	5	1370	G	N1-C2-N2	-6.22	110.60	116.20
36	5	1513	G	N9-C4-C5	6.22	107.89	105.40
1	2	1273	G	O4'-C1'-N9	6.21	113.17	108.20
36	1	347	G	C5-C6-O6	-6.21	124.87	128.60
36	1	633	C	C6-N1-C2	6.21	122.79	120.30
36	5	2942	C	N3-C4-N4	6.21	122.35	118.00
1	2	1782	A	C8-N9-C4	-6.21	103.31	105.80
36	5	2375	G	N3-C2-N2	6.21	124.25	119.90
36	5	2816	G	C6-C5-N7	6.21	134.13	130.40
36	1	716	A	C4-C5-N7	6.21	113.81	110.70
1	6	431	C	N1-C2-O2	6.21	122.63	118.90
36	5	1872	C	C4-C5-C6	6.21	120.51	117.40
36	1	1610	G	C8-N9-C4	-6.21	103.92	106.40
36	5	32	U	N1-C2-N3	6.21	118.63	114.90
36	5	995	U	C5-C6-N1	-6.21	119.60	122.70
36	1	1307	G	P-O3'-C3'	6.21	127.15	119.70
1	6	1269	U	N3-C2-O2	-6.21	117.86	122.20
36	1	913	A	C5-C6-N6	-6.20	118.74	123.70
36	5	3060	C	N3-C4-N4	6.20	122.34	118.00
36	5	1666	G	C5-C6-O6	6.20	132.32	128.60
36	5	824	C	C6-N1-C2	-6.20	117.82	120.30
36	1	953	G	C4-N9-C1'	-6.20	118.44	126.50
36	1	1376	C	C4-C5-C6	6.20	120.50	117.40
36	5	104	G	N1-C6-O6	6.20	123.62	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2300	G	N3-C2-N2	6.20	124.24	119.90
37	7	98	C	O5'-P-OP1	6.20	118.14	110.70
36	1	200	C	N3-C2-O2	-6.20	117.56	121.90
49	m3	47	ALA	C-N-CD	6.20	141.41	128.40
36	1	3306	U	C5-C4-O4	6.20	129.62	125.90
36	5	878	G	OP1-P-O3'	6.20	118.83	105.20
36	5	1300	G	C5-C6-O6	-6.20	124.88	128.60
1	6	1726	G	OP2-P-O3'	6.19	118.83	105.20
36	5	111	C	C6-N1-C2	6.19	122.78	120.30
36	5	3010	U	N3-C4-O4	-6.19	115.06	119.40
36	1	1445	U	N1-C2-O2	-6.19	118.47	122.80
36	1	2606	G	N1-C2-N2	-6.19	110.63	116.20
36	1	2870	C	N3-C4-C5	6.19	124.38	121.90
36	5	2424	A	N1-C6-N6	6.19	122.31	118.60
36	1	3092	C	O4'-C1'-N1	6.19	113.15	108.20
36	1	905	U	N1-C2-O2	-6.19	118.47	122.80
36	1	1507	G	C4-C5-C6	6.19	122.51	118.80
36	5	1586	G	N3-C4-N9	6.19	129.71	126.00
1	2	142	G	N3-C2-N2	-6.18	115.57	119.90
36	1	3175	U	O5'-P-OP2	-6.18	100.13	105.70
36	5	359	U	N1-C2-O2	-6.18	118.47	122.80
36	5	3060	C	C5-C4-N4	-6.18	115.87	120.20
36	5	399	A	O5'-P-OP1	-6.18	100.14	105.70
37	7	19	C	N3-C4-C5	6.18	124.37	121.90
38	8	80	A	C8-N9-C4	-6.18	103.33	105.80
1	2	619	A	OP2-P-O3'	6.18	118.80	105.20
36	1	1164	G	C5-C6-O6	6.18	132.31	128.60
36	1	2257	C	C6-N1-C2	-6.18	117.83	120.30
1	6	55	A	C8-N9-C4	6.18	108.27	105.80
36	5	1379	G	N3-C2-N2	6.18	124.23	119.90
36	1	2787	G	C2-N3-C4	6.18	114.99	111.90
36	5	1405	U	C5-C6-N1	-6.18	119.61	122.70
36	5	217	U	OP1-P-O3'	6.17	118.79	105.20
36	5	1379	G	C5-C6-O6	6.17	132.31	128.60
36	1	2369	G	N3-C4-C5	-6.17	125.51	128.60
36	5	1115	G	N3-C4-C5	-6.17	125.51	128.60
36	5	1426	C	C5-C4-N4	-6.17	115.88	120.20
1	2	1455	G	C4-C5-N7	-6.17	108.33	110.80
36	1	1447	G	O5'-P-OP2	-6.17	100.15	105.70
36	1	3041	U	N1-C2-O2	-6.17	118.48	122.80
36	5	2524	A	N9-C1'-C2'	6.17	122.02	114.00
36	5	350	C	O4'-C1'-N1	-6.17	103.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	892	U	N3-C4-C5	6.17	118.30	114.60
36	1	3218	A	P-O3'-C3'	6.16	127.09	119.70
1	6	163	G	C8-N9-C4	-6.16	103.94	106.40
1	6	297	U	N3-C4-O4	6.16	123.71	119.40
36	5	83	U	N3-C2-O2	-6.16	117.89	122.20
36	5	2295	A	N9-C4-C5	-6.16	103.34	105.80
77	q1	9	ARG	NE-CZ-NH2	-6.16	117.22	120.30
36	1	1429	G	N3-C4-N9	6.16	129.69	126.00
25	d3	33	LEU	CA-CB-CG	-6.16	101.14	115.30
1	6	1614	A	C5-N7-C8	-6.16	100.82	103.90
36	5	1371	G	C4-C5-N7	-6.16	108.34	110.80
36	1	867	G	N1-C2-N2	6.15	121.74	116.20
36	5	63	A	N1-C6-N6	6.15	122.29	118.60
36	1	1124	U	C5-C6-N1	6.15	125.78	122.70
36	1	2193	U	C5-C6-N1	-6.15	119.62	122.70
43	l6	30	LEU	CA-CB-CG	6.15	129.45	115.30
1	2	765	G	O4'-C1'-N9	-6.15	103.28	108.20
36	1	765	C	N3-C2-O2	-6.15	117.59	121.90
36	1	817	A	OP1-P-O3'	6.15	118.73	105.20
38	4	148	G	C5-C6-O6	6.15	132.29	128.60
36	5	573	C	N3-C4-C5	-6.15	119.44	121.90
36	5	2307	G	N3-C4-C5	-6.15	125.53	128.60
1	6	1478	G	C6-C5-N7	-6.15	126.71	130.40
36	1	1935	G	N1-C6-O6	-6.15	116.21	119.90
36	5	283	G	N1-C6-O6	6.15	123.59	119.90
1	6	637	C	O5'-P-OP2	-6.15	100.17	105.70
36	5	3316	A	N1-C6-N6	6.15	122.29	118.60
36	5	3049	A	C8-N9-C4	6.14	108.26	105.80
36	1	398	A	C5-C6-N6	-6.14	118.79	123.70
1	6	794	U	O4'-C1'-N1	6.14	113.11	108.20
36	5	40	A	O5'-P-OP1	-6.14	100.17	105.70
36	5	150	A	C5-C6-N6	-6.14	118.79	123.70
36	1	3050	U	N1-C2-O2	6.14	127.10	122.80
36	1	1313	G	C6-C5-N7	-6.14	126.72	130.40
36	1	2135	U	N1-C2-O2	6.14	127.10	122.80
1	6	542	A	N1-C6-N6	6.14	122.28	118.60
36	5	341	G	C8-N9-C4	-6.14	103.94	106.40
36	5	1116	G	N9-C4-C5	6.14	107.86	105.40
1	2	402	C	N1-C2-O2	-6.14	115.22	118.90
1	2	1782	A	N9-C4-C5	6.14	108.25	105.80
36	1	805	G	O5'-P-OP1	6.14	118.06	110.70
36	1	2920	U	N3-C4-C5	6.14	118.28	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2983	C	O5'-P-OP1	-6.14	100.18	105.70
37	3	94	C	N1-C2-O2	-6.13	115.22	118.90
36	1	907	G	O4'-C1'-N9	6.13	113.11	108.20
36	1	1351	U	N3-C2-O2	-6.13	117.91	122.20
36	5	2877	G	N1-C2-N2	-6.13	110.68	116.20
36	1	2309	A	N1-C6-N6	6.13	122.28	118.60
36	5	2700	G	C4-C5-N7	6.13	113.25	110.80
36	1	1161	G	N1-C6-O6	-6.13	116.22	119.90
36	5	2211	U	C6-N1-C2	-6.13	117.32	121.00
37	7	41	G	N9-C4-C5	-6.13	102.95	105.40
1	2	610	G	C5-C6-O6	-6.12	124.92	128.60
36	1	859	G	N3-C4-N9	6.12	129.68	126.00
1	2	1654	G	C6-N1-C2	-6.12	121.43	125.10
1	6	1280	C	N3-C4-C5	-6.12	119.45	121.90
36	5	613	G	N9-C4-C5	6.12	107.85	105.40
36	5	3098	G	O5'-P-OP2	-6.12	100.19	105.70
36	5	3185	U	O5'-P-OP2	-6.12	100.19	105.70
36	1	1420	C	C5-C4-N4	6.12	124.48	120.20
36	1	2370	G	C5-C6-N1	6.12	114.56	111.50
36	1	2572	C	C6-N1-C1'	-6.12	113.45	120.80
1	6	310	C	N1-C2-O2	-6.12	115.23	118.90
36	5	1057	A	C4-C5-N7	6.12	113.76	110.70
36	5	1115	G	N7-C8-N9	6.12	116.16	113.10
36	5	516	A	N1-C6-N6	6.12	122.27	118.60
36	1	953	G	N3-C4-N9	-6.12	122.33	126.00
36	5	922	U	C4-C5-C6	6.12	123.37	119.70
36	5	2145	A	C6-N1-C2	-6.12	114.93	118.60
1	2	145	A	C8-N9-C4	-6.12	103.35	105.80
1	6	1172	G	C8-N9-C4	-6.12	103.95	106.40
36	5	3174	A	C5-N7-C8	-6.12	100.84	103.90
36	1	2821	C	N3-C2-O2	6.11	126.18	121.90
36	5	218	G	N1-C6-O6	-6.11	116.23	119.90
41	L4	150	LEU	CA-CB-CG	6.11	129.35	115.30
36	5	520	U	N1-C2-O2	-6.11	118.52	122.80
1	2	1596	C	N1-C2-O2	6.11	122.56	118.90
36	1	1450	G	C8-N9-C4	6.11	108.84	106.40
37	7	21	G	C8-N9-C4	6.11	108.84	106.40
36	1	2392	C	C5-C4-N4	-6.11	115.93	120.20
47	m0	167	LEU	CA-CB-CG	6.11	129.34	115.30
36	1	99	A	C5'-C4'-O4'	6.10	116.42	109.10
36	1	1000	C	C5-C4-N4	-6.10	115.93	120.20
36	5	1665	C	N3-C4-C5	6.10	124.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2816	G	OP2-P-O3'	6.10	118.63	105.20
36	1	361	A	N1-C6-N6	-6.10	114.94	118.60
36	1	2687	G	C5-C6-O6	6.10	132.26	128.60
36	5	927	C	C2-N3-C4	-6.10	116.85	119.90
36	1	407	A	O5'-P-OP2	-6.10	100.21	105.70
36	1	2831	G	N1-C6-O6	6.10	123.56	119.90
36	5	705	A	O5'-P-OP2	-6.10	100.21	105.70
36	1	2152	A	C4-C5-N7	-6.09	107.65	110.70
36	1	2609	A	N1-C6-N6	-6.09	114.94	118.60
36	1	2826	U	N3-C4-C5	6.09	118.26	114.60
36	1	979	U	N3-C4-C5	-6.09	110.94	114.60
36	5	2992	U	N1-C2-O2	6.09	127.06	122.80
1	2	334	G	C2-N3-C4	-6.09	108.86	111.90
1	2	1456	C	N3-C2-O2	-6.09	117.64	121.90
36	1	2920	U	C5-C6-N1	-6.09	119.66	122.70
1	6	402	C	C6-N1-C2	6.09	122.74	120.30
36	5	150	A	N1-C6-N6	6.09	122.25	118.60
36	5	574	U	N1-C2-O2	-6.09	118.54	122.80
36	5	3049	A	C6-N1-C2	6.09	122.25	118.60
36	5	425	G	C8-N9-C4	6.09	108.83	106.40
36	1	922	U	N3-C2-O2	-6.09	117.94	122.20
36	1	947	G	N3-C2-N2	6.09	124.16	119.90
36	1	3207	U	C2-N1-C1'	-6.09	110.40	117.70
36	5	201	A	OP1-P-OP2	-6.09	110.47	119.60
54	m8	178	ARG	NE-CZ-NH2	-6.09	117.26	120.30
36	5	1886	A	N1-C6-N6	6.08	122.25	118.60
1	6	1755	A	C4-C5-N7	6.08	113.74	110.70
36	5	3123	A	C8-N9-C4	6.08	108.23	105.80
36	1	1820	U	P-O3'-C3'	6.08	127.00	119.70
36	1	2216	G	C4-C5-N7	-6.08	108.37	110.80
36	1	2281	A	N9-C4-C5	-6.08	103.37	105.80
36	1	2293	C	N3-C4-N4	6.08	122.25	118.00
36	1	3214	U	N1-C2-N3	6.08	118.55	114.90
1	2	1559	A	C5-N7-C8	-6.08	100.86	103.90
36	1	2115	G	C5-C6-O6	-6.07	124.95	128.60
36	1	2434	U	C5-C6-N1	-6.07	119.66	122.70
36	1	3319	U	P-O3'-C3'	6.07	126.99	119.70
36	1	2314	U	C5-C4-O4	-6.07	122.26	125.90
36	1	923	C	C6-N1-C2	6.07	122.73	120.30
36	5	354	U	N1-C2-O2	6.07	127.05	122.80
36	1	1308	A	O5'-P-OP1	6.07	117.98	110.70
36	5	426	G	C6-C5-N7	6.07	134.04	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	359	U	C5-C6-N1	-6.07	119.67	122.70
36	1	2586	G	C5-C6-O6	-6.07	124.96	128.60
36	1	2370	G	OP1-P-OP2	6.06	128.70	119.60
36	1	2618	G	C5-C6-N1	6.06	114.53	111.50
36	1	2632	G	N1-C6-O6	-6.06	116.26	119.90
36	5	2732	G	N3-C4-C5	-6.06	125.57	128.60
37	7	115	G	C8-N9-C4	-6.06	103.97	106.40
36	5	1484	U	C2-N3-C4	-6.06	123.36	127.00
50	m4	135	LEU	CA-CB-CG	6.06	129.24	115.30
36	1	785	G	N1-C6-O6	-6.06	116.26	119.90
36	1	1371	G	N1-C6-O6	-6.06	116.27	119.90
36	1	2649	A	C8-N9-C4	6.06	108.22	105.80
36	5	2800	G	N3-C4-N9	-6.06	122.36	126.00
36	1	60	A	N1-C6-N6	6.06	122.23	118.60
36	1	2522	G	C8-N9-C1'	-6.06	119.12	127.00
36	5	3154	C	C2-N3-C4	6.06	122.93	119.90
36	5	350	C	C6-N1-C2	-6.06	117.88	120.30
36	5	2830	G	N1-C2-N3	6.05	127.53	123.90
36	1	804	C	C2-N1-C1'	-6.05	112.14	118.80
36	5	2142	A	C5-C6-N1	6.05	120.73	117.70
36	1	2389	C	C5-C6-N1	-6.05	117.97	121.00
1	6	371	G	N1-C6-O6	6.05	123.53	119.90
1	6	977	A	N1-C6-N6	6.05	122.23	118.60
36	5	972	A	O5'-P-OP2	6.05	117.96	110.70
1	2	1761	U	P-O3'-C3'	6.05	126.96	119.70
36	1	3109	G	C5-N7-C8	6.05	107.32	104.30
36	5	702	C	C6-N1-C2	-6.05	117.88	120.30
36	5	1162	U	C2-N3-C4	-6.05	123.37	127.00
38	8	80	A	N7-C8-N9	6.05	116.82	113.80
36	1	2719	U	C2-N1-C1'	-6.05	110.44	117.70
36	5	1586	G	N3-C4-C5	-6.05	125.58	128.60
36	1	1724	U	O4'-C1'-N1	6.04	113.04	108.20
36	1	645	A	C5-C6-N1	6.04	120.72	117.70
36	1	1907	C	C2-N3-C4	6.04	122.92	119.90
36	1	2940	A	N1-C2-N3	6.04	132.32	129.30
36	5	589	A	N1-C6-N6	6.04	122.23	118.60
36	5	2278	C	N3-C4-N4	-6.04	113.77	118.00
36	5	2917	G	C8-N9-C1'	-6.04	119.14	127.00
36	1	1389	G	C4-C5-N7	6.04	113.22	110.80
36	1	2958	A	C5-C6-N1	6.04	120.72	117.70
1	6	696	C	C2-N1-C1'	-6.04	112.15	118.80
36	5	39	A	C5-C6-N6	-6.04	118.87	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	974	G	C4-N9-C1'	6.04	134.35	126.50
36	5	3185	U	C2-N3-C4	-6.04	123.38	127.00
1	6	349	U	O5'-P-OP2	-6.04	100.26	105.70
36	5	2707	C	O5'-P-OP2	-6.04	100.27	105.70
36	5	3343	G	N3-C4-N9	6.04	129.62	126.00
1	6	1522	U	O5'-P-OP2	-6.04	100.27	105.70
36	1	1499	C	N1-C2-O2	-6.03	115.28	118.90
36	1	2400	G	C2-N3-C4	-6.03	108.88	111.90
36	1	2909	U	N1-C2-O2	-6.03	118.58	122.80
36	5	2614	G	C5-N7-C8	6.03	107.32	104.30
36	5	584	G	C5-C6-O6	6.03	132.22	128.60
36	1	1604	G	C4-N9-C1'	6.03	134.34	126.50
36	5	1520	G	C2-N3-C4	6.03	114.92	111.90
36	1	797	U	C5-C6-N1	-6.03	119.69	122.70
21	c9	57	ARG	NE-CZ-NH1	6.03	123.31	120.30
36	1	2977	G	O5'-P-OP1	-6.03	100.28	105.70
36	1	228	U	N3-C2-O2	-6.02	117.98	122.20
36	1	1556	C	N1-C2-O2	6.02	122.51	118.90
36	1	2403	G	N3-C2-N2	6.02	124.12	119.90
36	1	3306	U	C2-N3-C4	-6.02	123.39	127.00
1	6	144	U	N1-C2-O2	6.02	127.02	122.80
36	1	847	A	N9-C4-C5	-6.02	103.39	105.80
1	6	1489	U	C5-C4-O4	-6.02	122.29	125.90
36	1	398	A	C6-C5-N7	-6.02	128.09	132.30
36	1	410	U	N1-C2-O2	-6.02	118.59	122.80
36	1	2216	G	C5-C6-O6	6.02	132.21	128.60
36	1	2388	U	N1-C2-O2	-6.02	118.59	122.80
36	1	3344	A	O4'-C1'-N9	6.02	113.02	108.20
1	6	1514	U	N3-C4-O4	-6.02	115.19	119.40
36	5	2618	G	C5-C6-O6	-6.02	124.99	128.60
36	5	3173	G	N1-C6-O6	6.02	123.51	119.90
36	1	972	A	N7-C8-N9	-6.02	110.79	113.80
36	5	2698	G	C8-N9-C4	6.02	108.81	106.40
36	5	2817	A	OP1-P-OP2	-6.02	110.58	119.60
36	1	953	G	C8-N9-C1'	6.01	134.82	127.00
1	6	1473	U	N1-C2-N3	6.01	118.51	114.90
36	5	880	G	C5-C6-O6	-6.01	124.99	128.60
36	5	2375	G	O5'-P-OP2	-6.01	100.29	105.70
36	1	940	G	N1-C6-O6	-6.01	116.29	119.90
36	1	2418	G	OP1-P-O3'	6.01	118.42	105.20
1	6	1783	C	O5'-P-OP2	-6.01	100.29	105.70
36	5	1050	U	N3-C2-O2	-6.01	117.99	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2801	A	N1-C2-N3	-6.01	126.29	129.30
1	2	1274	C	N3-C2-O2	-6.01	117.69	121.90
36	1	92	G	C5-C6-N1	6.01	114.50	111.50
36	1	2418	G	C2-N3-C4	6.01	114.91	111.90
12	c0	97	PRO	N-CA-CB	6.01	110.51	103.30
36	5	3140	G	C8-N9-C1'	-6.01	119.19	127.00
73	O7	65	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	6	371	G	C5-C6-O6	-6.01	125.00	128.60
36	5	2915	U	C2-N3-C4	-6.01	123.40	127.00
36	1	2293	C	C5-C4-N4	-6.00	116.00	120.20
1	6	942	G	N1-C6-O6	-6.00	116.30	119.90
37	7	110	G	O5'-P-OP2	-6.00	100.30	105.70
1	2	1119	G	N1-C6-O6	-6.00	116.30	119.90
36	1	805	G	C5-C6-N1	6.00	114.50	111.50
52	m6	37	ARG	NE-CZ-NH2	-6.00	117.30	120.30
36	1	784	A	N1-C6-N6	6.00	122.20	118.60
1	2	1119	G	C5-C6-O6	6.00	132.20	128.60
36	1	388	G	C8-N9-C4	-6.00	104.00	106.40
36	1	1125	U	OP1-P-OP2	-6.00	110.60	119.60
36	5	2623	G	C8-N9-C4	6.00	108.80	106.40
36	1	2679	A	N1-C6-N6	6.00	122.20	118.60
36	5	35	A	N1-C6-N6	6.00	122.20	118.60
36	5	1130	A	C2-N3-C4	6.00	113.60	110.60
36	1	3002	C	N3-C4-C5	5.99	124.30	121.90
36	1	1329	U	C6-N1-C2	-5.99	117.41	121.00
36	1	2788	C	O5'-P-OP2	-5.99	100.31	105.70
36	5	642	U	O5'-P-OP2	-5.99	100.31	105.70
36	1	635	G	N1-C6-O6	5.99	123.49	119.90
36	1	2864	A	C8-N9-C4	-5.99	103.41	105.80
12	c0	83	PRO	N-CA-CB	5.99	110.49	103.30
36	5	818	C	N1-C2-O2	-5.99	115.31	118.90
36	5	1878	G	C8-N9-C1'	-5.99	119.22	127.00
36	5	2345	A	C8-N9-C4	5.99	108.19	105.80
36	1	957	C	N3-C2-O2	5.99	126.09	121.90
36	1	1166	G	N1-C6-O6	5.99	123.49	119.90
36	1	2142	A	OP1-P-O3'	5.99	118.37	105.20
36	5	1284	C	C5-C6-N1	5.99	123.99	121.00
36	1	368	G	N1-C2-N2	-5.98	110.82	116.20
36	1	768	C	C6-N1-C2	-5.98	117.91	120.30
36	1	1351	U	N1-C2-O2	5.98	126.99	122.80
36	5	2650	U	C2-N3-C4	-5.98	123.41	127.00
36	1	85	A	C2-N3-C4	-5.98	107.61	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1064	A	N9-C4-C5	-5.98	103.41	105.80
36	5	1410	U	O5'-P-OP2	-5.98	100.32	105.70
36	5	1506	A	N9-C4-C5	5.98	108.19	105.80
37	7	94	C	N3-C4-C5	5.98	124.29	121.90
1	6	321	C	C6-N1-C2	-5.98	117.91	120.30
1	6	1503	A	O4'-C1'-N9	5.98	112.98	108.20
36	5	641	C	OP1-P-O3'	5.98	118.35	105.20
36	5	2794	G	C5-C6-N1	5.98	114.49	111.50
36	5	2995	A	N7-C8-N9	-5.98	110.81	113.80
1	2	1092	A	N1-C6-N6	5.98	122.19	118.60
36	1	973	A	C8-N9-C4	-5.98	103.41	105.80
36	1	1314	C	C6-N1-C2	-5.98	117.91	120.30
36	5	1163	A	O5'-P-OP2	-5.98	100.32	105.70
36	5	2938	G	OP1-P-OP2	5.98	128.56	119.60
36	1	648	C	OP1-P-OP2	5.98	128.56	119.60
36	5	1890	U	C5-C6-N1	-5.98	119.71	122.70
36	5	2392	C	C6-N1-C2	5.98	122.69	120.30
1	2	142	G	N1-C6-O6	5.97	123.48	119.90
36	5	960	U	N1-C2-O2	5.97	126.98	122.80
36	5	1200	A	C4-C5-C6	5.97	119.99	117.00
36	5	3215	A	C2-N3-C4	-5.97	107.61	110.60
1	2	543	C	N3-C2-O2	-5.97	117.72	121.90
36	1	766	U	O5'-P-OP1	-5.97	100.33	105.70
36	5	1365	G	N1-C2-N2	-5.97	110.83	116.20
36	5	2401	A	C2-N3-C4	5.97	113.58	110.60
36	1	747	A	N1-C6-N6	5.96	122.18	118.60
36	5	861	C	N3-C2-O2	5.96	126.08	121.90
36	5	3293	U	C6-N1-C2	5.96	124.58	121.00
1	6	1749	A	N1-C6-N6	5.96	122.18	118.60
36	1	2634	U	N1-C2-N3	5.96	118.48	114.90
1	6	767	U	C5-C4-O4	5.96	129.48	125.90
36	5	3107	U	N3-C2-O2	-5.96	118.03	122.20
36	1	817	A	C6-N1-C2	-5.96	115.03	118.60
36	1	1523	U	N1-C2-O2	-5.96	118.63	122.80
36	5	636	C	C5-C6-N1	-5.96	118.02	121.00
36	5	1154	A	C2-N3-C4	5.96	113.58	110.60
36	5	1605	A	O4'-C1'-N9	5.96	112.97	108.20
36	5	2278	C	N1-C2-O2	5.96	122.47	118.90
36	5	2396	G	N9-C4-C5	5.96	107.78	105.40
36	1	2409	G	N3-C2-N2	5.96	124.07	119.90
36	1	3143	C	N3-C2-O2	5.96	126.07	121.90
36	1	1192	C	N1-C2-O2	5.95	122.47	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	861	C	N3-C4-N4	5.95	122.17	118.00
36	5	2849	C	OP1-P-OP2	5.95	128.53	119.60
52	m6	84	LEU	CB-CG-CD1	-5.95	100.88	111.00
36	1	1493	G	O4'-C1'-N9	5.95	112.96	108.20
36	1	51	A	C5-C6-N6	-5.95	118.94	123.70
37	7	35	C	C6-N1-C2	5.95	122.68	120.30
36	1	196	G	N1-C6-O6	5.95	123.47	119.90
36	1	922	U	N3-C4-O4	-5.95	115.24	119.40
36	1	61	A	C2-N3-C4	-5.94	107.63	110.60
36	5	2719	U	C6-N1-C1'	5.94	129.52	121.20
36	1	1175	C	C5-C6-N1	-5.94	118.03	121.00
1	6	151	G	N3-C4-N9	-5.94	122.43	126.00
64	n8	73	LEU	CA-CB-CG	5.94	128.97	115.30
36	5	2928	C	C4-C5-C6	5.94	120.37	117.40
36	1	659	G	C6-C5-N7	-5.94	126.84	130.40
36	5	2285	C	C5-C6-N1	5.94	123.97	121.00
37	3	73	C	N1-C2-O2	5.94	122.46	118.90
45	l8	69	LEU	CA-CB-CG	5.94	128.96	115.30
36	1	1151	U	C6-N1-C2	-5.94	117.44	121.00
36	5	214	G	C8-N9-C4	5.94	108.78	106.40
1	2	1291	G	C2-N3-C4	-5.93	108.93	111.90
36	1	620	U	N1-C1'-C2'	5.93	121.72	114.00
36	5	1883	A	N1-C6-N6	-5.93	115.04	118.60
36	5	2377	G	N1-C6-O6	-5.93	116.34	119.90
36	1	3190	C	N3-C4-C5	5.93	124.27	121.90
36	1	622	A	N1-C6-N6	5.93	122.16	118.60
36	1	2606	G	N9-C4-C5	-5.93	103.03	105.40
36	1	2665	U	O5'-P-OP1	-5.93	100.36	105.70
1	6	102	U	O5'-P-OP1	-5.93	100.36	105.70
36	1	324	A	N3-C4-C5	-5.93	122.65	126.80
36	1	960	U	C2-N3-C4	-5.93	123.44	127.00
36	1	1494	U	N3-C4-O4	-5.93	115.25	119.40
36	1	2883	U	C5-C6-N1	5.93	125.66	122.70
37	3	88	G	C4-C5-N7	-5.93	108.43	110.80
36	1	2906	C	C2-N3-C4	-5.93	116.94	119.90
36	5	719	U	N3-C2-O2	-5.93	118.05	122.20
36	5	3092	C	O4'-C1'-N1	5.93	112.94	108.20
36	5	46	U	N1-C2-O2	5.92	126.95	122.80
78	Q2	87	ARG	NE-CZ-NH1	-5.92	117.34	120.30
36	5	1834	U	C6-N1-C2	-5.92	117.45	121.00
36	1	3083	G	N3-C4-C5	-5.92	125.64	128.60
36	5	389	A	C8-N9-C4	-5.92	103.43	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	102	C	N1-C2-O2	-5.92	115.35	118.90
36	1	3055	U	C2-N1-C1'	5.92	124.80	117.70
36	1	3101	G	C8-N9-C4	5.92	108.77	106.40
56	N0	115	ARG	NE-CZ-NH1	5.92	123.26	120.30
36	5	1083	G	OP1-P-OP2	5.92	128.47	119.60
36	5	3204	C	N3-C4-C5	5.92	124.27	121.90
36	1	1838	G	N9-C4-C5	-5.91	103.03	105.40
36	1	3264	G	O5'-P-OP1	-5.91	100.38	105.70
1	6	93	A	N9-C4-C5	-5.91	103.44	105.80
36	1	1173	U	C5-C6-N1	-5.91	119.74	122.70
36	1	2320	A	C2-N3-C4	-5.91	107.64	110.60
36	5	3060	C	N3-C2-O2	5.91	126.04	121.90
36	5	2930	A	N9-C4-C5	5.91	108.16	105.80
36	1	33	G	C8-N9-C4	-5.91	104.04	106.40
36	1	806	A	C5-C6-N6	-5.91	118.97	123.70
36	5	92	G	C5-C6-N1	5.91	114.45	111.50
36	1	2824	G	C8-N9-C4	-5.91	104.04	106.40
36	1	3344	A	C4-C5-N7	5.91	113.65	110.70
36	5	641	C	N1-C2-O2	-5.91	115.36	118.90
36	5	869	G	N1-C6-O6	-5.91	116.36	119.90
1	2	453	U	C5-C4-O4	5.90	129.44	125.90
36	1	2551	U	N1-C2-N3	5.90	118.44	114.90
36	5	631	U	N1-C2-N3	5.90	118.44	114.90
36	5	824	C	N3-C2-O2	-5.90	117.77	121.90
36	5	2928	C	N3-C2-O2	-5.90	117.77	121.90
36	1	3143	C	N1-C2-O2	-5.90	115.36	118.90
1	6	387	A	N1-C6-N6	-5.90	115.06	118.60
52	m6	128	ARG	NE-CZ-NH2	-5.90	117.35	120.30
36	1	637	C	C2-N3-C4	-5.90	116.95	119.90
36	1	2977	G	C5-C6-N1	5.90	114.45	111.50
1	2	1773	C	C5-C6-N1	5.90	123.95	121.00
38	4	94	C	N3-C4-C5	5.90	124.26	121.90
36	5	1390	A	C5-C6-N6	5.90	128.42	123.70
36	1	391	A	N1-C6-N6	-5.89	115.06	118.60
36	1	859	G	C8-N9-C1'	-5.89	119.34	127.00
36	1	2404	A	OP1-P-OP2	-5.89	110.76	119.60
36	5	2171	G	N1-C6-O6	-5.89	116.36	119.90
36	5	2350	C	C2-N3-C4	-5.89	116.95	119.90
36	1	3178	A	N1-C6-N6	5.89	122.14	118.60
54	M8	179	ARG	NE-CZ-NH2	-5.89	117.35	120.30
36	1	979	U	C5-C4-O4	5.89	129.43	125.90
36	1	2409	G	N3-C4-C5	-5.89	125.65	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2723	U	N3-C2-O2	5.89	126.32	122.20
36	5	2730	G	N1-C6-O6	5.89	123.44	119.90
36	1	114	A	N1-C6-N6	5.89	122.13	118.60
36	1	3112	G	C5-C6-O6	-5.89	125.07	128.60
36	5	2144	A	O4'-C1'-N9	5.89	112.91	108.20
36	1	2415	C	C5-C6-N1	-5.89	118.06	121.00
36	1	1048	A	N1-C2-N3	-5.89	126.36	129.30
36	1	949	C	C6-N1-C2	-5.88	117.95	120.30
36	1	2846	U	N1-C2-N3	5.88	118.43	114.90
36	1	2886	U	C5-C4-O4	-5.88	122.37	125.90
36	1	2820	A	C2-N3-C4	5.88	113.54	110.60
36	5	2408	U	N1-C2-N3	5.88	118.43	114.90
38	4	30	C	C5-C4-N4	5.88	124.31	120.20
36	5	344	A	C8-N9-C4	5.88	108.15	105.80
36	5	2514	U	O5'-P-OP1	-5.88	100.41	105.70
36	5	2658	G	C8-N9-C4	5.88	108.75	106.40
36	5	3097	C	C6-N1-C2	-5.88	117.95	120.30
36	1	652	G	N3-C2-N2	5.88	124.01	119.90
36	5	35	A	C2-N3-C4	-5.88	107.66	110.60
37	7	101	G	C8-N9-C4	5.88	108.75	106.40
37	7	120	C	C5-C6-N1	-5.88	118.06	121.00
1	6	1000	C	N3-C2-O2	-5.88	117.79	121.90
36	1	517	G	N9-C4-C5	5.87	107.75	105.40
36	5	1141	C	N1-C2-O2	-5.87	115.38	118.90
36	5	2777	G	C5-C6-O6	5.87	132.12	128.60
38	8	32	C	N3-C2-O2	5.87	126.01	121.90
36	1	2385	G	C8-N9-C4	5.87	108.75	106.40
36	5	2796	G	O5'-P-OP2	-5.87	100.42	105.70
37	7	67	G	N3-C2-N2	-5.87	115.79	119.90
36	1	3010	U	N3-C2-O2	-5.87	118.09	122.20
1	6	1470	C	N1-C2-O2	-5.87	115.38	118.90
36	5	2293	C	C2-N1-C1'	5.87	125.26	118.80
36	1	910	G	C5-C6-O6	5.87	132.12	128.60
36	1	1307	G	OP1-P-O3'	5.87	118.11	105.20
36	1	2149	A	C5-C6-N1	-5.87	114.77	117.70
36	1	3081	C	N3-C4-N4	-5.87	113.89	118.00
36	1	3209	A	C4-C5-N7	5.87	113.63	110.70
20	c8	116	LEU	CA-CB-CG	5.87	128.80	115.30
36	5	2855	U	C5-C6-N1	5.87	125.64	122.70
36	5	3374	U	N3-C4-O4	-5.87	115.29	119.40
37	3	81	U	C6-N1-C2	5.87	124.52	121.00
36	1	61	A	N1-C6-N6	5.87	122.12	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2340	U	N3-C4-O4	-5.87	115.29	119.40
36	1	3055	U	C6-N1-C1'	-5.87	112.99	121.20
1	6	402	C	O4'-C1'-N1	5.87	112.89	108.20
36	5	2620	G	C2-N3-C4	5.87	114.83	111.90
36	1	1152	G	C5-C6-O6	-5.86	125.08	128.60
36	1	2986	U	C5-C6-N1	-5.86	119.77	122.70
1	6	1432	U	O4'-C1'-N1	5.86	112.89	108.20
18	C6	28	LEU	CA-CB-CG	5.86	128.78	115.30
36	1	2306	C	C5-C4-N4	5.86	124.30	120.20
1	6	3	U	C6-N1-C2	5.86	124.52	121.00
36	5	75	G	O5'-P-OP2	-5.86	100.43	105.70
36	1	1349	G	C8-N9-C1'	-5.86	119.39	127.00
36	1	2391	G	N1-C2-N2	-5.86	110.93	116.20
1	2	554	C	C2-N1-C1'	5.86	125.24	118.80
36	1	1305	U	N1-C2-O2	5.86	126.90	122.80
37	3	85	G	OP2-P-O3'	5.86	118.08	105.20
37	3	97	A	N9-C4-C5	5.86	108.14	105.80
1	6	1596	C	C5-C4-N4	5.86	124.30	120.20
36	5	947	G	N1-C6-O6	-5.86	116.39	119.90
36	5	1208	U	N3-C4-O4	-5.86	115.30	119.40
36	5	1412	G	N3-C4-N9	-5.86	122.49	126.00
36	5	3093	C	C2-N1-C1'	-5.85	112.36	118.80
36	1	694	C	N3-C4-C5	5.85	124.24	121.90
36	1	1555	U	C5-C6-N1	-5.85	119.77	122.70
1	6	3	U	C5-C6-N1	-5.85	119.77	122.70
36	5	1338	C	N1-C2-O2	-5.85	115.39	118.90
36	5	1429	G	N3-C2-N2	5.85	124.00	119.90
36	5	2930	A	C5-C6-N1	5.85	120.62	117.70
1	2	1012	U	C2-N3-C4	5.85	130.51	127.00
1	2	1280	C	N3-C4-C5	-5.85	119.56	121.90
36	1	2979	U	C2-N3-C4	-5.85	123.49	127.00
36	5	840	C	N3-C2-O2	-5.85	117.81	121.90
36	1	1494	U	C2-N3-C4	-5.85	123.49	127.00
1	6	371	G	C6-C5-N7	-5.85	126.89	130.40
1	6	965	U	N1-C2-O2	5.85	126.89	122.80
36	5	1159	A	N1-C2-N3	-5.85	126.38	129.30
36	5	2730	G	C5-C6-O6	-5.85	125.09	128.60
36	1	2335	G	C8-N9-C4	5.85	108.74	106.40
36	1	905	U	N1-C2-N3	5.84	118.41	114.90
36	1	1364	C	C2-N3-C4	-5.84	116.98	119.90
38	4	21	C	C6-N1-C2	5.84	122.64	120.30
36	1	397	A	N1-C6-N6	-5.84	115.09	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1380	G	C2-N3-C4	-5.84	108.98	111.90
1	6	1097	U	P-O3'-C3'	5.84	126.71	119.70
36	5	1615	C	O5'-P-OP1	-5.84	100.44	105.70
36	1	3096	C	O5'-P-OP1	-5.84	100.44	105.70
36	1	3344	A	N1-C2-N3	5.84	132.22	129.30
38	4	103	G	N3-C4-C5	-5.84	125.68	128.60
36	5	1303	A	O5'-P-OP1	-5.84	100.44	105.70
36	1	2137	U	O4'-C1'-N1	5.84	112.87	108.20
1	6	1670	G	O5'-P-OP2	-5.84	100.44	105.70
36	5	919	U	N1-C2-N3	5.84	118.40	114.90
36	5	3118	C	C6-N1-C2	-5.84	117.96	120.30
36	5	3198	U	C5-C4-O4	-5.84	122.40	125.90
36	5	2134	G	N1-C6-O6	-5.84	116.40	119.90
1	2	577	G	C5-N7-C8	-5.84	101.38	104.30
25	D3	23	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	6	402	C	O5'-P-OP1	5.84	117.70	110.70
1	6	901	G	C5-N7-C8	-5.84	101.38	104.30
36	5	505	G	N9-C4-C5	5.84	107.73	105.40
36	5	1059	G	C5-C6-O6	-5.84	125.10	128.60
36	5	1371	G	C5-N7-C8	5.84	107.22	104.30
1	2	1129	U	N3-C4-C5	5.83	118.10	114.60
1	2	1479	A	N1-C6-N6	5.83	122.10	118.60
36	1	2372	A	C8-N9-C4	-5.83	103.47	105.80
1	6	1793	G	N9-C4-C5	5.83	107.73	105.40
21	c9	57	ARG	NE-CZ-NH2	-5.83	117.38	120.30
36	5	3143	C	N3-C2-O2	5.83	125.98	121.90
36	1	282	G	C2'-C3'-O3'	5.83	123.03	113.70
36	5	1787	A	N1-C6-N6	5.83	122.10	118.60
1	2	1748	G	C5-C6-O6	5.83	132.10	128.60
36	1	2397	A	O5'-P-OP2	-5.83	100.45	105.70
36	5	1057	A	C5-C6-N6	-5.83	119.04	123.70
36	5	2800	G	N3-C2-N2	-5.83	115.82	119.90
36	1	221	A	O5'-P-OP2	-5.83	100.46	105.70
36	1	2938	G	OP1-P-O3'	5.83	118.02	105.20
36	1	14	U	O5'-P-OP2	-5.83	100.46	105.70
36	1	2249	G	P-O3'-C3'	5.83	126.69	119.70
36	5	3005	A	C5-N7-C8	5.83	106.81	103.90
36	5	3214	U	N3-C4-O4	-5.83	115.32	119.40
37	7	11	A	N1-C6-N6	5.83	122.09	118.60
36	1	2752	U	N3-C4-O4	-5.82	115.32	119.40
1	6	769	A	N1-C6-N6	-5.82	115.11	118.60
36	1	1440	G	N3-C2-N2	5.82	123.97	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1902	G	N3-C4-N9	5.82	129.49	126.00
36	1	2756	C	C2-N1-C1'	5.82	125.20	118.80
36	1	1433	A	O5'-P-OP1	-5.82	100.46	105.70
36	1	341	G	C5-C6-O6	-5.82	125.11	128.60
36	1	611	A	O5'-P-OP1	5.82	117.68	110.70
1	6	864	U	N3-C4-O4	-5.82	115.33	119.40
36	5	2162	U	C2-N3-C4	-5.82	123.51	127.00
36	1	926	A	N1-C6-N6	5.81	122.09	118.60
36	5	3245	A	C8-N9-C4	-5.81	103.47	105.80
36	1	44	U	C5-C6-N1	-5.81	119.80	122.70
1	6	557	G	N1-C6-O6	-5.81	116.42	119.90
36	5	3362	A	N1-C2-N3	5.81	132.20	129.30
36	1	3269	U	N3-C2-O2	-5.81	118.14	122.20
1	6	337	G	C5-N7-C8	-5.81	101.40	104.30
36	5	1177	G	N9-C4-C5	5.81	107.72	105.40
36	1	200	C	C2-N1-C1'	5.80	125.18	118.80
36	5	1483	G	O4'-C1'-N9	5.80	112.84	108.20
52	m6	27	LEU	CB-CG-CD1	-5.80	101.13	111.00
36	5	1190	A	N1-C6-N6	-5.80	115.12	118.60
36	5	1157	G	C5-C6-O6	5.80	132.08	128.60
36	5	2618	G	N9-C4-C5	-5.80	103.08	105.40
36	1	283	G	O4'-C1'-N9	-5.80	103.56	108.20
36	1	304	G	N1-C2-N2	5.80	121.42	116.20
36	1	1893	A	N1-C6-N6	-5.80	115.12	118.60
36	1	2802	A	N1-C6-N6	-5.80	115.12	118.60
1	6	287	G	C5-C6-O6	-5.80	125.12	128.60
36	5	2950	G	O4'-C1'-N9	5.80	112.84	108.20
36	1	2279	A	N1-C6-N6	5.79	122.08	118.60
1	2	580	A	C8-N9-C4	-5.79	103.48	105.80
1	2	1190	C	C6-N1-C2	5.79	122.62	120.30
1	6	1680	G	C5-C6-O6	-5.79	125.12	128.60
36	5	83	U	N1-C2-O2	5.79	126.85	122.80
36	1	2911	A	C8-N9-C4	5.79	108.12	105.80
1	2	213	A	C8-N9-C4	5.79	108.12	105.80
36	1	651	G	C8-N9-C1'	-5.79	119.47	127.00
36	1	704	U	O5'-P-OP2	-5.79	100.49	105.70
36	1	1858	A	N3-C4-C5	-5.79	122.75	126.80
36	1	1890	U	C6-N1-C2	5.79	124.47	121.00
36	1	2176	U	N3-C2-O2	-5.79	118.15	122.20
36	1	2424	A	C5-C6-N6	-5.79	119.07	123.70
1	6	1389	C	N1-C2-O2	5.79	122.37	118.90
1	6	1735	U	N3-C4-O4	-5.79	115.35	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	718	G	N3-C4-N9	-5.79	122.53	126.00
36	1	895	A	N3-C4-C5	5.79	130.85	126.80
54	M8	178	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	2	1096	C	N1-C2-O2	5.79	122.37	118.90
36	1	1326	A	C8-N9-C4	5.79	108.11	105.80
36	1	2913	C	O5'-P-OP1	-5.79	100.49	105.70
1	6	1020	A	N1-C2-N3	5.79	132.19	129.30
36	5	39	A	N9-C4-C5	-5.79	103.49	105.80
36	5	103	G	C5-C6-O6	5.79	132.07	128.60
36	5	424	G	O5'-P-OP2	-5.79	100.49	105.70
36	5	2141	U	OP2-P-O3'	5.79	117.93	105.20
36	1	2307	G	N1-C6-O6	-5.78	116.43	119.90
36	1	678	G	C5-C6-O6	-5.78	125.13	128.60
36	1	1615	C	C2-N3-C4	-5.78	117.01	119.90
36	1	2647	A	N1-C2-N3	5.78	132.19	129.30
1	6	400	A	OP2-P-O3'	5.78	117.91	105.20
36	5	2767	U	C5-C4-O4	5.78	129.37	125.90
36	5	2176	U	N3-C2-O2	-5.78	118.16	122.20
1	6	1078	C	N3-C4-N4	-5.77	113.96	118.00
36	5	650	C	C2-N3-C4	-5.77	117.01	119.90
36	5	753	C	C2-N1-C1'	5.77	125.15	118.80
36	5	2307	G	C8-N9-C4	-5.77	104.09	106.40
36	1	1408	G	O5'-P-OP1	-5.77	100.50	105.70
36	1	1140	G	C8-N9-C1'	-5.77	119.50	127.00
36	5	931	C	C2-N3-C4	-5.77	117.02	119.90
36	5	952	A	C5-C6-N6	-5.77	119.08	123.70
36	5	2113	A	C8-N9-C4	5.77	108.11	105.80
36	5	3302	U	N3-C4-C5	5.77	118.06	114.60
36	1	2309	A	C8-N9-C4	5.77	108.11	105.80
36	5	1389	G	C5-C6-O6	-5.77	125.14	128.60
36	5	2968	G	N7-C8-N9	-5.77	110.22	113.10
36	5	3377	G	C5-C6-O6	-5.77	125.14	128.60
36	1	2818	U	O5'-P-OP1	-5.76	100.51	105.70
36	5	817	A	O5'-P-OP1	-5.76	100.51	105.70
36	1	2872	A	C8-N9-C4	5.76	108.11	105.80
36	1	2827	U	N1-C2-N3	5.76	118.36	114.90
1	6	102	U	N1-C2-O2	-5.76	118.77	122.80
1	6	308	C	C2-N1-C1'	-5.76	112.46	118.80
36	5	33	G	C6-N1-C2	-5.76	121.64	125.10
36	5	3372	A	N1-C6-N6	-5.76	115.14	118.60
36	1	41	G	N1-C6-O6	-5.76	116.44	119.90
36	1	917	A	C5-C6-N6	5.76	128.31	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2726	C	C4-C5-C6	5.76	120.28	117.40
36	1	2880	U	OP2-P-O3'	5.76	117.87	105.20
1	6	1000	C	C4-C5-C6	5.76	120.28	117.40
1	6	1747	G	O5'-P-OP2	-5.76	100.52	105.70
36	5	1402	C	C4-C5-C6	5.76	120.28	117.40
36	5	3047	U	N3-C2-O2	-5.76	118.17	122.20
1	6	1361	U	C2-N1-C1'	5.76	124.61	117.70
1	6	1766	A	N1-C6-N6	5.76	122.05	118.60
36	5	434	U	O5'-P-OP1	5.76	117.61	110.70
36	5	437	G	N3-C4-N9	-5.76	122.55	126.00
36	5	2954	U	O4'-C1'-N1	5.76	112.81	108.20
36	5	3335	A	O5'-P-OP2	-5.76	100.52	105.70
49	m3	46	ILE	CG1-CB-CG2	-5.76	98.73	111.40
36	5	1481	A	N7-C8-N9	5.75	116.68	113.80
36	1	2986	U	N1-C2-N3	5.75	118.35	114.90
36	5	880	G	N1-C6-O6	5.75	123.35	119.90
36	5	1171	G	N1-C2-N2	-5.75	111.02	116.20
3	S1	70	LEU	CA-CB-CG	5.75	128.53	115.30
36	1	1604	G	C8-N9-C1'	-5.75	119.52	127.00
36	1	2408	U	N3-C2-O2	-5.75	118.17	122.20
36	5	3138	U	N1-C2-O2	-5.75	118.77	122.80
36	1	1595	U	C2-N1-C1'	-5.75	110.80	117.70
36	5	1452	A	N9-C4-C5	-5.75	103.50	105.80
36	5	2758	A	C8-N9-C4	-5.75	103.50	105.80
1	2	610	G	N1-C6-O6	5.75	123.35	119.90
1	2	1280	C	N3-C4-N4	5.75	122.02	118.00
36	1	894	G	OP1-P-O3'	5.75	117.85	105.20
36	1	913	A	N1-C6-N6	5.75	122.05	118.60
40	L3	266	ARG	NE-CZ-NH2	-5.75	117.43	120.30
36	5	52	A	N1-C6-N6	5.75	122.05	118.60
36	5	85	A	O5'-P-OP2	-5.75	100.53	105.70
36	5	1437	C	C2-N1-C1'	5.75	125.12	118.80
36	1	413	U	C2-N3-C4	-5.75	123.55	127.00
36	1	1868	G	C4-N9-C1'	5.75	133.97	126.50
36	1	2192	C	C5-C6-N1	-5.75	118.13	121.00
36	1	2885	C	C6-N1-C2	5.75	122.60	120.30
36	5	3035	A	C8-N9-C4	5.75	108.10	105.80
37	7	121	U	O4'-C1'-N1	-5.75	103.60	108.20
52	m6	66	LYS	CD-CE-NZ	5.75	124.92	111.70
1	6	1	U	C2-N1-C1'	5.75	124.59	117.70
36	1	3277	U	N3-C2-O2	-5.74	118.18	122.20
1	6	1773	C	N3-C2-O2	5.74	125.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	994	G	O5'-P-OP2	-5.74	100.53	105.70
1	6	299	A	O5'-P-OP2	-5.74	100.53	105.70
36	5	1343	A	C5-C6-N1	-5.74	114.83	117.70
36	5	2323	G	N9-C4-C5	5.74	107.70	105.40
36	1	2952	G	N9-C4-C5	-5.74	103.10	105.40
36	5	2651	G	OP2-P-O3'	5.74	117.83	105.20
36	1	776	U	N3-C4-C5	-5.74	111.16	114.60
36	1	2706	G	C5-C6-O6	-5.74	125.16	128.60
36	5	852	U	OP2-P-O3'	5.74	117.82	105.20
36	1	970	A	C5-N7-C8	-5.74	101.03	103.90
1	2	1553	G	O5'-P-OP1	-5.74	100.54	105.70
36	5	1430	U	O5'-P-OP1	-5.74	100.54	105.70
36	5	2524	A	N7-C8-N9	5.74	116.67	113.80
36	1	711	A	N1-C6-N6	-5.73	115.16	118.60
36	5	2370	G	C6-N1-C2	-5.73	121.66	125.10
37	7	8	G	N3-C2-N2	5.73	123.91	119.90
1	6	44	U	N3-C2-O2	5.73	126.21	122.20
1	6	380	U	N3-C2-O2	-5.73	118.19	122.20
36	5	32	U	C4-C5-C6	5.73	123.14	119.70
36	5	1316	C	N1-C2-O2	-5.73	115.46	118.90
36	5	1484	U	C5-C6-N1	-5.73	119.83	122.70
36	5	2725	U	N3-C4-C5	5.73	118.04	114.60
38	4	25	G	C4-C5-N7	-5.73	108.51	110.80
36	5	503	C	N3-C4-C5	5.73	124.19	121.90
36	5	708	G	C4-C5-N7	5.73	113.09	110.80
36	5	3228	C	N3-C2-O2	-5.73	117.89	121.90
36	1	659	G	N3-C2-N2	5.73	123.91	119.90
37	7	85	G	C5-C6-O6	5.73	132.04	128.60
1	6	1100	G	C8-N9-C1'	-5.73	119.56	127.00
36	5	354	U	N3-C2-O2	-5.73	118.19	122.20
36	1	1425	U	C5-C6-N1	-5.72	119.84	122.70
36	5	648	C	C4-C5-C6	5.72	120.26	117.40
36	5	3295	A	OP2-P-O3'	5.72	117.79	105.20
38	8	25	G	O5'-P-OP2	-5.72	100.55	105.70
36	1	1715	A	O4'-C1'-N9	-5.72	103.62	108.20
36	5	1908	A	N3-C4-C5	-5.72	122.79	126.80
36	5	2891	U	C2-N3-C4	-5.72	123.57	127.00
38	8	106	C	C6-N1-C2	5.72	122.59	120.30
1	2	1339	C	C5-C6-N1	5.72	123.86	121.00
36	1	644	G	C6-C5-N7	-5.72	126.97	130.40
36	5	3350	C	C6-N1-C2	-5.72	118.01	120.30
36	5	2920	U	C4-C5-C6	5.72	123.13	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2975	U	N1-C2-O2	5.72	126.80	122.80
36	1	580	C	N1-C2-O2	-5.72	115.47	118.90
36	1	2314	U	C2-N1-C1'	5.72	124.56	117.70
37	3	83	U	C2-N3-C4	-5.72	123.57	127.00
1	6	459	G	N1-C6-O6	5.72	123.33	119.90
36	5	800	G	C5-N7-C8	5.72	107.16	104.30
36	1	944	C	C5-C6-N1	5.71	123.86	121.00
36	1	1124	U	N1-C2-O2	5.71	126.80	122.80
36	1	1433	A	OP1-P-O3'	5.71	117.77	105.20
36	1	1437	C	C2-N1-C1'	5.71	125.08	118.80
36	1	1611	G	C6-C5-N7	-5.71	126.97	130.40
36	5	2650	U	N3-C4-C5	5.71	118.03	114.60
36	5	2290	C	C4-C5-C6	5.71	120.25	117.40
1	6	378	A	O5'-P-OP1	5.71	117.55	110.70
36	5	1049	C	N3-C4-C5	5.71	124.18	121.90
36	5	2899	C	C2-N3-C4	-5.71	117.05	119.90
1	2	734	A	P-O3'-C3'	5.71	126.55	119.70
36	5	649	A	C8-N9-C4	-5.71	103.52	105.80
36	5	1556	C	N1-C2-O2	5.71	122.32	118.90
36	1	153	U	N3-C4-C5	-5.70	111.18	114.60
38	4	64	U	N3-C2-O2	-5.70	118.21	122.20
36	5	2651	G	OP1-P-O3'	-5.70	92.65	105.20
49	m3	21	ARG	NE-CZ-NH1	-5.70	117.45	120.30
36	1	3373	U	C5-C6-N1	-5.70	119.85	122.70
1	6	66	U	P-O3'-C3'	5.70	126.54	119.70
36	5	2113	A	C4-C5-C6	-5.70	114.15	117.00
36	5	2403	G	C2-N3-C4	5.70	114.75	111.90
36	5	2550	U	N3-C2-O2	-5.70	118.21	122.20
36	1	439	C	C5-C6-N1	5.70	123.85	121.00
36	1	2634	U	C4-C5-C6	5.70	123.12	119.70
36	5	1215	U	C5-C4-O4	-5.70	122.48	125.90
1	2	402	C	N3-C2-O2	5.70	125.89	121.90
1	2	1455	G	O5'-P-OP2	-5.70	100.57	105.70
1	2	1560	U	C6-N1-C2	-5.70	117.58	121.00
36	1	1152	G	N1-C6-O6	5.70	123.32	119.90
1	2	1657	U	O4'-C1'-N1	5.69	112.75	108.20
36	1	1665	C	C5-C4-N4	-5.69	116.21	120.20
38	4	47	C	C4-C5-C6	5.69	120.25	117.40
36	5	2682	C	N3-C4-C5	5.69	124.18	121.90
36	1	267	G	O4'-C1'-N9	-5.69	103.65	108.20
36	1	825	U	N3-C4-O4	-5.69	115.42	119.40
36	1	2247	G	N1-C6-O6	5.69	123.32	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	992	A	N3-C4-C5	5.69	130.78	126.80
36	1	427	C	N1-C2-O2	-5.69	115.49	118.90
36	1	1343	A	N1-C6-N6	5.69	122.02	118.60
1	6	1666	U	N1-C2-O2	-5.69	118.82	122.80
36	5	673	U	C2-N3-C4	-5.69	123.58	127.00
36	5	2833	A	C4-C5-N7	-5.69	107.86	110.70
1	6	448	C	N3-C4-C5	-5.69	119.62	121.90
1	2	158	U	P-O3'-C3'	5.69	126.53	119.70
1	2	934	C	C2-N1-C1'	5.69	125.06	118.80
36	1	3275	U	C6-N1-C2	-5.69	117.59	121.00
37	3	99	G	O5'-P-OP2	-5.69	100.58	105.70
36	5	2854	U	OP2-P-O3'	5.69	117.71	105.20
1	2	469	C	N3-C2-O2	5.69	125.88	121.90
36	1	3369	G	C5-C6-O6	-5.69	125.19	128.60
37	7	101	G	C5-C6-O6	-5.69	125.19	128.60
36	1	3303	G	O4'-C1'-N9	5.68	112.75	108.20
37	3	67	G	N1-C6-O6	5.68	123.31	119.90
36	5	1901	A	C4-C5-C6	5.68	119.84	117.00
36	5	3120	C	O5'-P-OP1	-5.68	100.58	105.70
1	2	159	U	C2-N1-C1'	-5.68	110.88	117.70
36	1	339	C	OP1-P-OP2	-5.68	111.08	119.60
36	1	1122	U	N3-C4-C5	5.68	118.01	114.60
36	1	913	A	N3-C4-N9	5.68	131.94	127.40
1	6	1246	C	N3-C2-O2	-5.68	117.92	121.90
36	5	675	C	C6-N1-C2	-5.68	118.03	120.30
36	1	1152	G	O4'-C1'-N9	5.68	112.74	108.20
36	5	613	G	C4-C5-N7	-5.68	108.53	110.80
36	5	2386	A	N7-C8-N9	5.68	116.64	113.80
1	2	404	G	C5-C6-O6	-5.68	125.19	128.60
36	1	3268	A	N1-C6-N6	5.68	122.01	118.60
1	6	1031	U	O5'-P-OP2	-5.68	100.59	105.70
36	1	887	G	N1-C6-O6	5.67	123.31	119.90
36	1	976	U	O5'-P-OP2	-5.67	100.59	105.70
38	4	103	G	N1-C6-O6	-5.67	116.50	119.90
1	6	1058	U	OP1-P-O3'	5.67	117.69	105.20
36	5	38	U	O5'-P-OP1	5.67	117.51	110.70
36	5	2889	C	N3-C4-C5	5.67	124.17	121.90
36	1	2376	G	N3-C4-N9	5.67	129.40	126.00
36	1	315	C	O5'-P-OP1	-5.67	100.60	105.70
36	1	3109	G	C4-C5-N7	-5.67	108.53	110.80
36	5	2381	G	O5'-P-OP1	5.67	117.50	110.70
36	5	2918	G	O5'-P-OP2	-5.67	100.60	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2334	U	N3-C2-O2	-5.67	118.23	122.20
36	1	3101	G	N7-C8-N9	-5.67	110.27	113.10
36	5	214	G	N7-C8-N9	-5.67	110.27	113.10
36	5	659	G	C5-C6-N1	5.67	114.33	111.50
36	5	701	G	C4-C5-N7	-5.67	108.53	110.80
1	2	1455	G	C5-C6-N1	-5.67	108.67	111.50
36	5	424	G	OP1-P-OP2	5.67	128.10	119.60
36	1	801	A	O5'-P-OP1	5.66	117.50	110.70
36	1	1121	U	N1-C2-O2	-5.66	118.84	122.80
36	1	2375	G	N9-C4-C5	-5.66	103.13	105.40
36	1	2758	A	C2-N3-C4	5.66	113.43	110.60
36	1	3362	A	C6-C5-N7	-5.66	128.34	132.30
36	5	2367	A	O5'-P-OP1	-5.66	100.60	105.70
36	1	155	G	C5-C6-N1	5.66	114.33	111.50
1	6	390	G	C5-C6-O6	-5.66	125.20	128.60
36	1	650	C	C5-C6-N1	-5.66	118.17	121.00
50	M4	135	LEU	CA-CB-CG	5.66	128.31	115.30
36	5	1389	G	C4-C5-N7	5.66	113.06	110.80
36	5	2393	G	C4-C5-N7	5.66	113.06	110.80
36	1	941	G	C8-N9-C4	-5.65	104.14	106.40
36	1	2707	C	C6-N1-C2	-5.65	118.04	120.30
52	M6	84	LEU	CB-CG-CD2	-5.65	101.39	111.00
1	2	1114	G	O4'-C1'-N9	5.65	112.72	108.20
36	1	666	A	C5-N7-C8	5.65	106.73	103.90
36	1	931	C	C2-N3-C4	-5.65	117.07	119.90
1	6	1000	C	C2-N1-C1'	5.65	125.02	118.80
1	6	1615	C	N1-C2-O2	-5.65	115.51	118.90
36	5	1103	A	OP2-P-O3'	5.65	117.63	105.20
36	5	2142	A	OP1-P-OP2	-5.65	111.12	119.60
36	5	2572	C	C6-N1-C2	-5.65	118.04	120.30
36	1	111	C	N3-C4-C5	5.65	124.16	121.90
36	1	30	G	O5'-P-OP2	-5.65	100.62	105.70
36	1	351	A	C8-N9-C4	5.65	108.06	105.80
36	1	1403	C	C2-N3-C4	-5.65	117.08	119.90
37	3	93	C	N3-C4-C5	5.65	124.16	121.90
1	6	859	A	O5'-P-OP2	-5.65	100.62	105.70
36	5	339	C	C2-N1-C1'	-5.65	112.59	118.80
36	5	825	U	N3-C2-O2	-5.65	118.25	122.20
36	1	933	A	C4-C5-C6	5.65	119.82	117.00
36	1	2617	U	C2-N3-C4	-5.65	123.61	127.00
1	6	100	A	C8-N9-C4	5.65	108.06	105.80
36	1	3171	U	C5-C4-O4	-5.64	122.51	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1178	G	N3-C2-N2	-5.64	115.95	119.90
36	5	1392	G	N7-C8-N9	-5.64	110.28	113.10
36	5	1889	G	C4-N9-C1'	5.64	133.84	126.50
36	5	2870	C	C2-N1-C1'	-5.64	112.59	118.80
36	5	3020	U	C5-C4-O4	-5.64	122.51	125.90
1	2	829	A	P-O3'-C3'	5.64	126.47	119.70
39	L2	242	ARG	NE-CZ-NH2	-5.64	117.48	120.30
36	1	1329	U	N3-C2-O2	-5.64	118.25	122.20
36	5	891	G	N3-C2-N2	5.64	123.85	119.90
36	5	2872	A	C5-C6-N6	-5.64	119.19	123.70
36	1	2693	C	C6-N1-C2	5.64	122.55	120.30
36	1	3005	A	N1-C6-N6	-5.64	115.22	118.60
64	N8	115	LYS	C-N-CA	-5.64	110.46	122.30
36	5	1064	A	C5-C6-N6	-5.64	119.19	123.70
36	5	2818	U	C5'-C4'-O4'	-5.64	102.34	109.10
1	2	864	U	N3-C2-O2	-5.63	118.26	122.20
36	1	2314	U	C5-C6-N1	5.63	125.52	122.70
36	5	1786	G	N3-C4-N9	5.63	129.38	126.00
36	5	1840	U	N3-C2-O2	-5.63	118.25	122.20
36	5	2917	G	C4-N9-C1'	5.63	133.82	126.50
37	7	36	C	N3-C4-N4	-5.63	114.06	118.00
36	1	813	G	N1-C6-O6	-5.63	116.52	119.90
36	1	3214	U	N3-C4-O4	-5.63	115.46	119.40
36	5	341	G	OP1-P-O3'	5.63	117.59	105.20
36	1	1152	G	C6-C5-N7	-5.63	127.02	130.40
36	1	2870	C	N3-C4-N4	-5.63	114.06	118.00
1	6	858	G	C5-N7-C8	-5.63	101.48	104.30
36	5	343	U	O5'-P-OP1	-5.63	100.63	105.70
36	5	1307	G	OP1-P-OP2	5.63	128.05	119.60
36	5	2794	G	C5-C6-O6	-5.63	125.22	128.60
79	q3	4	ARG	NE-CZ-NH1	5.63	123.12	120.30
36	1	3375	A	P-O3'-C3'	5.63	126.45	119.70
36	5	1858	A	O4'-C1'-N9	5.63	112.70	108.20
1	2	610	G	C4-N9-C1'	5.63	133.82	126.50
36	1	1115	G	C8-N9-C1'	-5.63	119.68	127.00
36	1	2985	C	N3-C4-C5	-5.63	119.65	121.90
36	1	3245	A	N9-C4-C5	-5.63	103.55	105.80
36	5	2859	U	C5-C4-O4	5.63	129.28	125.90
36	5	3047	U	N3-C4-O4	-5.63	115.46	119.40
38	4	53	A	N3-C4-C5	-5.63	122.86	126.80
1	6	337	G	N1-C6-O6	5.63	123.28	119.90
1	6	1058	U	P-O3'-C3'	5.63	126.45	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	974	G	N3-C4-N9	5.63	129.38	126.00
36	5	2255	A	O5'-P-OP1	-5.63	100.64	105.70
36	5	928	C	C4-C5-C6	5.62	120.21	117.40
36	1	577	C	C4-C5-C6	5.62	120.21	117.40
36	1	2334	U	N1-C2-O2	5.62	126.74	122.80
36	1	2885	C	N3-C4-C5	5.62	124.15	121.90
1	6	448	C	O4'-C1'-N1	5.62	112.70	108.20
36	1	2614	G	C4-C5-N7	-5.62	108.55	110.80
52	m6	94	ARG	NE-CZ-NH2	5.62	123.11	120.30
36	1	831	G	C8-N9-C4	5.62	108.65	106.40
1	6	970	A	P-O3'-C3'	5.62	126.44	119.70
36	1	28	C	C6-N1-C2	5.62	122.55	120.30
36	1	97	U	N1-C2-N3	5.62	118.27	114.90
36	1	828	A	N9-C4-C5	5.62	108.05	105.80
68	O2	33	ARG	NE-CZ-NH1	5.62	123.11	120.30
36	5	31	C	OP1-P-OP2	-5.62	111.17	119.60
36	5	1469	C	C6-N1-C2	-5.62	118.05	120.30
36	5	2403	G	O5'-P-OP2	-5.62	100.64	105.70
36	5	2997	G	O5'-P-OP1	-5.62	100.64	105.70
1	6	579	A	P-O3'-C3'	5.62	126.44	119.70
36	1	1307	G	N3-C2-N2	5.62	123.83	119.90
36	5	3069	G	C5-C6-O6	-5.62	125.23	128.60
36	5	216	G	C4-C5-N7	5.61	113.05	110.80
1	2	1559	A	N7-C8-N9	5.61	116.61	113.80
36	1	54	C	N3-C4-N4	-5.61	114.07	118.00
36	1	2940	A	C4-C5-C6	5.61	119.81	117.00
36	5	2639	G	N3-C4-N9	5.61	129.37	126.00
37	7	35	C	O5'-P-OP2	-5.61	100.65	105.70
36	1	639	G	N3-C2-N2	-5.61	115.97	119.90
36	1	2868	U	C5-C6-N1	-5.61	119.89	122.70
37	7	51	A	C8-N9-C4	-5.61	103.56	105.80
36	1	1411	C	OP1-P-O3'	5.61	117.53	105.20
36	1	2356	A	N1-C2-N3	-5.61	126.50	129.30
36	5	928	C	O5'-P-OP2	-5.61	100.65	105.70
36	5	3326	G	N1-C6-O6	-5.61	116.53	119.90
36	1	1365	G	N3-C2-N2	5.61	123.82	119.90
36	1	1518	U	C5-C6-N1	-5.61	119.90	122.70
36	5	12	A	N1-C6-N6	5.61	121.96	118.60
36	5	2213	A	N7-C8-N9	-5.61	111.00	113.80
36	5	2317	A	O5'-P-OP2	-5.61	100.66	105.70
36	5	2414	G	N1-C6-O6	5.61	123.26	119.90
36	5	2703	A	N9-C4-C5	5.61	108.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	120	C	N1-C2-O2	-5.60	115.54	118.90
36	5	2550	U	N1-C2-N3	5.60	118.26	114.90
36	5	2930	A	C4-C5-C6	-5.60	114.20	117.00
36	1	799	G	O5'-P-OP1	-5.60	100.66	105.70
36	1	1483	G	O4'-C1'-N9	5.60	112.68	108.20
36	5	2753	G	N3-C2-N2	-5.60	115.98	119.90
36	5	2934	A	C5-N7-C8	5.60	106.70	103.90
36	1	1004	U	N1-C2-O2	5.60	126.72	122.80
36	1	1364	C	N3-C4-C5	5.60	124.14	121.90
36	1	2614	G	O5'-P-OP1	-5.60	100.66	105.70
36	1	2618	G	N3-C4-C5	-5.60	125.80	128.60
44	L7	179	LEU	CA-CB-CG	5.60	128.18	115.30
36	5	1832	C	C6-N1-C2	5.60	122.54	120.30
36	5	2188	A	N7-C8-N9	-5.60	111.00	113.80
36	1	651	G	N3-C4-N9	5.60	129.36	126.00
36	1	1733	G	C4-N9-C1'	5.60	133.77	126.50
36	5	2385	G	C5-C6-O6	-5.60	125.24	128.60
1	6	1643	U	C5-C6-N1	-5.59	119.90	122.70
36	5	435	C	N3-C4-C5	5.59	124.14	121.90
36	5	1116	G	N3-C2-N2	-5.59	115.98	119.90
36	1	2714	G	C4-C5-C6	-5.59	115.44	118.80
36	5	2211	U	N3-C4-C5	-5.59	111.24	114.60
36	1	365	A	N1-C6-N6	5.59	121.95	118.60
36	1	1868	G	C6-C5-N7	-5.59	127.05	130.40
36	5	1317	A	OP2-P-O3'	5.59	117.50	105.20
36	5	2148	U	C2-N1-C1'	-5.59	110.99	117.70
36	5	2290	C	O5'-P-OP2	-5.59	100.67	105.70
36	5	3211	C	C6-N1-C2	5.59	122.54	120.30
36	5	3235	C	N1-C2-O2	5.59	122.25	118.90
36	1	109	A	C8-N9-C4	-5.59	103.56	105.80
36	1	1149	G	O4'-C1'-N9	5.59	112.67	108.20
36	1	1409	G	C6-C5-N7	5.59	133.75	130.40
36	1	1596	C	N1-C2-O2	-5.59	115.55	118.90
36	5	3141	A	N9-C4-C5	5.59	108.04	105.80
36	1	947	G	N3-C4-C5	-5.59	125.81	128.60
1	6	926	A	N1-C6-N6	5.59	121.95	118.60
36	5	93	C	N3-C4-C5	-5.59	119.67	121.90
36	5	986	U	N1-C2-O2	5.59	126.71	122.80
36	1	197	G	O5'-P-OP1	-5.59	100.67	105.70
36	1	502	U	N1-C2-O2	5.59	126.71	122.80
36	1	1494	U	N3-C4-C5	5.59	117.95	114.60
36	5	2870	C	N3-C4-N4	-5.59	114.09	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3382	U	C2-N1-C1'	5.59	124.40	117.70
36	1	2152	A	C5-N7-C8	5.58	106.69	103.90
37	3	97	A	O5'-P-OP2	-5.58	100.67	105.70
36	5	420	G	C6-N1-C2	-5.58	121.75	125.10
36	1	1117	G	C8-N9-C4	5.58	108.63	106.40
38	4	113	U	C5-C4-O4	5.58	129.25	125.90
36	5	963	G	C8-N9-C4	5.58	108.63	106.40
36	5	2203	U	C5-C4-O4	-5.58	122.55	125.90
36	1	333	G	C5-C6-O6	5.58	131.95	128.60
20	c8	15	LEU	CA-CB-CG	5.58	128.14	115.30
36	5	1133	A	N9-C4-C5	5.58	108.03	105.80
36	5	1138	U	C2-N3-C4	-5.58	123.65	127.00
36	5	2329	C	N1-C2-O2	-5.58	115.55	118.90
36	1	500	C	C4-C5-C6	5.58	120.19	117.40
36	1	3362	A	N1-C6-N6	5.58	121.95	118.60
1	6	55	A	N7-C8-N9	-5.58	111.01	113.80
36	5	573	C	C6-N1-C2	-5.58	118.07	120.30
36	5	1906	G	C6-N1-C2	-5.58	121.75	125.10
36	5	1172	G	N1-C6-O6	-5.58	116.55	119.90
36	5	1399	A	N9-C4-C5	-5.58	103.57	105.80
36	1	2216	G	N9-C4-C5	5.58	107.63	105.40
36	1	2343	C	C6-N1-C2	5.58	122.53	120.30
36	1	3209	A	C6-C5-N7	-5.58	128.40	132.30
37	7	112	G	C8-N9-C4	-5.58	104.17	106.40
36	5	2830	G	C8-N9-C4	-5.57	104.17	106.40
36	1	1404	G	C8-N9-C4	5.57	108.63	106.40
36	1	2278	C	N3-C4-C5	5.57	124.13	121.90
36	5	3016	A	OP2-P-O3'	5.57	117.46	105.20
36	1	52	A	O5'-P-OP2	-5.57	100.69	105.70
36	1	1416	C	N3-C4-N4	-5.57	114.10	118.00
36	5	426	G	C8-N9-C4	5.57	108.63	106.40
36	5	931	C	N3-C4-C5	5.57	124.13	121.90
36	5	3145	C	C6-N1-C2	5.57	122.53	120.30
36	1	31	C	N3-C2-O2	-5.57	118.00	121.90
36	1	1342	C	C2-N3-C4	-5.57	117.11	119.90
36	1	2417	U	N1-C2-O2	-5.57	118.90	122.80
36	1	2550	U	N3-C2-O2	-5.57	118.30	122.20
36	5	577	C	N1-C2-O2	-5.57	115.56	118.90
36	5	3047	U	N1-C2-O2	5.57	126.70	122.80
36	1	819	U	N1-C2-O2	-5.57	118.91	122.80
36	1	971	G	C5-C6-N1	5.57	114.28	111.50
36	1	2824	G	N9-C4-C5	5.57	107.63	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3150	A	C8-N9-C4	5.57	108.03	105.80
1	6	194	U	C5-C6-N1	5.57	125.48	122.70
36	5	1520	G	C5-C6-N1	5.57	114.28	111.50
1	2	1196	A	P-O3'-C3'	5.56	126.38	119.70
36	1	369	A	C8-N9-C4	-5.56	103.58	105.80
36	1	1140	G	C4-N9-C1'	5.56	133.73	126.50
36	5	1124	U	C4-C5-C6	-5.56	116.36	119.70
36	1	2296	A	N1-C6-N6	5.56	121.94	118.60
1	6	1596	C	N3-C4-N4	-5.56	114.11	118.00
36	1	336	A	C2-N3-C4	5.56	113.38	110.60
36	1	2246	G	N3-C2-N2	-5.56	116.01	119.90
36	1	2804	A	O5'-P-OP2	-5.56	100.70	105.70
36	5	974	G	C2-N3-C4	5.56	114.68	111.90
36	5	2956	A	N7-C8-N9	5.56	116.58	113.80
36	1	573	C	N3-C4-C5	5.56	124.12	121.90
1	6	87	C	N1-C2-O2	-5.56	115.57	118.90
36	5	216	G	C5-C6-O6	-5.56	125.27	128.60
36	5	2400	G	N9-C4-C5	-5.56	103.18	105.40
1	6	1698	G	P-O3'-C3'	5.56	126.37	119.70
36	1	968	G	N9-C4-C5	5.55	107.62	105.40
36	5	1908	A	C2-N3-C4	5.55	113.38	110.60
36	1	1481	A	O4'-C1'-N9	5.55	112.64	108.20
36	1	282	G	P-O3'-C3'	5.55	126.36	119.70
36	5	987	U	O5'-P-OP1	-5.55	100.70	105.70
36	5	3062	G	C8-N9-C4	-5.55	104.18	106.40
36	5	3266	G	C5-C6-O6	5.55	131.93	128.60
36	1	677	A	O5'-P-OP1	-5.55	100.71	105.70
36	1	1192	C	C2-N1-C1'	5.55	124.90	118.80
36	1	2412	G	N7-C8-N9	5.55	115.88	113.10
36	1	2891	U	N3-C4-O4	5.55	123.28	119.40
36	1	3043	C	OP2-P-O3'	5.55	117.41	105.20
36	5	1336	U	O5'-P-OP2	-5.55	100.71	105.70
36	5	1429	G	N9-C4-C5	-5.55	103.18	105.40
36	1	1412	G	O5'-P-OP1	-5.55	100.71	105.70
1	2	1129	U	N3-C4-O4	-5.55	115.52	119.40
1	2	1766	A	C8-N9-C4	5.55	108.02	105.80
36	1	788	C	C6-N1-C2	5.55	122.52	120.30
36	1	1130	A	C2-N3-C4	5.55	113.37	110.60
36	1	2799	A	C8-N9-C4	-5.55	103.58	105.80
36	1	3219	G	O5'-P-OP1	-5.55	100.71	105.70
1	6	1776	A	O5'-P-OP2	-5.55	100.71	105.70
36	5	32	U	N1-C2-O2	-5.55	118.92	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1306	G	N9-C4-C5	-5.55	103.18	105.40
1	6	362	G	C8-N9-C1'	-5.54	119.79	127.00
36	1	800	G	C5-C6-O6	5.54	131.93	128.60
36	1	955	U	C2-N3-C4	-5.54	123.67	127.00
36	1	2606	G	OP2-P-O3'	5.54	117.39	105.20
36	5	2385	G	C4-C5-N7	5.54	113.02	110.80
1	2	1747	G	C2-N3-C4	-5.54	109.13	111.90
36	1	2400	G	C5-C6-O6	-5.54	125.28	128.60
36	1	2620	G	C5-C6-O6	-5.54	125.28	128.60
36	1	2938	G	C8-N9-C4	-5.54	104.18	106.40
38	4	25	G	C5-N7-C8	5.54	107.07	104.30
36	5	2881	C	C2-N3-C4	-5.54	117.13	119.90
37	7	92	A	C8-N9-C4	5.54	108.02	105.80
1	2	1324	G	N9-C4-C5	5.54	107.62	105.40
36	1	1132	C	C5-C6-N1	-5.54	118.23	121.00
36	1	1153	A	O5'-P-OP1	-5.54	100.72	105.70
39	L2	122	ASP	CB-CG-OD2	5.54	123.28	118.30
1	6	1568	C	P-O3'-C3'	5.54	126.34	119.70
36	5	1108	U	OP1-P-OP2	5.54	127.91	119.60
36	5	2308	C	N1-C2-O2	-5.54	115.58	118.90
36	1	758	C	N1-C2-O2	-5.54	115.58	118.90
1	6	1781	A	C5-C6-N1	-5.54	114.93	117.70
36	1	980	A	N1-C2-N3	5.54	132.07	129.30
36	5	1155	C	N3-C4-C5	5.54	124.11	121.90
1	2	720	G	P-O3'-C3'	5.53	126.34	119.70
36	1	304	G	C6-C5-N7	5.53	133.72	130.40
36	5	102	C	N3-C4-N4	5.53	121.87	118.00
36	5	2865	U	C5-C6-N1	5.53	125.47	122.70
36	1	317	A	N1-C6-N6	5.53	121.92	118.60
36	5	2270	A	N1-C6-N6	5.53	121.92	118.60
36	5	3311	C	C5-C4-N4	5.53	124.07	120.20
1	2	1524	A	N1-C6-N6	-5.53	115.28	118.60
37	7	49	G	N3-C2-N2	-5.53	116.03	119.90
1	2	1291	G	N3-C2-N2	-5.53	116.03	119.90
36	1	104	G	OP1-P-O3'	5.53	117.35	105.20
1	2	1432	U	O5'-P-OP1	-5.52	100.73	105.70
1	2	1654	G	C5-C6-N1	5.52	114.26	111.50
36	1	3217	C	N3-C2-O2	-5.52	118.03	121.90
36	5	425	G	N7-C8-N9	-5.52	110.34	113.10
24	D2	104	LEU	CA-CB-CG	5.52	128.00	115.30
36	1	1847	A	O5'-P-OP1	-5.52	100.73	105.70
38	4	31	G	C8-N9-C4	5.52	108.61	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	101	G	C4-C5-N7	5.52	113.01	110.80
36	1	1489	A	C8-N9-C4	5.52	108.01	105.80
36	1	1483	G	N1-C6-O6	-5.52	116.59	119.90
36	5	2309	A	OP1-P-OP2	5.52	127.88	119.60
36	5	3144	G	N9-C4-C5	5.52	107.61	105.40
36	1	2305	G	N3-C4-N9	5.52	129.31	126.00
36	1	2792	A	C2-N3-C4	5.52	113.36	110.60
1	6	1781	A	C4-C5-C6	5.52	119.76	117.00
36	5	2115	G	N3-C2-N2	-5.52	116.04	119.90
36	5	2116	G	N1-C6-O6	5.52	123.21	119.90
36	5	2935	U	OP1-P-O3'	5.52	117.34	105.20
36	1	2165	G	C8-N9-C4	-5.52	104.19	106.40
1	2	1097	U	O4'-C1'-N1	5.51	112.61	108.20
36	1	2585	G	N3-C4-C5	-5.51	125.84	128.60
1	6	363	G	C5-C6-O6	-5.51	125.29	128.60
36	1	918	C	OP2-P-O3'	5.51	117.33	105.20
36	1	1153	A	C6-C5-N7	-5.51	128.44	132.30
36	1	2836	C	N3-C4-C5	-5.51	119.69	121.90
36	1	3182	G	OP2-P-O3'	5.51	117.32	105.20
36	5	2352	A	C2-N3-C4	-5.51	107.84	110.60
36	5	2408	U	C5-C6-N1	-5.51	119.94	122.70
36	1	936	A	C5-C6-N6	-5.51	119.29	123.70
36	5	1190	A	C5-C6-N6	5.51	128.11	123.70
36	5	1429	G	C8-N9-C4	5.51	108.60	106.40
36	5	1879	A	C8-N9-C4	-5.51	103.60	105.80
36	1	907	G	N3-C4-N9	5.51	129.31	126.00
36	1	2177	G	N1-C6-O6	-5.51	116.59	119.90
36	1	2412	G	OP1-P-O3'	5.51	117.32	105.20
1	6	1096	C	C6-N1-C2	5.51	122.50	120.30
36	5	894	G	N3-C4-N9	5.51	129.31	126.00
36	1	788	C	C2-N1-C1'	-5.51	112.74	118.80
36	1	2321	A	C2-N3-C4	-5.51	107.85	110.60
1	6	1768	G	O5'-P-OP2	5.51	117.31	110.70
36	5	2735	U	C5-C6-N1	5.51	125.45	122.70
36	1	1489	A	N9-C4-C5	-5.50	103.60	105.80
1	6	18	C	C6-N1-C2	-5.50	118.10	120.30
36	5	337	G	N3-C4-C5	-5.50	125.85	128.60
1	2	623	A	O5'-P-OP1	-5.50	100.75	105.70
24	D2	65	LEU	CA-CB-CG	5.50	127.96	115.30
36	1	498	A	N1-C6-N6	-5.50	115.30	118.60
36	1	2943	G	C4-C5-N7	5.50	113.00	110.80
78	Q2	87	ARG	NE-CZ-NH2	5.50	123.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2278	C	C4-C5-C6	-5.50	114.65	117.40
36	5	2996	U	N1-C2-O2	5.50	126.65	122.80
36	1	828	A	C8-N9-C4	-5.50	103.60	105.80
36	1	2150	G	N1-C2-N2	-5.50	111.25	116.20
36	1	2838	A	C2-N3-C4	-5.50	107.85	110.60
36	5	1906	G	C5-C6-O6	-5.50	125.30	128.60
36	1	1316	C	N1-C2-N3	5.50	123.05	119.20
1	6	119	A	C2-N3-C4	-5.50	107.85	110.60
36	5	2366	C	C5-C6-N1	5.50	123.75	121.00
36	1	2800	G	C6-N1-C2	-5.50	121.80	125.10
1	6	328	A	O5'-P-OP2	-5.50	100.75	105.70
36	5	578	A	N1-C6-N6	5.50	121.90	118.60
36	5	909	G	N7-C8-N9	-5.50	110.35	113.10
36	1	847	A	C5-C6-N6	-5.50	119.30	123.70
36	1	1432	C	C6-N1-C2	-5.50	118.10	120.30
36	1	2811	A	C8-N9-C4	-5.50	103.60	105.80
36	1	2940	A	C6-N1-C2	-5.50	115.30	118.60
36	1	3119	U	N1-C2-O2	5.50	126.65	122.80
36	5	1928	G	C5-C6-N1	-5.50	108.75	111.50
36	5	3043	C	OP1-P-OP2	-5.50	111.35	119.60
36	1	704	U	C5-C6-N1	-5.50	119.95	122.70
36	1	630	A	C5-C6-N1	5.49	120.45	117.70
36	1	1157	G	N3-C4-N9	-5.49	122.70	126.00
36	1	1931	U	C2-N1-C1'	-5.49	111.11	117.70
36	1	2396	G	C4-C5-N7	-5.49	108.60	110.80
36	1	2672	G	C8-N9-C4	5.49	108.60	106.40
36	1	2862	U	N3-C2-O2	-5.49	118.36	122.20
36	5	586	C	N1-C2-O2	-5.49	115.60	118.90
36	5	1114	U	C5-C4-O4	-5.49	122.60	125.90
36	1	3142	A	C2-N3-C4	-5.49	107.85	110.60
1	2	75	U	C2-N1-C1'	5.49	124.29	117.70
36	1	83	U	N3-C4-C5	5.49	117.89	114.60
36	1	3309	G	C4-C5-N7	5.49	113.00	110.80
1	6	1019	A	C8-N9-C4	5.49	108.00	105.80
36	5	212	G	OP1-P-O3'	5.49	117.28	105.20
36	5	365	A	N9-C4-C5	-5.49	103.60	105.80
36	5	1484	U	C5-C4-O4	-5.49	122.61	125.90
1	2	8	U	O5'-P-OP2	-5.49	100.76	105.70
36	1	1113	G	N3-C2-N2	-5.49	116.06	119.90
1	6	1749	A	C2-N3-C4	-5.49	107.86	110.60
1	6	56	U	C5-C6-N1	-5.49	119.96	122.70
36	5	2135	U	C2-N3-C4	-5.49	123.71	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2572	C	C6-N1-C1'	-5.49	114.22	120.80
36	5	2830	G	OP2-P-O3'	5.49	117.27	105.20
1	2	323	A	C8-N9-C4	-5.49	103.61	105.80
37	3	96	U	OP2-P-O3'	5.49	117.27	105.20
1	6	1003	A	C8-N9-C4	5.49	107.99	105.80
1	6	1783	C	O5'-P-OP1	5.49	117.28	110.70
36	5	651	G	C8-N9-C4	-5.49	104.21	106.40
36	5	1441	G	O5'-P-OP2	-5.49	100.76	105.70
36	5	2148	U	N1-C2-O2	-5.49	118.96	122.80
37	7	38	U	C2-N3-C4	-5.49	123.71	127.00
36	1	192	C	C6-N1-C2	-5.48	118.11	120.30
1	6	597	G	N1-C6-O6	-5.48	116.61	119.90
1	6	1503	A	C5-N7-C8	-5.48	101.16	103.90
36	5	1496	C	OP1-P-OP2	-5.48	111.38	119.60
36	5	2794	G	C4-C5-N7	5.48	112.99	110.80
36	5	2524	A	C4-C5-N7	5.48	113.44	110.70
36	5	3225	C	C2-N1-C1'	5.48	124.83	118.80
1	2	627	C	C5-C4-N4	-5.48	116.36	120.20
4	s2	148	LEU	CA-CB-CG	5.48	127.90	115.30
1	2	402	C	O5'-P-OP2	5.48	117.27	110.70
36	1	1119	C	N3-C4-N4	-5.48	114.17	118.00
36	1	1292	C	C6-N1-C2	5.48	122.49	120.30
36	1	2656	A	C2-N3-C4	5.48	113.34	110.60
36	1	2836	C	N1-C2-N3	5.48	123.03	119.20
59	n3	45	ARG	NE-CZ-NH1	-5.48	117.56	120.30
79	q3	4	ARG	NE-CZ-NH2	-5.48	117.56	120.30
38	4	79	A	N7-C8-N9	5.48	116.54	113.80
61	N5	34	LEU	CA-CB-CG	5.48	127.90	115.30
36	5	981	U	C6-N1-C2	-5.48	117.71	121.00
1	6	308	C	C4-C5-C6	5.47	120.14	117.40
36	5	1064	A	C4-C5-N7	5.47	113.44	110.70
38	8	29	U	C2-N3-C4	-5.47	123.72	127.00
36	1	407	A	N1-C6-N6	5.47	121.88	118.60
36	5	1158	A	C5-C6-N6	-5.47	119.32	123.70
36	5	1371	G	C5-C6-N1	5.47	114.24	111.50
36	1	49	A	C5-C6-N1	-5.47	114.97	117.70
36	5	2345	A	N1-C6-N6	5.47	121.88	118.60
1	2	830	U	C2-N1-C1'	5.47	124.26	117.70
1	2	1258	U	N3-C2-O2	-5.47	118.37	122.20
36	1	2371	G	OP2-P-O3'	5.47	117.23	105.20
1	6	901	G	C6-C5-N7	-5.47	127.12	130.40
1	6	1481	C	C6-N1-C2	-5.47	118.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	909	G	C8-N9-C4	5.47	108.59	106.40
36	5	970	A	C8-N9-C4	5.47	107.99	105.80
36	1	72	C	N1-C2-O2	-5.47	115.62	118.90
36	1	2836	C	N3-C4-N4	-5.47	114.17	118.00
1	2	1456	C	C6-N1-C2	-5.46	118.11	120.30
36	1	2733	A	N1-C6-N6	5.46	121.88	118.60
36	1	3029	A	C8-N9-C4	-5.46	103.61	105.80
1	6	185	U	N1-C2-O2	5.46	126.62	122.80
1	6	1596	C	N1-C2-N3	5.46	123.03	119.20
36	5	412	G	N9-C4-C5	5.46	107.59	105.40
36	1	2343	C	C2-N3-C4	-5.46	117.17	119.90
1	6	1414	U	N3-C2-O2	-5.46	118.38	122.20
36	5	1327	C	N1-C2-O2	5.46	122.18	118.90
36	5	2691	A	C8-N9-C4	-5.46	103.61	105.80
36	1	990	U	N3-C4-C5	5.46	117.88	114.60
36	1	1113	G	O5'-P-OP1	-5.46	100.78	105.70
36	1	2121	G	C5-C6-O6	5.46	131.88	128.60
36	1	2786	G	N9-C4-C5	5.46	107.58	105.40
36	5	2634	U	N3-C4-O4	5.46	123.22	119.40
36	1	426	G	N3-C2-N2	5.46	123.72	119.90
1	6	639	U	C2-N1-C1'	5.46	124.25	117.70
36	1	345	G	C6-N1-C2	-5.46	121.82	125.10
36	1	407	A	N9-C4-C5	-5.46	103.62	105.80
1	6	627	C	O5'-P-OP1	-5.46	100.79	105.70
36	5	2830	G	N9-C4-C5	5.46	107.58	105.40
37	7	85	G	O5'-P-OP1	-5.46	100.79	105.70
1	2	720	G	OP1-P-O3'	5.46	117.20	105.20
36	1	859	G	N3-C2-N2	5.46	123.72	119.90
36	1	1515	A	C2-N3-C4	-5.46	107.87	110.60
36	5	702	C	N3-C2-O2	-5.46	118.08	121.90
36	5	782	U	N1-C2-N3	5.46	118.17	114.90
36	5	1138	U	N3-C4-C5	5.46	117.87	114.60
36	5	1929	G	C2-N3-C4	-5.46	109.17	111.90
36	5	1162	U	C5-C6-N1	-5.46	119.97	122.70
1	2	1454	G	C5-C6-O6	5.45	131.87	128.60
36	1	76	G	N3-C4-N9	5.45	129.27	126.00
1	6	638	U	N3-C2-O2	-5.45	118.38	122.20
36	5	1427	U	N3-C4-O4	-5.45	115.58	119.40
36	5	3202	G	C5-C6-O6	5.45	131.87	128.60
1	2	1751	C	N3-C4-C5	5.45	124.08	121.90
36	1	1156	C	N3-C4-N4	-5.45	114.18	118.00
36	5	908	G	O4'-C1'-N9	-5.45	103.84	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3050	U	C5-C4-O4	5.45	129.17	125.90
36	1	400	G	N1-C2-N2	5.45	121.11	116.20
36	1	1365	G	N1-C6-O6	-5.45	116.63	119.90
36	1	1851	G	N3-C4-N9	5.45	129.27	126.00
36	1	2611	U	O5'-P-OP1	5.45	117.24	110.70
36	1	3151	U	O5'-P-OP2	-5.45	100.79	105.70
36	5	2666	C	N1-C2-O2	-5.45	115.63	118.90
36	1	191	U	N1-C2-N3	5.45	118.17	114.90
36	5	815	G	C5-C6-N1	5.45	114.22	111.50
36	5	1178	G	C6-N1-C2	-5.45	121.83	125.10
36	5	2191	U	N3-C2-O2	-5.45	118.39	122.20
36	1	2736	A	O5'-P-OP2	-5.45	100.80	105.70
37	7	101	G	C6-C5-N7	-5.45	127.13	130.40
36	1	2402	A	C4-C5-C6	5.45	119.72	117.00
1	6	1745	G	N3-C4-N9	5.45	129.27	126.00
36	5	30	G	OP1-P-O3'	5.45	117.18	105.20
36	1	2960	C	C4-C5-C6	5.44	120.12	117.40
36	1	2794	G	N3-C2-N2	5.44	123.71	119.90
36	1	3109	G	N7-C8-N9	-5.44	110.38	113.10
1	6	1121	C	N3-C2-O2	-5.44	118.09	121.90
36	5	804	C	C6-N1-C2	5.44	122.48	120.30
36	5	892	U	C6-N1-C2	5.44	124.27	121.00
36	5	2991	A	C8-N9-C4	-5.44	103.62	105.80
36	1	2719	U	C2-N3-C4	-5.44	123.74	127.00
36	1	2846	U	N3-C4-O4	-5.44	115.59	119.40
36	5	395	A	O5'-P-OP2	-5.44	100.80	105.70
36	5	741	U	O5'-P-OP1	-5.44	100.80	105.70
36	5	2531	C	N1-C2-O2	5.44	122.16	118.90
36	5	2816	G	O5'-P-OP1	-5.44	100.80	105.70
36	5	2861	U	N1-C2-O2	-5.44	118.99	122.80
36	5	2258	U	N3-C2-O2	-5.44	118.39	122.20
36	1	634	C	OP2-P-O3'	5.44	117.16	105.20
36	1	859	G	N1-C2-N2	-5.44	111.31	116.20
36	1	947	G	C6-C5-N7	-5.44	127.14	130.40
68	O2	33	ARG	NE-CZ-NH2	-5.44	117.58	120.30
36	5	300	G	N3-C4-N9	-5.44	122.74	126.00
36	5	1719	G	N1-C6-O6	5.44	123.16	119.90
36	5	2190	U	N1-C2-N3	5.44	118.16	114.90
36	5	3133	C	N3-C4-C5	-5.44	119.72	121.90
1	2	1658	G	C4-C5-N7	5.44	112.97	110.80
36	1	2818	U	C5'-C4'-O4'	-5.44	102.58	109.10
36	5	909	G	C5-N7-C8	5.44	107.02	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2619	G	N1-C6-O6	5.44	123.16	119.90
4	S2	113	LEU	CA-CB-CG	5.43	127.80	115.30
36	1	949	C	N1-C2-O2	-5.43	115.64	118.90
36	1	1425	U	N3-C2-O2	-5.43	118.40	122.20
36	1	2186	U	N3-C4-O4	-5.43	115.60	119.40
36	1	2366	C	C4-C5-C6	-5.43	114.68	117.40
1	6	1010	C	O5'-P-OP2	-5.43	100.81	105.70
36	5	419	G	N9-C4-C5	-5.43	103.23	105.40
36	5	1846	C	C4-C5-C6	5.43	120.12	117.40
36	5	2794	G	O4'-C1'-N9	5.43	112.55	108.20
36	1	1519	G	N1-C6-O6	5.43	123.16	119.90
36	1	1838	G	C6-C5-N7	-5.43	127.14	130.40
36	1	2910	A	C5-N7-C8	-5.43	101.18	103.90
36	1	3109	G	C2-N3-C4	5.43	114.62	111.90
36	5	816	A	N9-C4-C5	5.43	107.97	105.80
37	7	26	C	C4-C5-C6	5.43	120.12	117.40
36	1	2585	G	N3-C4-N9	5.43	129.26	126.00
36	1	2942	C	N1-C2-O2	-5.43	115.64	118.90
36	5	1397	C	N1-C2-O2	-5.43	115.64	118.90
1	2	139	C	P-O3'-C3'	5.43	126.22	119.70
1	6	515	A	O5'-P-OP2	-5.43	100.81	105.70
1	6	1127	G	C2-N3-C4	-5.43	109.19	111.90
1	6	1396	U	C6-N1-C2	-5.43	117.74	121.00
1	2	1462	G	N1-C6-O6	5.43	123.16	119.90
36	1	936	A	OP2-P-O3'	5.43	117.14	105.20
36	5	1592	G	C6-N1-C2	5.43	128.36	125.10
1	2	1059	U	C2-N1-C1'	5.43	124.21	117.70
36	1	37	U	OP1-P-O3'	5.43	117.14	105.20
36	1	716	A	N3-C4-C5	5.43	130.60	126.80
36	1	2632	G	N3-C2-N2	5.43	123.70	119.90
36	5	189	G	C8-N9-C4	-5.42	104.23	106.40
1	6	1584	G	OP1-P-O3'	5.42	117.13	105.20
27	D5	95	HIS	N-CA-C	5.42	125.64	111.00
29	D7	29	ARG	NE-CZ-NH1	5.42	123.01	120.30
36	1	754	G	OP2-P-O3'	5.42	117.13	105.20
36	1	1329	U	O4'-C1'-N1	5.42	112.54	108.20
36	1	2995	A	C8-N9-C4	5.42	107.97	105.80
36	5	1415	U	OP1-P-O3'	5.42	117.13	105.20
36	1	325	A	N1-C6-N6	-5.42	115.35	118.60
36	1	2153	U	C6-N1-C2	-5.42	117.75	121.00
1	6	139	C	P-O3'-C3'	5.42	126.20	119.70
36	5	2362	C	N1-C2-O2	5.42	122.15	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2904	U	C5-C6-N1	-5.42	119.99	122.70
1	2	1274	C	C4-C5-C6	5.42	120.11	117.40
36	1	297	G	O4'-C1'-N9	5.42	112.53	108.20
36	1	2959	C	OP2-P-O3'	5.42	117.12	105.20
1	6	144	U	C6-N1-C2	-5.42	117.75	121.00
1	6	539	G	N3-C4-N9	-5.42	122.75	126.00
1	6	1572	G	N1-C6-O6	5.42	123.15	119.90
36	5	2887	A	C4-C5-C6	5.42	119.71	117.00
52	M6	78	ARG	NE-CZ-NH1	5.42	123.01	120.30
36	5	861	C	C5-C4-N4	-5.42	116.41	120.20
36	5	3086	A	N9-C4-C5	-5.42	103.63	105.80
36	1	681	U	C5-C4-O4	-5.42	122.65	125.90
36	1	896	A	O4'-C1'-N9	5.42	112.53	108.20
36	5	869	G	N3-C4-C5	-5.42	125.89	128.60
36	1	1363	A	N1-C6-N6	-5.41	115.35	118.60
36	1	2692	A	C8-N9-C4	-5.41	103.64	105.80
1	6	39	A	O4'-C1'-N9	5.41	112.53	108.20
1	6	397	A	C2-N3-C4	-5.41	107.89	110.60
36	5	328	U	N3-C4-O4	-5.41	115.61	119.40
36	1	1054	A	O5'-P-OP2	-5.41	100.83	105.70
36	1	1911	A	C5-C6-N6	-5.41	119.37	123.70
36	5	1522	U	N3-C2-O2	-5.41	118.41	122.20
36	5	3154	C	N3-C2-O2	-5.41	118.11	121.90
36	1	338	A	OP2-P-O3'	5.41	117.10	105.20
38	4	21	C	N3-C2-O2	5.41	125.69	121.90
36	5	1199	C	C5-C6-N1	-5.41	118.30	121.00
36	5	2930	A	C8-N9-C1'	5.41	137.44	127.70
38	8	19	C	C4-C5-C6	5.41	120.11	117.40
36	5	2153	U	C5-C6-N1	-5.41	120.00	122.70
36	5	2430	A	C8-N9-C4	-5.41	103.64	105.80
36	1	959	C	C5-C6-N1	-5.41	118.30	121.00
1	6	1124	A	C2-N3-C4	-5.41	107.90	110.60
1	6	1514	U	O5'-P-OP1	-5.41	100.83	105.70
36	1	678	G	N1-C6-O6	5.41	123.14	119.90
36	5	1428	A	O5'-P-OP1	-5.41	100.83	105.70
36	5	2804	A	C8-N9-C4	5.41	107.96	105.80
36	5	2981	U	C2-N1-C1'	5.41	124.19	117.70
36	5	637	C	C2-N1-C1'	-5.40	112.86	118.80
36	1	284	A	O4'-C1'-N9	5.40	112.52	108.20
36	1	2415	C	N3-C2-O2	-5.40	118.12	121.90
36	1	2714	G	C8-N9-C1'	5.40	134.02	127.00
1	6	146	U	N3-C4-O4	-5.40	115.62	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	594	U	C2-N3-C4	-5.40	123.76	127.00
36	5	2706	G	O5'-P-OP2	-5.40	100.84	105.70
36	5	2892	A	N1-C6-N6	-5.40	115.36	118.60
36	5	3076	C	N3-C4-N4	-5.40	114.22	118.00
1	2	1144	U	N3-C2-O2	-5.40	118.42	122.20
36	1	947	G	N3-C4-N9	5.40	129.24	126.00
36	1	2237	C	C6-N1-C2	5.40	122.46	120.30
36	1	2278	C	C5-C6-N1	5.40	123.70	121.00
38	4	39	G	N1-C6-O6	-5.40	116.66	119.90
36	5	1379	G	N1-C2-N2	-5.40	111.34	116.20
36	1	69	C	C4-C5-C6	5.40	120.10	117.40
1	6	1164	G	C5-C6-O6	-5.40	125.36	128.60
36	5	416	A	C8-N9-C4	-5.40	103.64	105.80
37	7	111	U	C5-C4-O4	-5.40	122.66	125.90
36	1	916	G	P-O3'-C3'	5.40	126.18	119.70
1	6	1092	A	N1-C6-N6	5.40	121.84	118.60
36	5	1655	G	C5-C6-O6	-5.40	125.36	128.60
36	5	2191	U	N1-C2-O2	5.40	126.58	122.80
1	2	323	A	N7-C8-N9	5.39	116.50	113.80
36	1	392	G	N1-C6-O6	5.39	123.14	119.90
38	4	32	C	N3-C2-O2	5.39	125.68	121.90
1	6	1540	G	N1-C6-O6	-5.39	116.66	119.90
36	5	592	A	N1-C6-N6	5.39	121.84	118.60
1	2	1668	G	N9-C4-C5	5.39	107.56	105.40
1	2	1745	G	C5-C6-O6	-5.39	125.36	128.60
36	1	663	C	N1-C2-O2	-5.39	115.67	118.90
36	1	2132	C	C5-C6-N1	-5.39	118.30	121.00
48	M1	112	LEU	CA-CB-CG	5.39	127.70	115.30
1	6	1428	G	C8-N9-C4	-5.39	104.24	106.40
36	5	411	U	N1-C2-O2	-5.39	119.03	122.80
36	5	520	U	C2-N1-C1'	-5.39	111.23	117.70
36	5	2281	A	O4'-C1'-N9	5.39	112.52	108.20
36	5	2645	G	N1-C6-O6	-5.39	116.66	119.90
36	1	1888	U	C2-N3-C4	-5.39	123.77	127.00
1	6	339	C	N1-C2-O2	-5.39	115.67	118.90
36	5	1148	G	N9-C4-C5	-5.39	103.24	105.40
36	5	2606	G	C5-C6-O6	5.39	131.83	128.60
36	1	1196	C	C5-C6-N1	-5.39	118.31	121.00
36	1	1901	A	N1-C6-N6	-5.39	115.37	118.60
36	1	2305	G	C5-C6-O6	-5.39	125.37	128.60
36	1	2978	U	N3-C2-O2	-5.39	118.43	122.20
36	5	1701	C	C6-N1-C2	-5.39	118.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2416	U	C6-N1-C2	-5.39	117.77	121.00
36	5	3366	G	C8-N9-C4	-5.39	104.25	106.40
1	2	73	U	P-O3'-C3'	5.38	126.16	119.70
36	1	719	U	O5'-P-OP1	-5.38	100.86	105.70
36	1	1060	U	C2-N3-C4	-5.38	123.77	127.00
36	1	1585	C	N3-C4-C5	5.38	124.05	121.90
36	1	2257	C	N3-C2-O2	-5.38	118.13	121.90
36	1	2936	A	N1-C6-N6	-5.38	115.37	118.60
36	5	121	A	C8-N9-C4	5.38	107.95	105.80
36	5	698	U	N1-C2-O2	-5.38	119.03	122.80
36	5	1897	G	C5-C6-O6	-5.38	125.37	128.60
1	2	448	C	O5'-P-OP2	-5.38	100.86	105.70
36	1	196	G	N3-C4-N9	5.38	129.23	126.00
36	1	909	G	N7-C8-N9	-5.38	110.41	113.10
36	1	2391	G	C5-C6-O6	5.38	131.83	128.60
1	6	434	G	C5'-C4'-O4'	5.38	115.56	109.10
1	6	801	G	N1-C6-O6	-5.38	116.67	119.90
1	6	1772	C	OP2-P-O3'	5.38	117.03	105.20
37	7	35	C	C5-C6-N1	-5.38	118.31	121.00
38	4	15	G	C5-C6-O6	-5.38	125.37	128.60
41	L4	313	LEU	CA-CB-CG	5.38	127.67	115.30
36	5	2389	C	C2-N3-C4	-5.38	117.21	119.90
68	o2	39	ASP	CB-CG-OD1	-5.38	113.46	118.30
36	1	2192	C	C4-C5-C6	5.38	120.09	117.40
36	1	2944	U	N3-C2-O2	-5.38	118.44	122.20
36	1	2954	U	C6-N1-C2	5.38	124.23	121.00
36	5	214	G	C5-N7-C8	5.38	106.99	104.30
36	5	2278	C	C5-C4-N4	5.38	123.96	120.20
38	8	22	U	O4'-C1'-N1	5.38	112.50	108.20
36	1	286	U	N1-C2-N3	5.38	118.12	114.90
36	5	1855	U	C5-C6-N1	-5.38	120.01	122.70
36	1	881	C	N1-C2-O2	5.37	122.12	118.90
36	1	993	G	O4'-C1'-N9	5.37	112.50	108.20
36	5	1934	G	C2-N3-C4	-5.37	109.21	111.90
36	5	3138	U	C2-N3-C4	-5.37	123.78	127.00
1	2	1573	A	P-O3'-C3'	5.37	126.14	119.70
36	1	295	A	O5'-P-OP1	-5.37	100.87	105.70
36	1	701	G	OP2-P-O3'	5.37	117.02	105.20
36	1	1127	G	N1-C2-N2	5.37	121.03	116.20
1	6	824	G	C4-C5-N7	5.37	112.95	110.80
36	5	654	C	OP2-P-O3'	5.37	117.02	105.20
36	5	690	A	C8-N9-C4	5.37	107.95	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2116	G	N3-C4-N9	5.37	129.22	126.00
36	5	2950	G	N9-C4-C5	-5.37	103.25	105.40
36	1	3079	U	O5'-P-OP1	-5.37	100.87	105.70
36	5	400	G	C8-N9-C4	-5.37	104.25	106.40
36	5	3076	C	N3-C4-C5	5.37	124.05	121.90
36	1	1592	G	C8-N9-C4	-5.37	104.25	106.40
36	1	2411	U	C4-C5-C6	-5.37	116.48	119.70
36	5	1404	G	C5-C6-O6	5.37	131.82	128.60
36	1	163	C	C6-N1-C2	-5.37	118.15	120.30
36	1	196	G	C6-C5-N7	-5.37	127.18	130.40
36	1	2408	U	C2-N1-C1'	5.37	124.14	117.70
36	1	1868	G	C8-N9-C1'	-5.37	120.02	127.00
36	1	2152	A	N9-C4-C5	5.37	107.95	105.80
36	1	3318	G	C8-N9-C4	-5.37	104.25	106.40
1	6	402	C	N3-C4-C5	5.37	124.05	121.90
36	5	420	G	N1-C2-N2	-5.37	111.37	116.20
36	5	2182	A	N9-C4-C5	5.37	107.95	105.80
1	2	1503	A	N1-C6-N6	5.36	121.82	118.60
36	1	651	G	C4-N9-C1'	5.36	133.47	126.50
36	1	1334	U	C5-C6-N1	-5.36	120.02	122.70
36	1	3044	G	N1-C6-O6	-5.36	116.68	119.90
37	3	28	C	N3-C4-N4	5.36	121.75	118.00
1	6	1796	C	N3-C4-N4	-5.36	114.25	118.00
36	5	1368	U	N3-C4-C5	5.36	117.82	114.60
36	5	2141	U	C5-C4-O4	-5.36	122.68	125.90
36	1	681	U	N3-C4-O4	5.36	123.15	119.40
1	6	437	A	N1-C2-N3	5.36	131.98	129.30
1	6	992	A	O5'-P-OP1	-5.36	100.87	105.70
36	1	1891	A	N7-C8-N9	-5.36	111.12	113.80
15	c3	22	ALA	C-N-CD	-5.36	108.81	120.60
36	5	1055	A	O5'-P-OP2	-5.36	100.88	105.70
36	5	159	A	C8-N9-C4	5.36	107.94	105.80
36	5	1900	A	OP1-P-O3'	5.36	116.99	105.20
36	5	2188	A	N9-C1'-C2'	-5.36	106.11	112.00
1	2	497	G	P-O3'-C3'	5.36	126.13	119.70
36	1	2978	U	O4'-C1'-N1	5.36	112.49	108.20
40	L3	266	ARG	NE-CZ-NH1	5.36	122.98	120.30
36	5	189	G	C5-C6-O6	5.36	131.81	128.60
36	5	3179	U	O5'-P-OP1	-5.36	100.88	105.70
36	5	3308	C	C6-N1-C2	-5.36	118.16	120.30
36	1	2952	G	C2-N3-C4	-5.36	109.22	111.90
1	6	385	A	C2-N3-C4	-5.36	107.92	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1539	G	N3-C4-C5	5.36	131.28	128.60
36	5	943	U	C2-N3-C4	-5.36	123.79	127.00
36	5	1371	G	C2-N3-C4	5.36	114.58	111.90
36	5	1495	U	C2-N1-C1'	5.36	124.13	117.70
36	5	2420	C	C5-C4-N4	-5.36	116.45	120.20
36	5	2767	U	N3-C4-O4	-5.36	115.65	119.40
36	1	422	A	C2-N3-C4	5.35	113.28	110.60
1	6	1549	C	C6-N1-C2	-5.35	118.16	120.30
1	2	992	A	C2-N3-C4	-5.35	107.92	110.60
36	5	1420	C	OP2-P-O3'	5.35	116.98	105.20
36	1	625	G	OP1-P-O3'	5.35	116.97	105.20
37	3	96	U	C6-N1-C2	5.35	124.21	121.00
1	6	305	C	C2-N1-C1'	-5.35	112.91	118.80
36	5	101	G	O4'-C1'-N9	5.35	112.48	108.20
36	1	1825	G	O5'-P-OP1	5.35	117.12	110.70
36	1	3207	U	C6-N1-C1'	5.35	128.69	121.20
36	5	1469	C	C4-C5-C6	5.35	120.07	117.40
36	1	2980	U	N1-C2-N3	5.34	118.11	114.90
47	M0	4	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	6	54	C	N3-C4-C5	5.34	124.04	121.90
36	5	1846	C	N1-C2-N3	5.34	122.94	119.20
36	5	2726	C	C4-C5-C6	5.34	120.07	117.40
38	4	85	G	N1-C6-O6	5.34	123.11	119.90
37	7	102	A	C2-N3-C4	-5.34	107.93	110.60
36	1	2731	U	N1-C2-O2	-5.34	119.06	122.80
36	1	2993	G	N9-C4-C5	-5.34	103.26	105.40
38	4	47	C	C5-C6-N1	-5.34	118.33	121.00
1	6	1246	C	N1-C2-O2	5.34	122.11	118.90
1	6	1649	G	N3-C2-N2	5.34	123.64	119.90
24	D2	93	LEU	CA-CB-CG	5.34	127.58	115.30
36	1	878	G	C5-C6-O6	-5.34	125.40	128.60
36	1	2662	G	C6-C5-N7	-5.34	127.20	130.40
36	1	2800	G	N7-C8-N9	-5.34	110.43	113.10
38	4	16	G	N1-C6-O6	5.34	123.10	119.90
81	e1	100	LEU	CA-CB-CG	5.34	127.58	115.30
36	5	1724	U	O4'-C1'-N1	5.34	112.47	108.20
36	5	2647	A	N9-C4-C5	5.34	107.94	105.80
36	5	2831	G	C4-C5-N7	-5.34	108.66	110.80
36	1	2179	C	C5-C4-N4	-5.34	116.46	120.20
38	4	114	G	C8-N9-C4	5.34	108.53	106.40
36	1	279	U	O5'-P-OP2	5.34	117.10	110.70
36	1	592	A	N9-C4-C5	-5.34	103.67	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1082	U	C2-N1-C1'	5.34	124.10	117.70
36	1	1858	A	C4-N9-C1'	5.34	135.91	126.30
36	5	2285	C	C6-N1-C2	-5.34	118.17	120.30
36	1	1349	G	C4-N9-C1'	5.33	133.44	126.50
1	2	704	C	N1-C2-O2	5.33	122.10	118.90
1	2	1600	A	P-O3'-C3'	5.33	126.10	119.70
36	1	2155	G	O5'-P-OP2	-5.33	100.90	105.70
1	6	187	G	P-O3'-C3'	5.33	126.10	119.70
1	6	904	G	N3-C4-N9	5.33	129.20	126.00
36	5	2282	U	C6-N1-C2	5.33	124.20	121.00
36	5	2696	A	O5'-P-OP1	-5.33	100.90	105.70
36	5	2798	C	N3-C4-N4	-5.33	114.27	118.00
1	2	1661	U	OP2-P-O3'	5.33	116.93	105.20
36	1	880	G	C4-N9-C1'	-5.33	119.57	126.50
36	1	953	G	N3-C4-C5	5.33	131.27	128.60
36	1	2619	G	N7-C8-N9	-5.33	110.43	113.10
36	5	3012	A	O5'-P-OP2	-5.33	100.90	105.70
36	1	98	G	N1-C6-O6	-5.33	116.70	119.90
36	1	304	G	C5-C6-N1	5.33	114.17	111.50
36	1	2281	A	O4'-C1'-N9	5.33	112.46	108.20
37	3	82	G	N1-C2-N2	-5.33	111.40	116.20
36	5	1177	G	C8-N9-C4	-5.33	104.27	106.40
36	5	1499	C	N1-C2-O2	-5.33	115.70	118.90
36	1	2400	G	C8-N9-C4	5.33	108.53	106.40
36	5	3076	C	N1-C2-O2	5.33	122.10	118.90
36	1	63	A	N1-C2-N3	-5.33	126.64	129.30
1	6	1091	A	OP2-P-O3'	5.33	116.92	105.20
1	2	542	A	C4-N9-C1'	5.33	135.88	126.30
1	6	1	U	O4'-C1'-N1	5.33	112.46	108.20
1	6	545	A	O5'-P-OP2	-5.33	100.91	105.70
1	6	1634	C	C6-N1-C1'	-5.33	114.41	120.80
51	m5	76	PRO	C-N-CA	-5.33	108.39	121.70
36	1	2650	U	C5-C4-O4	5.32	129.09	125.90
1	6	362	G	C4-N9-C1'	5.32	133.42	126.50
36	5	351	A	C8-N9-C4	5.32	107.93	105.80
36	5	938	C	C2-N3-C4	-5.32	117.24	119.90
52	m6	94	ARG	NE-CZ-NH1	-5.32	117.64	120.30
36	1	1073	U	N1-C2-O2	-5.32	119.08	122.80
36	5	1886	A	C5-C6-N6	-5.32	119.44	123.70
36	1	398	A	N9-C4-C5	-5.32	103.67	105.80
36	1	2945	G	O5'-P-OP1	5.32	117.08	110.70
36	5	3077	A	N1-C6-N6	-5.32	115.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3287	U	N1-C2-O2	5.32	126.52	122.80
40	13	334	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	2	42	G	N1-C6-O6	-5.32	116.71	119.90
36	1	677	A	N1-C6-N6	5.32	121.79	118.60
36	1	1000	C	C6-N1-C1'	-5.32	114.42	120.80
36	5	3075	G	OP1-P-O3'	5.32	116.90	105.20
36	1	637	C	N3-C4-N4	-5.32	114.28	118.00
36	1	785	G	O5'-P-OP2	-5.32	100.92	105.70
36	1	818	C	N1-C2-N3	5.32	122.92	119.20
38	4	140	G	N9-C4-C5	5.32	107.53	105.40
1	6	1600	A	C2-N3-C4	-5.32	107.94	110.60
36	5	2400	G	C4-C5-N7	5.32	112.93	110.80
36	5	2858	U	C2-N1-C1'	5.32	124.08	117.70
36	5	3343	G	N9-C4-C5	-5.32	103.27	105.40
37	7	76	A	O4'-C1'-N9	5.32	112.45	108.20
1	2	1039	A	O4'-C1'-N9	5.32	112.45	108.20
36	1	159	A	N1-C6-N6	5.32	121.79	118.60
36	1	413	U	C5-C6-N1	-5.32	120.04	122.70
36	1	2945	G	N7-C8-N9	-5.32	110.44	113.10
1	2	507	U	N1-C2-O2	5.31	126.52	122.80
1	6	1755	A	C5-C6-N6	-5.31	119.45	123.70
36	5	2802	A	OP2-P-O3'	5.31	116.89	105.20
1	2	1600	A	C5-C6-N1	-5.31	115.04	117.70
36	1	2249	G	C2'-C3'-O3'	5.31	122.20	113.70
36	1	2350	C	C2-N3-C4	-5.31	117.24	119.90
36	5	2182	A	N1-C6-N6	-5.31	115.41	118.60
1	2	404	G	N9-C4-C5	-5.31	103.28	105.40
1	2	973	A	C5-C6-N1	-5.31	115.05	117.70
36	5	297	G	N1-C6-O6	-5.31	116.71	119.90
36	5	1380	G	N9-C4-C5	-5.31	103.28	105.40
36	1	876	A	O5'-P-OP2	-5.31	100.92	105.70
1	6	362	G	N1-C2-N2	-5.31	111.42	116.20
1	6	629	U	O5'-P-OP1	-5.31	100.92	105.70
36	5	439	C	C6-N1-C2	-5.31	118.18	120.30
36	5	631	U	N3-C4-O4	-5.31	115.68	119.40
36	5	1095	U	N3-C2-O2	-5.31	118.48	122.20
36	5	2293	C	N3-C4-N4	5.31	121.72	118.00
36	5	2338	C	N3-C4-N4	5.31	121.72	118.00
1	2	992	A	N3-C4-N9	-5.31	123.16	127.40
36	1	941	G	N9-C4-C5	5.31	107.52	105.40
36	1	973	A	N9-C4-C5	5.31	107.92	105.80
36	1	2302	G	N1-C2-N2	-5.31	111.42	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	3	3	U	C5-C6-N1	-5.31	120.05	122.70
1	6	1697	G	N3-C4-C5	-5.31	125.95	128.60
36	5	2636	A	O5'-P-OP1	-5.31	100.92	105.70
36	5	3309	G	C5-C6-N1	5.31	114.15	111.50
36	1	197	G	N1-C6-O6	5.31	123.08	119.90
36	1	2409	G	N9-C4-C5	5.31	107.52	105.40
1	2	1455	G	N9-C4-C5	5.30	107.52	105.40
25	D3	111	GLY	N-CA-C	-5.30	99.84	113.10
36	1	2144	A	C5-C6-N6	-5.30	119.46	123.70
36	1	3173	G	C5-N7-C8	-5.30	101.65	104.30
1	6	1103	U	OP2-P-O3'	5.30	116.87	105.20
36	5	267	G	O4'-C1'-N9	-5.30	103.96	108.20
36	5	361	A	N1-C6-N6	-5.30	115.42	118.60
36	5	2956	A	C5-C6-N1	-5.30	115.05	117.70
36	5	3050	U	N3-C2-O2	-5.30	118.49	122.20
36	5	3351	U	C6-N1-C2	-5.30	117.82	121.00
36	1	806	A	O4'-C1'-N9	-5.30	103.96	108.20
36	1	957	C	N3-C4-N4	5.30	121.71	118.00
36	1	1307	G	OP2-P-O3'	-5.30	93.53	105.20
36	5	43	A	C8-N9-C4	-5.30	103.68	105.80
36	5	339	C	C6-N1-C1'	5.30	127.16	120.80
1	2	554	C	N3-C4-C5	-5.30	119.78	121.90
1	2	777	C	C6-N1-C2	-5.30	118.18	120.30
36	1	421	G	N1-C2-N2	-5.30	111.43	116.20
36	1	634	C	N3-C2-O2	-5.30	118.19	121.90
36	1	1484	U	OP2-P-O3'	5.30	116.86	105.20
36	1	2434	U	N3-C4-O4	-5.30	115.69	119.40
6	S4	164	LEU	CA-CB-CG	5.30	127.49	115.30
36	1	99	A	O5'-P-OP1	5.30	117.06	110.70
36	1	608	A	N1-C6-N6	5.30	121.78	118.60
36	1	1114	U	N1-C2-N3	-5.30	111.72	114.90
36	5	2889	C	C2-N3-C4	-5.30	117.25	119.90
36	1	2409	G	N1-C6-O6	-5.30	116.72	119.90
36	1	2954	U	OP1-P-O3'	5.30	116.86	105.20
36	5	3126	C	N3-C4-C5	5.30	124.02	121.90
1	6	1305	U	N1-C2-O2	-5.30	119.09	122.80
36	5	2851	A	N1-C2-N3	5.30	131.95	129.30
47	m0	88	ARG	NE-CZ-NH1	-5.30	117.65	120.30
36	1	1412	G	N1-C6-O6	-5.29	116.72	119.90
36	1	2848	G	O5'-P-OP2	-5.29	100.94	105.70
36	5	86	G	C5-C6-N1	5.29	114.15	111.50
36	5	2315	G	N7-C8-N9	-5.29	110.45	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	933	A	C8-N9-C4	-5.29	103.68	105.80
1	2	1119	G	C8-N9-C4	-5.29	104.28	106.40
36	1	1846	C	C4-C5-C6	5.29	120.05	117.40
36	1	2816	G	O4'-C1'-N9	5.29	112.44	108.20
36	1	2971	A	N1-C6-N6	5.29	121.78	118.60
1	2	1389	C	N3-C2-O2	-5.29	118.20	121.90
1	6	610	G	C8-N9-C1'	-5.29	120.12	127.00
64	N8	116	GLY	N-CA-C	5.29	126.32	113.10
36	5	1306	G	C8-N9-C4	5.29	108.52	106.40
36	1	2200	U	C6-N1-C2	-5.29	117.83	121.00
38	4	125	U	C5-C6-N1	5.29	125.34	122.70
1	6	542	A	C4-C5-N7	5.29	113.34	110.70
21	C9	57	ARG	NE-CZ-NH1	5.29	122.94	120.30
36	1	824	C	N3-C4-N4	-5.29	114.30	118.00
69	O3	67	MET	CG-SD-CE	-5.29	91.74	100.20
1	6	1480	G	C8-N9-C4	-5.29	104.28	106.40
36	5	2369	G	N3-C4-N9	5.29	129.17	126.00
36	5	2831	G	N3-C4-C5	-5.29	125.96	128.60
40	l3	266	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	6	1535	U	N1-C2-N3	5.29	118.07	114.90
36	5	41	G	OP2-P-O3'	5.29	116.83	105.20
36	5	1365	G	N3-C2-N2	5.29	123.60	119.90
1	2	784	C	N1-C2-O2	-5.28	115.73	118.90
36	1	1140	G	N3-C4-C5	-5.28	125.96	128.60
1	6	1389	C	C2-N1-C1'	5.28	124.61	118.80
36	5	588	G	N3-C4-C5	-5.28	125.96	128.60
36	5	2245	C	N3-C2-O2	-5.28	118.20	121.90
37	7	111	U	C2-N1-C1'	5.28	124.04	117.70
36	1	2305	G	C6-C5-N7	-5.28	127.23	130.40
36	1	2977	G	N7-C8-N9	-5.28	110.46	113.10
41	L4	95	ARG	NE-CZ-NH1	-5.28	117.66	120.30
36	5	413	U	N3-C4-O4	5.28	123.10	119.40
36	5	1889	G	C8-N9-C1'	-5.28	120.13	127.00
1	2	1554	U	N3-C4-C5	-5.28	111.43	114.60
36	1	344	A	N1-C6-N6	-5.28	115.43	118.60
36	1	890	C	O5'-P-OP2	-5.28	100.95	105.70
36	1	1152	G	C4-C5-N7	5.28	112.91	110.80
36	1	1420	C	OP2-P-O3'	5.28	116.82	105.20
38	4	64	U	N1-C2-N3	5.28	118.07	114.90
1	6	1420	C	OP2-P-O3'	5.28	116.81	105.20
36	5	1846	C	OP2-P-O3'	5.28	116.82	105.20
36	1	1452	A	C8-N9-C4	5.28	107.91	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	577	C	C5-C6-N1	-5.28	118.36	121.00
36	5	2883	U	N3-C2-O2	-5.28	118.50	122.20
36	1	1430	U	C5-C6-N1	5.28	125.34	122.70
36	1	3183	A	O5'-P-OP1	-5.28	100.95	105.70
41	L4	139	GLY	N-CA-C	-5.28	99.91	113.10
36	5	431	U	O5'-P-OP2	-5.28	100.95	105.70
36	5	1193	A	C6-C5-N7	-5.28	128.60	132.30
36	5	3244	A	C2-N3-C4	-5.28	107.96	110.60
1	2	553	G	C4-C5-N7	5.28	112.91	110.80
36	1	2904	U	N3-C4-C5	5.28	117.77	114.60
49	M3	47	ALA	C-N-CD	5.28	139.48	128.40
1	6	565	C	O5'-P-OP1	-5.28	100.95	105.70
38	8	18	U	C5-C4-O4	5.28	129.06	125.90
1	2	142	G	N3-C4-N9	-5.27	122.84	126.00
1	6	1614	A	C4-C5-N7	5.27	113.34	110.70
15	C3	22	ALA	C-N-CA	5.27	144.15	122.00
36	1	2373	A	C5'-C4'-O4'	-5.27	102.77	109.10
36	1	2392	C	N3-C4-N4	5.27	121.69	118.00
36	5	528	U	N1-C2-O2	5.27	126.49	122.80
36	5	2385	G	C2-N3-C4	-5.27	109.26	111.90
36	5	3277	U	N3-C2-O2	-5.27	118.51	122.20
37	7	91	G	OP1-P-OP2	5.27	127.51	119.60
36	5	2390	A	OP2-P-O3'	5.27	116.80	105.20
36	1	633	C	C5-C6-N1	-5.27	118.36	121.00
1	6	957	G	C5-C6-N1	-5.27	108.86	111.50
36	5	2167	A	N1-C6-N6	-5.27	115.44	118.60
36	1	54	C	C2-N1-C1'	-5.27	113.00	118.80
36	1	371	G	N9-C4-C5	-5.27	103.29	105.40
36	1	869	G	N3-C4-C5	-5.27	125.97	128.60
36	1	1695	U	C5-C6-N1	-5.27	120.07	122.70
36	1	2731	U	N3-C2-O2	5.27	125.89	122.20
1	6	47	A	O5'-P-OP1	-5.27	100.96	105.70
36	5	2825	C	O5'-P-OP2	-5.27	100.96	105.70
36	1	328	U	OP2-P-O3'	5.27	116.79	105.20
36	1	2700	G	C5-C6-O6	-5.27	125.44	128.60
40	L3	4	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	2	1486	G	O4'-C1'-N9	5.26	112.41	108.20
36	1	1323	G	N1-C6-O6	-5.26	116.74	119.90
36	1	1329	U	N1-C2-N3	5.26	118.06	114.90
36	1	1381	A	N1-C6-N6	5.26	121.76	118.60
1	6	945	U	N1-C2-O2	5.26	126.49	122.80
1	6	1150	G	C4-N9-C1'	-5.26	119.66	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1149	G	C5-C6-O6	-5.26	125.44	128.60
36	5	1305	U	N3-C2-O2	5.26	125.89	122.20
36	5	2178	A	C8-N9-C4	5.26	107.91	105.80
36	5	2417	U	N3-C4-O4	5.26	123.08	119.40
36	5	2898	G	O4'-C1'-N9	-5.26	103.99	108.20
1	6	65	A	N1-C6-N6	5.26	121.76	118.60
12	c0	88	PRO	N-CA-CB	5.26	109.62	103.30
36	1	676	G	C8-N9-C4	-5.26	104.30	106.40
36	1	1101	G	O5'-P-OP2	-5.26	100.96	105.70
36	1	1437	C	C5-C6-N1	5.26	123.63	121.00
36	5	1879	A	C5-C6-N6	-5.26	119.49	123.70
36	5	3200	G	C5-C6-O6	-5.26	125.44	128.60
36	1	153	U	C6-N1-C2	-5.26	117.84	121.00
36	1	2972	G	N3-C2-N2	-5.26	116.22	119.90
36	5	280	U	C2-N3-C4	-5.26	123.84	127.00
36	5	1143	A	C6-N1-C2	5.26	121.76	118.60
36	5	1842	A	C2-N3-C4	-5.26	107.97	110.60
36	5	3093	C	N1-C2-O2	-5.26	115.74	118.90
36	1	1115	G	C4-N9-C1'	5.26	133.34	126.50
36	5	403	C	OP2-P-O3'	5.26	116.77	105.20
36	5	861	C	O5'-P-OP1	5.26	117.01	110.70
36	5	1051	U	C2-N3-C4	-5.26	123.84	127.00
36	5	1389	G	N1-C6-O6	5.26	123.06	119.90
13	C1	88	ARG	NE-CZ-NH2	-5.26	117.67	120.30
36	1	2357	A	N1-C6-N6	5.26	121.75	118.60
36	1	2700	G	C6-C5-N7	-5.26	127.25	130.40
36	5	1820	U	O4'-C1'-N1	5.26	112.41	108.20
37	7	102	A	N1-C6-N6	5.26	121.75	118.60
37	7	111	U	C6-N1-C1'	-5.26	113.84	121.20
36	1	284	A	C8-N9-C4	-5.25	103.70	105.80
36	1	764	U	P-O3'-C3'	5.25	126.00	119.70
36	1	2184	U	C4-C5-C6	-5.25	116.55	119.70
1	6	1150	G	C8-N9-C4	5.25	108.50	106.40
36	5	25	U	C4-C5-C6	5.25	122.85	119.70
36	5	957	C	N3-C4-C5	5.25	124.00	121.90
36	5	41	G	OP1-P-OP2	-5.25	111.72	119.60
36	5	1495	U	O4'-C1'-N1	5.25	112.40	108.20
36	5	2375	G	N1-C2-N2	-5.25	111.47	116.20
36	5	2989	U	C6-N1-C2	5.25	124.15	121.00
36	1	666	A	N1-C6-N6	-5.25	115.45	118.60
36	1	870	G	C5-C6-O6	-5.25	125.45	128.60
36	1	2371	G	N1-C6-O6	5.25	123.05	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2883	U	O5'-P-OP2	-5.25	100.98	105.70
36	1	3109	G	O5'-P-OP2	5.25	117.00	110.70
1	6	957	G	N3-C2-N2	-5.25	116.23	119.90
36	5	1112	A	C6-C5-N7	-5.25	128.63	132.30
37	7	49	G	O5'-P-OP2	5.25	117.00	110.70
75	o9	23	LEU	CA-CB-CG	5.25	127.37	115.30
36	1	652	G	N3-C4-N9	5.25	129.15	126.00
36	1	2383	C	C5-C6-N1	-5.25	118.38	121.00
36	1	2700	G	N1-C6-O6	5.25	123.05	119.90
36	1	2871	G	O5'-P-OP2	-5.25	100.98	105.70
1	6	163	G	N7-C8-N9	5.25	115.72	113.10
1	6	538	A	O4'-C1'-N9	5.25	112.40	108.20
1	6	760	A	N1-C6-N6	5.25	121.75	118.60
36	1	110	G	C5'-C4'-O4'	5.25	115.39	109.10
1	6	403	G	N3-C2-N2	5.25	123.57	119.90
1	2	704	C	O4'-C1'-N1	5.24	112.39	108.20
49	M3	85	LEU	CA-CB-CG	5.24	127.36	115.30
1	6	1299	G	N3-C4-C5	-5.24	125.98	128.60
1	6	1415	U	N3-C2-O2	-5.24	118.53	122.20
36	5	1180	A	C2-N3-C4	-5.24	107.98	110.60
37	7	21	G	N9-C4-C5	-5.24	103.30	105.40
36	5	1152	G	N1-C2-N3	5.24	127.05	123.90
36	5	2930	A	N1-C2-N3	-5.24	126.68	129.30
37	7	47	C	C2-N3-C4	-5.24	117.28	119.90
36	1	2860	U	C5-C4-O4	-5.24	122.76	125.90
1	6	93	A	C8-N9-C4	5.24	107.90	105.80
4	s2	58	LEU	CA-CB-CG	5.24	127.35	115.30
36	5	1206	G	N9-C4-C5	5.24	107.50	105.40
1	2	1370	U	P-O3'-C3'	5.24	125.98	119.70
36	1	2975	U	N1-C2-O2	5.24	126.47	122.80
36	5	1312	C	C5-C6-N1	5.24	123.62	121.00
36	5	2660	G	C5-C6-O6	-5.24	125.46	128.60
36	1	1148	G	N7-C8-N9	-5.24	110.48	113.10
36	1	1425	U	N3-C4-O4	-5.24	115.73	119.40
37	3	86	U	C6-N1-C1'	-5.24	113.87	121.20
36	5	1404	G	N1-C6-O6	-5.24	116.76	119.90
36	1	295	A	N7-C8-N9	5.23	116.42	113.80
36	1	347	G	C6-N1-C2	-5.23	121.96	125.10
36	5	195	U	C4-C5-C6	5.23	122.84	119.70
36	5	2122	G	N1-C6-O6	-5.23	116.76	119.90
36	5	1381	A	C8-N9-C4	5.23	107.89	105.80
36	5	1520	G	N3-C4-C5	-5.23	125.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3010	U	OP2-P-O3'	5.23	116.71	105.20
73	O7	24	ARG	CG-CD-NE	-5.23	100.81	111.80
36	5	1429	G	C2-N3-C4	-5.23	109.28	111.90
36	5	3049	A	N7-C8-N9	-5.23	111.19	113.80
36	1	1081	U	C5-C6-N1	5.23	125.31	122.70
36	1	3177	G	C2-N3-C4	5.23	114.52	111.90
1	6	354	C	N3-C4-N4	-5.23	114.34	118.00
36	5	2660	G	N7-C8-N9	-5.23	110.49	113.10
1	2	426	G	C4-N9-C1'	5.23	133.29	126.50
36	1	34	A	OP2-P-O3'	5.23	116.70	105.20
36	1	637	C	C5-C6-N1	-5.23	118.39	121.00
36	1	1173	U	N3-C4-O4	-5.23	115.74	119.40
36	1	2611	U	C5-C6-N1	-5.23	120.09	122.70
36	1	2752	U	N3-C4-C5	5.23	117.74	114.60
36	5	1884	A	OP2-P-O3'	5.23	116.70	105.20
36	1	1390	A	N1-C6-N6	-5.23	115.46	118.60
36	1	2133	U	C2-N1-C1'	-5.23	111.43	117.70
1	6	305	C	N1-C2-O2	-5.23	115.76	118.90
62	n6	60	ARG	NE-CZ-NH1	-5.23	117.69	120.30
36	1	817	A	N9-C1'-C2'	5.22	120.79	114.00
36	1	1445	U	C2-N3-C4	-5.22	123.86	127.00
1	6	782	U	N3-C2-O2	-5.22	118.54	122.20
36	5	2131	A	N1-C6-N6	5.22	121.73	118.60
38	8	6	U	C2-N3-C4	-5.22	123.87	127.00
1	2	1174	C	N1-C2-O2	5.22	122.03	118.90
36	1	716	A	O4'-C1'-N9	-5.22	104.02	108.20
36	1	2993	G	N3-C2-N2	5.22	123.56	119.90
1	6	194	U	N3-C2-O2	-5.22	118.55	122.20
1	6	362	G	N3-C4-C5	-5.22	125.99	128.60
1	6	1572	G	C6-C5-N7	-5.22	127.27	130.40
36	5	1202	A	O5'-P-OP1	-5.22	101.00	105.70
36	5	1909	A	C8-N9-C4	5.22	107.89	105.80
36	1	1547	G	N7-C8-N9	-5.22	110.49	113.10
36	5	911	C	C6-N1-C2	5.22	122.39	120.30
36	5	2305	G	N3-C2-N2	5.22	123.56	119.90
36	5	2341	A	N9-C4-C5	-5.22	103.71	105.80
36	1	832	G	C8-N9-C4	5.22	108.49	106.40
36	1	1180	A	O4'-C1'-N9	-5.22	104.02	108.20
36	1	1428	A	OP2-P-O3'	5.22	116.68	105.20
36	1	2923	U	C5-C4-O4	-5.22	122.77	125.90
62	N6	83	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	6	646	C	C6-N1-C2	-5.22	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	858	G	N7-C8-N9	5.22	115.71	113.10
1	6	864	U	N1-C2-O2	5.22	126.45	122.80
36	5	1205	A	C5-C6-N6	-5.22	119.53	123.70
36	5	1511	U	C5-C6-N1	-5.22	120.09	122.70
36	5	2830	G	N3-C4-C5	-5.22	125.99	128.60
36	1	2957	G	C5-N7-C8	5.22	106.91	104.30
36	5	3277	U	N1-C2-O2	5.22	126.45	122.80
36	1	2772	C	O4'-C1'-N1	5.22	112.37	108.20
46	L9	166	ARG	NE-CZ-NH2	5.22	122.91	120.30
36	1	417	A	O5'-P-OP2	-5.21	101.01	105.70
36	1	916	G	C6-N1-C2	5.21	128.23	125.10
36	1	1145	G	C5-C6-O6	-5.21	125.47	128.60
36	1	2935	U	C2-N3-C4	5.21	130.13	127.00
36	5	398	A	C8-N9-C4	-5.21	103.71	105.80
36	5	891	G	N1-C6-O6	-5.21	116.77	119.90
36	5	1171	G	C2-N3-C4	-5.21	109.29	111.90
36	5	2119	A	C5-C6-N6	-5.21	119.53	123.70
36	5	3271	G	O5'-P-OP1	5.21	116.96	110.70
1	2	1200	G	C6-C5-N7	-5.21	127.27	130.40
1	2	1778	G	N1-C6-O6	-5.21	116.77	119.90
36	1	30	G	N1-C2-N2	-5.21	111.51	116.20
36	1	936	A	P-O3'-C3'	5.21	125.95	119.70
36	1	1329	U	C2-N1-C1'	5.21	123.95	117.70
36	1	2883	U	C4-C5-C6	-5.21	116.57	119.70
36	5	2340	U	N3-C2-O2	-5.21	118.55	122.20
1	2	1096	C	C5-C6-N1	5.21	123.61	121.00
1	6	1514	U	N3-C2-O2	-5.21	118.55	122.20
36	5	26	A	O5'-P-OP1	-5.21	101.01	105.70
36	5	1302	A	C8-N9-C4	-5.21	103.72	105.80
40	l3	205	VAL	CB-CA-C	-5.21	101.50	111.40
36	1	1323	G	OP2-P-O3'	5.21	116.66	105.20
36	1	2422	C	N1-C2-O2	5.21	122.03	118.90
36	1	2600	C	C2-N1-C1'	5.21	124.53	118.80
37	7	95	A	C8-N9-C4	5.21	107.88	105.80
36	1	1320	C	O5'-P-OP2	-5.21	101.01	105.70
36	1	1591	G	C5-C6-O6	5.21	131.72	128.60
36	5	2369	G	O5'-P-OP1	-5.21	101.01	105.70
36	5	2692	A	N1-C6-N6	-5.21	115.48	118.60
36	5	2816	G	C4-N9-C1'	-5.21	119.73	126.50
36	5	2857	C	C6-N1-C2	5.21	122.38	120.30
36	5	2944	U	C4-C5-C6	-5.21	116.58	119.70
36	5	3104	U	N3-C4-C5	5.21	117.72	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2586	G	N1-C6-O6	5.20	123.02	119.90
36	1	3136	G	N3-C4-N9	5.20	129.12	126.00
36	5	2812	C	OP1-P-OP2	5.20	127.41	119.60
36	5	2917	G	O5'-P-OP2	-5.20	101.02	105.70
1	2	359	A	N1-C2-N3	-5.20	126.70	129.30
36	1	944	C	C6-N1-C2	-5.20	118.22	120.30
36	1	1152	G	OP1-P-OP2	5.20	127.40	119.60
38	4	30	C	N3-C4-N4	-5.20	114.36	118.00
38	4	42	G	N1-C6-O6	5.20	123.02	119.90
1	6	4	C	O5'-P-OP1	-5.20	101.02	105.70
36	5	376	G	C5-C6-N1	5.20	114.10	111.50
36	5	942	U	C4-C5-C6	5.20	122.82	119.70
36	5	2865	U	N3-C4-C5	5.20	117.72	114.60
38	8	29	U	C5-C6-N1	-5.20	120.10	122.70
36	5	2798	C	C5-C4-N4	5.20	123.84	120.20
1	2	1241	G	O4'-C1'-N9	5.20	112.36	108.20
36	1	2331	C	C5-C6-N1	-5.20	118.40	121.00
1	6	1410	A	N1-C6-N6	5.20	121.72	118.60
36	5	1192	C	C4-C5-C6	5.20	120.00	117.40
36	5	1214	U	C6-N1-C2	-5.20	117.88	121.00
37	7	104	A	N1-C6-N6	5.20	121.72	118.60
36	1	1458	U	C6-N1-C2	5.20	124.12	121.00
36	1	2623	G	C6-C5-N7	-5.20	127.28	130.40
36	1	3222	U	N3-C2-O2	-5.20	118.56	122.20
36	5	426	G	C5-N7-C8	5.20	106.90	104.30
36	5	1522	U	N1-C2-O2	5.20	126.44	122.80
36	5	2732	G	N3-C4-N9	5.20	129.12	126.00
36	5	2930	A	O4'-C1'-N9	5.20	112.36	108.20
36	5	921	A	O4'-C1'-N9	-5.19	104.05	108.20
36	5	2945	G	OP1-P-OP2	-5.19	111.81	119.60
36	1	2935	U	O5'-P-OP2	-5.19	101.03	105.70
36	1	2986	U	C2-N3-C4	-5.19	123.89	127.00
36	1	3195	U	C2-N1-C1'	5.19	123.93	117.70
36	5	712	G	C8-N9-C4	-5.19	104.32	106.40
36	5	1212	A	O5'-P-OP2	-5.19	101.03	105.70
36	5	2632	G	C5-C6-O6	5.19	131.72	128.60
36	5	2689	A	C8-N9-C4	-5.19	103.72	105.80
36	5	2702	A	N9-C4-C5	5.19	107.88	105.80
36	5	2889	C	N3-C4-N4	-5.19	114.36	118.00
36	1	521	A	C4-C5-N7	5.19	113.30	110.70
36	1	2605	G	N3-C2-N2	-5.19	116.27	119.90
36	1	2939	G	N3-C2-N2	-5.19	116.27	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	589	A	O4'-C1'-N9	-5.19	104.05	108.20
36	5	2639	G	N3-C4-C5	-5.19	126.00	128.60
36	1	963	G	O5'-P-OP1	5.19	116.93	110.70
36	1	2192	C	C2-N3-C4	-5.19	117.31	119.90
36	5	1309	U	N1-C2-O2	-5.19	119.17	122.80
35	SM	134	ASP	CB-CG-OD2	5.19	122.97	118.30
36	1	1124	U	N3-C4-C5	5.19	117.71	114.60
36	1	2541	U	P-O3'-C3'	5.19	125.93	119.70
36	1	2940	A	C5-N7-C8	5.19	106.49	103.90
36	1	3361	G	N3-C4-N9	5.19	129.11	126.00
36	5	1496	C	C2-N1-C1'	5.19	124.51	118.80
1	2	1537	C	C5-C4-N4	-5.19	116.57	120.20
36	1	46	U	C5-C4-O4	5.19	129.01	125.90
36	5	2896	A	N1-C6-N6	-5.19	115.49	118.60
40	l3	2	SER	N-CA-C	-5.19	97.00	111.00
1	2	569	C	C6-N1-C2	-5.18	118.23	120.30
1	2	1559	A	O4'-C1'-N9	5.18	112.35	108.20
36	1	804	C	C6-N1-C1'	5.18	127.02	120.80
36	1	1200	A	O4'-C1'-N9	5.18	112.35	108.20
1	6	407	A	O5'-P-OP2	5.18	116.92	110.70
36	5	630	A	C5-C6-N1	-5.18	115.11	117.70
36	5	2310	U	O5'-P-OP2	-5.18	101.03	105.70
37	7	22	A	N3-C4-C5	-5.18	123.17	126.80
1	2	581	U	C6-N1-C1'	-5.18	113.94	121.20
36	1	1144	U	N3-C4-C5	5.18	117.71	114.60
36	1	1149	G	C4-N9-C1'	-5.18	119.76	126.50
36	1	1604	G	C2-N3-C4	5.18	114.49	111.90
36	1	2714	G	C4-C5-N7	5.18	112.87	110.80
36	1	2817	A	C5-C6-N6	-5.18	119.55	123.70
36	1	2827	U	OP1-P-O3'	5.18	116.60	105.20
36	5	838	G	C6-C5-N7	5.18	133.51	130.40
36	5	2341	A	N1-C2-N3	-5.18	126.71	129.30
36	1	2351	U	N1-C2-O2	5.18	126.43	122.80
1	6	1489	U	C2-N1-C1'	5.18	123.92	117.70
1	2	321	C	C6-N1-C2	-5.18	118.23	120.30
36	5	992	A	C8-N9-C4	5.18	107.87	105.80
36	5	1330	A	N1-C2-N3	-5.18	126.71	129.30
36	5	1538	G	C8-N9-C4	5.18	108.47	106.40
36	5	2989	U	C2-N1-C1'	-5.18	111.48	117.70
36	1	608	A	N9-C4-C5	-5.18	103.73	105.80
36	1	1797	A	N1-C6-N6	-5.18	115.49	118.60
1	6	1032	G	N9-C4-C5	-5.18	103.33	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2365	C	OP1-P-OP2	5.18	127.37	119.60
38	8	88	A	N1-C6-N6	5.18	121.71	118.60
1	6	558	U	P-O3'-C3'	5.18	125.91	119.70
36	5	1370	G	N3-C2-N2	5.18	123.52	119.90
36	5	1588	A	C8-N9-C4	5.18	107.87	105.80
36	1	795	G	N7-C8-N9	-5.17	110.51	113.10
36	1	881	C	N3-C2-O2	-5.17	118.28	121.90
36	1	1399	A	C8-N9-C4	5.17	107.87	105.80
38	4	17	A	C8-N9-C4	5.17	107.87	105.80
1	6	1568	C	C6-N1-C2	-5.17	118.23	120.30
36	5	104	G	C2-N3-C4	-5.17	109.31	111.90
36	5	2648	G	OP1-P-O3'	5.17	116.58	105.20
36	5	2909	U	N1-C2-O2	-5.17	119.18	122.80
36	1	2362	C	C5-C6-N1	5.17	123.59	121.00
36	1	2827	U	N3-C4-O4	-5.17	115.78	119.40
1	6	1020	A	C4-C5-C6	5.17	119.59	117.00
36	5	103	G	N9-C4-C5	5.17	107.47	105.40
1	2	1611	A	C2-N3-C4	-5.17	108.02	110.60
36	5	3218	A	P-O3'-C3'	5.17	125.91	119.70
36	1	2639	G	N9-C4-C5	-5.17	103.33	105.40
36	1	616	G	C5-C6-O6	-5.17	125.50	128.60
36	1	2423	U	C2-N1-C1'	5.17	123.90	117.70
1	6	1414	U	N1-C2-N3	5.17	118.00	114.90
36	5	2290	C	C5-C4-N4	-5.17	116.58	120.20
36	5	3287	U	C5-C6-N1	5.17	125.28	122.70
36	1	2384	A	C4-C5-N7	5.17	113.28	110.70
36	1	2979	U	C5-C6-N1	-5.17	120.12	122.70
37	3	81	U	N1-C2-O2	5.17	126.42	122.80
36	1	827	A	N7-C8-N9	-5.17	111.22	113.80
1	6	858	G	C4-C5-N7	5.17	112.87	110.80
36	5	708	G	C5-C6-O6	-5.17	125.50	128.60
36	5	1533	U	O5'-P-OP2	-5.17	101.05	105.70
36	1	345	G	N3-C4-C5	-5.16	126.02	128.60
36	1	2801	A	OP1-P-OP2	5.16	127.34	119.60
38	4	26	U	N3-C2-O2	-5.16	118.58	122.20
1	6	1034	C	C4-C5-C6	5.16	119.98	117.40
1	6	1549	C	N3-C4-C5	-5.16	119.83	121.90
36	5	1890	U	C4-C5-C6	5.16	122.80	119.70
36	5	2349	U	OP1-P-O3'	5.16	116.56	105.20
36	5	2964	G	N1-C6-O6	-5.16	116.80	119.90
1	2	9	U	O5'-P-OP1	-5.16	101.05	105.70
36	5	426	G	C4-C5-N7	-5.16	108.73	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	926	A	C5-C6-N6	-5.16	119.57	123.70
36	5	1057	A	N9-C4-C5	-5.16	103.73	105.80
36	1	1155	C	N1-C2-O2	-5.16	115.80	118.90
36	1	1458	U	C5-C6-N1	-5.16	120.12	122.70
36	1	2797	C	N1-C2-O2	-5.16	115.80	118.90
1	6	826	U	C6-N1-C2	-5.16	117.90	121.00
36	5	888	A	C5-C6-N1	-5.16	115.12	117.70
36	5	1141	C	O5'-P-OP1	-5.16	101.06	105.70
36	5	1180	A	O4'-C1'-N9	-5.16	104.07	108.20
36	5	2113	A	N1-C2-N3	-5.16	126.72	129.30
1	2	1679	G	C8-N9-C4	-5.16	104.34	106.40
36	5	92	G	C2-N3-C4	5.16	114.48	111.90
37	7	49	G	O4'-C1'-N9	5.16	112.33	108.20
1	2	1189	A	C8-N9-C4	5.16	107.86	105.80
36	1	71	A	N9-C4-C5	5.16	107.86	105.80
36	1	1898	G	O4'-C1'-N9	5.16	112.33	108.20
1	6	403	G	C4-C5-N7	5.16	112.86	110.80
36	1	1784	G	N3-C4-N9	-5.16	122.91	126.00
36	1	3312	U	OP2-P-O3'	5.16	116.54	105.20
36	5	1197	A	C5-C6-N6	-5.16	119.58	123.70
44	17	100	ARG	NE-CZ-NH2	-5.16	117.72	120.30
36	1	1423	C	OP2-P-O3'	5.15	116.54	105.20
36	1	2876	C	N1-C2-O2	5.15	121.99	118.90
1	6	826	U	C5-C6-N1	5.15	125.28	122.70
1	2	1199	G	O5'-P-OP2	-5.15	101.06	105.70
36	1	21	G	C5-C6-O6	5.15	131.69	128.60
36	1	1146	C	O5'-P-OP2	-5.15	101.06	105.70
36	1	2938	G	N3-C2-N2	-5.15	116.29	119.90
72	O6	27	SER	N-CA-C	-5.15	97.09	111.00
1	6	32	U	C2-N3-C4	-5.15	123.91	127.00
1	6	901	G	N1-C6-O6	5.15	122.99	119.90
36	5	1321	G	C5-C6-N1	-5.15	108.92	111.50
1	2	1596	C	C6-N1-C2	-5.15	118.24	120.30
36	1	1349	G	N3-C4-C5	-5.15	126.02	128.60
36	1	1929	G	C8-N9-C4	5.15	108.46	106.40
36	1	3171	U	N3-C2-O2	5.15	125.81	122.20
1	6	1208	A	O4'-C1'-N9	5.15	112.32	108.20
36	5	516	A	N9-C4-C5	-5.15	103.74	105.80
36	5	1178	G	N3-C4-C5	-5.15	126.03	128.60
36	1	2606	G	C6-C5-N7	-5.15	127.31	130.40
1	6	144	U	O4'-C1'-N1	5.15	112.32	108.20
36	1	760	G	O4'-C1'-N9	5.15	112.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1002	A	C8-N9-C4	5.15	107.86	105.80
36	1	1435	A	C8-N9-C4	-5.15	103.74	105.80
1	6	1293	U	N3-C4-C5	5.15	117.69	114.60
36	5	519	A	C6-C5-N7	-5.15	128.70	132.30
36	5	1331	U	N3-C4-C5	5.15	117.69	114.60
36	5	2719	U	O4'-C1'-N1	5.15	112.32	108.20
36	1	2927	C	OP2-P-O3'	5.15	116.52	105.20
36	5	883	A	OP1-P-OP2	-5.15	111.88	119.60
36	5	919	U	OP1-P-OP2	-5.15	111.88	119.60
36	5	1177	G	O4'-C1'-N9	5.15	112.32	108.20
36	5	1322	U	N3-C4-O4	-5.15	115.80	119.40
36	5	2757	U	C2-N3-C4	-5.15	123.91	127.00
36	1	2306	C	C6-N1-C2	-5.14	118.24	120.30
36	1	2850	G	O5'-P-OP2	-5.14	101.07	105.70
38	4	51	G	N9-C4-C5	-5.14	103.34	105.40
36	5	993	G	O4'-C1'-N9	5.14	112.31	108.20
36	5	1003	A	C8-N9-C4	5.14	107.86	105.80
36	5	1392	G	N3-C4-N9	5.14	129.09	126.00
36	5	1412	G	C8-N9-C4	-5.14	104.34	106.40
36	1	1168	U	C2-N1-C1'	5.14	123.87	117.70
36	1	1509	A	N1-C6-N6	5.14	121.69	118.60
1	6	1300	A	N1-C6-N6	-5.14	115.51	118.60
1	6	1600	A	P-O3'-C3'	5.14	125.87	119.70
36	5	221	A	C8-N9-C4	5.14	107.86	105.80
36	5	988	U	C5-C4-O4	5.14	128.99	125.90
36	1	805	G	N1-C6-O6	-5.14	116.82	119.90
36	1	2166	A	C2-N3-C4	5.14	113.17	110.60
36	1	2244	A	N1-C6-N6	-5.14	115.52	118.60
36	1	2802	A	OP2-P-O3'	5.14	116.51	105.20
36	1	3009	G	OP2-P-O3'	5.14	116.51	105.20
36	5	2805	G	C8-N9-C4	5.14	108.46	106.40
1	2	795	U	N3-C2-O2	-5.14	118.60	122.20
1	2	1486	G	C4-C5-N7	5.14	112.86	110.80
36	1	676	G	N3-C4-C5	-5.14	126.03	128.60
36	1	1122	U	C2-N3-C4	-5.14	123.92	127.00
36	1	2142	A	N3-C4-C5	-5.14	123.20	126.80
36	1	2201	G	N3-C2-N2	5.14	123.50	119.90
36	1	2625	C	OP1-P-OP2	5.14	127.31	119.60
36	1	2625	C	O5'-P-OP2	-5.14	101.08	105.70
36	5	73	C	C5-C6-N1	-5.14	118.43	121.00
36	5	403	C	OP1-P-OP2	5.14	127.31	119.60
36	5	2142	A	OP1-P-O3'	5.14	116.51	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3005	A	C4-C5-N7	-5.14	108.13	110.70
36	1	1120	A	N1-C6-N6	-5.14	115.52	118.60
36	1	1494	U	C6-N1-C2	5.14	124.08	121.00
36	5	2819	A	OP1-P-OP2	-5.14	111.89	119.60
36	5	3096	C	C2-N3-C4	-5.14	117.33	119.90
1	2	551	G	C4-C5-N7	5.14	112.86	110.80
36	1	664	U	C5-C4-O4	-5.14	122.82	125.90
36	1	2148	U	C5-C6-N1	-5.14	120.13	122.70
36	1	2747	A	C5-C6-N6	5.14	127.81	123.70
36	5	423	A	C5-N7-C8	5.14	106.47	103.90
36	5	1148	G	N7-C8-N9	-5.14	110.53	113.10
1	2	1096	C	C6-N1-C1'	-5.13	114.64	120.80
36	1	600	G	N3-C4-C5	-5.13	126.03	128.60
1	6	87	C	N1-C2-N3	5.13	122.80	119.20
1	6	351	C	N3-C2-O2	-5.13	118.31	121.90
1	6	1139	A	N1-C6-N6	-5.13	115.52	118.60
36	5	3309	G	C8-N9-C1'	-5.13	120.33	127.00
1	6	1743	U	OP2-P-O3'	5.13	116.49	105.20
36	1	1480	G	C4-C5-N7	5.13	112.85	110.80
36	1	2175	U	C5-C6-N1	-5.13	120.13	122.70
1	6	352	A	N1-C6-N6	-5.13	115.52	118.60
1	6	543	C	C4-C5-C6	-5.13	114.83	117.40
1	2	1600	A	OP1-P-O3'	5.13	116.49	105.20
36	1	80	G	N1-C6-O6	-5.13	116.82	119.90
36	1	2374	C	C6-N1-C2	-5.13	118.25	120.30
36	1	2719	U	N1-C2-N3	5.13	117.98	114.90
1	6	965	U	N3-C2-O2	-5.13	118.61	122.20
36	5	392	G	C5-C6-O6	-5.13	125.52	128.60
36	5	1161	G	C5-C6-N1	5.13	114.06	111.50
1	2	736	C	C5-C6-N1	5.13	123.56	121.00
36	1	660	A	N1-C2-N3	-5.13	126.74	129.30
36	1	2334	U	O5'-P-OP2	-5.13	101.08	105.70
1	6	359	A	C8-N9-C4	5.13	107.85	105.80
36	5	2346	C	N3-C4-C5	5.13	123.95	121.90
36	1	2605	G	N1-C2-N2	5.13	120.81	116.20
36	5	676	G	OP2-P-O3'	5.13	116.48	105.20
36	5	1330	A	C5-C6-N6	-5.13	119.60	123.70
36	5	1491	A	OP2-P-O3'	5.13	116.48	105.20
36	5	2621	G	N1-C6-O6	5.13	122.98	119.90
36	5	2969	A	N1-C2-N3	-5.13	126.74	129.30
36	5	3095	U	N3-C4-O4	-5.13	115.81	119.40
36	5	1405	U	C2-N3-C4	-5.12	123.92	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1596	C	C2-N1-C1'	5.12	124.44	118.80
36	1	659	G	N1-C2-N2	-5.12	111.59	116.20
36	1	985	U	N1-C2-N3	-5.12	111.83	114.90
36	1	1157	G	C4-C5-N7	-5.12	108.75	110.80
36	1	2621	G	C5-C6-O6	-5.12	125.53	128.60
36	1	2758	A	N7-C8-N9	-5.12	111.24	113.80
36	5	926	A	N1-C6-N6	5.12	121.67	118.60
36	1	1399	A	C6-N1-C2	5.12	121.67	118.60
36	1	2395	G	N7-C8-N9	-5.12	110.54	113.10
36	1	3280	U	O4'-C1'-N1	5.12	112.30	108.20
38	4	30	C	C6-N1-C2	-5.12	118.25	120.30
1	6	1190	C	C6-N1-C2	5.12	122.35	120.30
36	5	186	U	N1-C2-O2	5.12	126.39	122.80
36	5	679	U	N1-C2-N3	5.12	117.97	114.90
36	5	3309	G	C8-N9-C4	-5.12	104.35	106.40
37	7	103	A	N1-C6-N6	5.12	121.67	118.60
38	8	125	U	C2-N1-C1'	5.12	123.85	117.70
1	2	1456	C	C4-C5-C6	5.12	119.96	117.40
36	1	2952	G	C5-N7-C8	-5.12	101.74	104.30
36	5	1047	A	C5-C6-N6	-5.12	119.60	123.70
36	1	1468	A	OP1-P-OP2	5.12	127.28	119.60
36	5	2136	C	C4-C5-C6	5.12	119.96	117.40
1	2	322	G	OP1-P-O3'	5.12	116.46	105.20
1	2	367	A	N1-C6-N6	5.12	121.67	118.60
36	1	3110	C	C6-N1-C2	-5.12	118.25	120.30
1	6	1418	G	N9-C4-C5	-5.12	103.35	105.40
36	5	3142	A	O5'-P-OP1	-5.12	101.09	105.70
1	2	1559	A	C4-C5-N7	5.12	113.26	110.70
36	1	439	C	N3-C4-N4	5.12	121.58	118.00
36	1	2177	G	C5-C6-N1	5.12	114.06	111.50
1	6	987	G	C5-C6-O6	-5.12	125.53	128.60
36	5	33	G	C5-C6-N1	5.12	114.06	111.50
36	5	407	A	N7-C8-N9	5.12	116.36	113.80
36	5	679	U	C5-C4-O4	5.12	128.97	125.90
36	5	1327	C	N3-C2-O2	-5.12	118.32	121.90
36	5	1374	G	N1-C2-N2	-5.12	111.60	116.20
36	5	1377	G	C8-N9-C4	-5.12	104.35	106.40
36	5	1906	G	N1-C2-N3	5.12	126.97	123.90
36	5	1911	A	N1-C6-N6	5.12	121.67	118.60
36	5	1933	A	N1-C6-N6	5.12	121.67	118.60
36	5	2340	U	C2-N3-C4	-5.12	123.93	127.00
36	5	2892	A	C5-C6-N6	5.12	127.79	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3287	U	C2-N1-C1'	5.12	123.84	117.70
40	l3	3	HIS	N-CA-C	-5.12	97.19	111.00
36	1	426	G	N3-C4-C5	-5.11	126.04	128.60
36	1	505	G	N3-C4-N9	-5.11	122.93	126.00
36	1	1716	U	P-O3'-C3'	5.11	125.84	119.70
36	1	2153	U	N3-C2-O2	-5.11	118.62	122.20
36	1	2385	G	C2-N3-C4	-5.11	109.34	111.90
36	1	3056	U	N1-C2-O2	-5.11	119.22	122.80
38	4	125	U	C6-N1-C1'	-5.11	114.04	121.20
36	5	1154	A	N1-C6-N6	-5.11	115.53	118.60
36	5	2246	G	N1-C6-O6	-5.11	116.83	119.90
36	5	2707	C	C6-N1-C2	5.11	122.34	120.30
1	2	543	C	N1-C2-O2	5.11	121.97	118.90
1	2	737	A	O4'-C1'-N9	5.11	112.29	108.20
36	5	3141	A	C8-N9-C4	-5.11	103.75	105.80
36	1	706	A	C2-N3-C4	-5.11	108.05	110.60
36	1	1901	A	C2-N3-C4	5.11	113.16	110.60
1	6	158	U	C5-C4-O4	-5.11	122.83	125.90
36	5	1152	G	C8-N9-C4	-5.11	104.36	106.40
36	5	2606	G	N1-C6-O6	-5.11	116.83	119.90
36	5	3200	G	N1-C6-O6	5.11	122.97	119.90
36	1	1055	A	C8-N9-C4	5.11	107.84	105.80
1	6	1280	C	C6-N1-C2	-5.11	118.26	120.30
1	2	30	G	C5-C6-O6	-5.11	125.53	128.60
36	1	821	U	N3-C4-O4	-5.11	115.83	119.40
36	1	1480	G	C5-C6-O6	-5.11	125.53	128.60
1	6	891	A	C8-N9-C4	5.11	107.84	105.80
36	5	363	G	OP1-P-O3'	5.11	116.44	105.20
36	5	927	C	N3-C4-C5	5.11	123.94	121.90
36	5	1101	G	N3-C2-N2	5.11	123.47	119.90
36	5	3096	C	C4-C5-C6	5.11	119.95	117.40
18	C6	40	GLU	C-N-CD	-5.11	109.37	120.60
36	1	44	U	N3-C4-O4	-5.11	115.83	119.40
36	1	3041	U	N3-C2-O2	5.11	125.77	122.20
36	1	3129	A	C8-N9-C4	5.11	107.84	105.80
36	1	3334	U	N1-C2-N3	5.11	117.96	114.90
36	1	3361	G	N3-C2-N2	5.11	123.47	119.90
1	6	1749	A	N9-C4-C5	-5.11	103.76	105.80
36	5	1206	G	C5-C6-O6	5.11	131.66	128.60
36	5	1901	A	C8-N9-C1'	-5.11	118.51	127.70
36	5	1931	U	N3-C2-O2	5.11	125.77	122.20
36	5	2524	A	C3'-C2'-C1'	-5.11	97.42	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2531	C	C2-N1-C1'	5.11	124.42	118.80
36	1	74	G	N1-C6-O6	-5.10	116.84	119.90
36	1	422	A	C5-C6-N1	5.10	120.25	117.70
36	1	2642	A	OP2-P-O3'	5.10	116.43	105.20
1	6	647	G	N1-C2-N2	5.10	120.79	116.20
36	1	304	G	N3-C2-N2	-5.10	116.33	119.90
36	1	2314	U	C6-N1-C1'	-5.10	114.06	121.20
36	1	2879	C	N1-C2-O2	-5.10	115.84	118.90
36	5	712	G	N3-C4-C5	-5.10	126.05	128.60
36	5	2323	G	C5-C6-O6	5.10	131.66	128.60
36	5	2342	U	N3-C4-C5	5.10	117.66	114.60
36	5	2892	A	N9-C4-C5	5.10	107.84	105.80
59	n3	42	SER	N-CA-C	5.10	124.78	111.00
36	1	101	G	O4'-C1'-N9	5.10	112.28	108.20
36	1	1313	G	C5-N7-C8	-5.10	101.75	104.30
54	M8	99	THR	N-CA-C	5.10	124.77	111.00
1	6	1172	G	O5'-P-OP1	-5.10	101.11	105.70
36	5	416	A	OP2-P-O3'	5.10	116.42	105.20
36	1	3109	G	C5-C6-N1	5.10	114.05	111.50
1	6	17	C	N3-C2-O2	-5.10	118.33	121.90
36	5	3124	G	N9-C4-C5	5.10	107.44	105.40
38	8	26	U	OP2-P-O3'	5.10	116.42	105.20
1	2	427	C	N3-C2-O2	-5.10	118.33	121.90
1	2	1793	G	N1-C6-O6	-5.10	116.84	119.90
36	1	1102	A	OP1-P-O3'	5.10	116.41	105.20
36	1	1333	C	O5'-P-OP1	5.10	116.82	110.70
36	1	2953	U	N1-C2-O2	-5.10	119.23	122.80
37	7	41	G	N3-C2-N2	5.10	123.47	119.90
1	2	360	A	C4-C5-C6	-5.10	114.45	117.00
36	1	1371	G	N7-C8-N9	-5.10	110.55	113.10
37	3	47	C	O5'-P-OP2	-5.10	101.11	105.70
38	4	148	G	N3-C2-N2	5.10	123.47	119.90
36	5	726	G	N9-C4-C5	-5.10	103.36	105.40
36	5	2618	G	N3-C4-N9	5.10	129.06	126.00
1	2	1217	A	O4'-C1'-N9	-5.09	104.12	108.20
1	2	1629	G	N1-C2-N2	-5.09	111.61	116.20
36	1	2142	A	C2-N3-C4	5.09	113.15	110.60
36	1	2202	C	O5'-P-OP2	5.09	116.81	110.70
36	5	2145	A	C5-C6-N1	5.09	120.25	117.70
1	2	158	U	N3-C2-O2	-5.09	118.64	122.20
36	1	2817	A	O5'-P-OP2	5.09	116.81	110.70
36	5	966	U	O5'-P-OP2	-5.09	101.12	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	971	G	N3-C2-N2	-5.09	116.34	119.90
36	5	1147	G	OP2-P-O3'	5.09	116.40	105.20
36	5	2171	G	C5-C6-O6	5.09	131.66	128.60
36	5	2355	G	C5-C6-N1	5.09	114.05	111.50
36	5	2403	G	N3-C4-N9	5.09	129.06	126.00
36	5	2878	G	C4-C5-C6	-5.09	115.75	118.80
1	2	453	U	C6-N1-C1'	-5.09	114.07	121.20
36	1	212	G	C5-N7-C8	5.09	106.84	104.30
36	1	421	G	C5-C6-N1	5.09	114.05	111.50
36	1	1148	G	N3-C2-N2	5.09	123.46	119.90
36	1	1555	U	OP2-P-O3'	5.09	116.40	105.20
36	1	1908	A	C8-N9-C4	5.09	107.84	105.80
1	6	864	U	C5-C4-O4	5.09	128.95	125.90
1	6	1796	C	C5-C6-N1	-5.09	118.45	121.00
36	5	975	C	OP1-P-OP2	5.09	127.23	119.60
36	5	1113	G	N1-C2-N3	5.09	126.95	123.90
36	5	3141	A	C4-C5-C6	5.09	119.55	117.00
36	1	910	G	C4-C5-N7	-5.09	108.77	110.80
36	1	1184	A	C2-N3-C4	-5.09	108.06	110.60
36	1	1204	A	N1-C6-N6	5.09	121.65	118.60
36	1	1929	G	N9-C4-C5	-5.09	103.36	105.40
1	6	1185	U	N1-C2-O2	5.09	126.36	122.80
1	6	1742	U	OP2-P-O3'	5.09	116.39	105.20
36	5	104	G	C5-C6-O6	-5.09	125.55	128.60
36	5	948	C	OP1-P-OP2	-5.09	111.97	119.60
1	2	359	A	N9-C4-C5	-5.09	103.77	105.80
36	1	60	A	C5-C6-N6	-5.09	119.63	123.70
36	1	76	G	C4-N9-C1'	5.09	133.11	126.50
36	1	217	U	N1-C2-N3	5.09	117.95	114.90
36	1	1399	A	C5-C6-N1	-5.09	115.16	117.70
36	1	2138	A	N9-C4-C5	5.09	107.83	105.80
36	1	3344	A	N1-C6-N6	5.09	121.65	118.60
1	6	977	A	C5-C6-N6	-5.09	119.63	123.70
68	o2	24	ARG	NE-CZ-NH1	-5.09	117.76	120.30
36	1	1467	A	N9-C4-C5	5.08	107.83	105.80
1	6	1091	A	C5-C6-N1	-5.08	115.16	117.70
36	5	1343	A	C2-N3-C4	-5.08	108.06	110.60
37	7	35	C	O5'-P-OP1	5.08	116.80	110.70
37	7	53	U	N1-C2-O2	-5.08	119.24	122.80
36	1	53	G	C5-C6-N1	5.08	114.04	111.50
36	1	118	U	C2-N3-C4	-5.08	123.95	127.00
36	1	709	A	C5-C6-N6	-5.08	119.63	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1319	G	N7-C8-N9	-5.08	110.56	113.10
36	1	1859	A	O5'-P-OP2	-5.08	101.12	105.70
36	1	2651	G	C6-C5-N7	5.08	133.45	130.40
36	5	1158	A	N1-C6-N6	5.08	121.65	118.60
36	5	2169	G	N1-C6-O6	-5.08	116.85	119.90
36	5	3366	G	N3-C4-C5	-5.08	126.06	128.60
38	8	6	U	C5-C4-O4	-5.08	122.85	125.90
68	o2	43	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	2	1144	U	O5'-P-OP1	-5.08	101.13	105.70
1	2	1602	C	N3-C4-C5	5.08	123.93	121.90
36	1	1831	U	C5-C4-O4	5.08	128.95	125.90
36	1	2651	G	N9-C4-C5	5.08	107.43	105.40
36	5	3012	A	OP2-P-O3'	5.08	116.38	105.20
36	1	434	U	N1-C2-O2	5.08	126.36	122.80
1	6	92	A	C8-N9-C4	5.08	107.83	105.80
1	6	1293	U	C5-C6-N1	-5.08	120.16	122.70
36	5	107	A	N1-C6-N6	-5.08	115.55	118.60
1	2	1745	G	C6-C5-N7	-5.08	127.35	130.40
36	1	60	A	N9-C4-C5	-5.08	103.77	105.80
36	1	1838	G	N3-C4-N9	5.08	129.05	126.00
38	4	51	G	C5-C6-O6	-5.08	125.55	128.60
36	5	1294	A	OP2-P-O3'	5.08	116.37	105.20
36	5	2968	G	N1-C6-O6	-5.08	116.85	119.90
36	1	111	C	C2-N3-C4	-5.08	117.36	119.90
36	1	2316	G	O5'-P-OP2	-5.08	101.13	105.70
6	s4	38	LEU	CA-CB-CG	5.08	126.98	115.30
36	5	873	C	P-O3'-C3'	5.08	125.79	119.70
41	14	206	LEU	CA-CB-CG	5.08	126.98	115.30
36	1	1127	G	N3-C4-C5	5.08	131.14	128.60
36	1	3094	A	C5-C6-N1	5.08	120.24	117.70
1	6	305	C	C6-N1-C1'	5.08	126.89	120.80
36	5	389	A	N9-C4-C5	5.08	107.83	105.80
36	5	2860	U	C4-C5-C6	-5.08	116.66	119.70
36	1	286	U	N3-C2-O2	-5.07	118.65	122.20
36	1	779	G	N3-C4-N9	5.07	129.04	126.00
36	1	2747	A	N9-C4-C5	5.07	107.83	105.80
1	6	1509	C	N1-C2-O2	5.07	121.94	118.90
1	6	1681	A	O4'-C1'-N9	5.07	112.26	108.20
1	6	1751	C	C6-N1-C2	5.07	122.33	120.30
36	5	644	G	C5-N7-C8	5.07	106.84	104.30
36	5	674	G	C2-N3-C4	-5.07	109.36	111.90
36	5	2208	A	O4'-C1'-N9	5.07	112.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	626	U	OP1-P-O3'	5.07	116.36	105.20
36	5	2287	C	N3-C4-N4	-5.07	114.45	118.00
36	1	786	A	C5-N7-C8	5.07	106.44	103.90
38	4	23	U	C2-N3-C4	-5.07	123.96	127.00
38	4	28	C	C2-N1-C1'	5.07	124.38	118.80
36	5	644	G	N9-C4-C5	5.07	107.43	105.40
36	5	1207	G	C5-C6-N1	5.07	114.03	111.50
36	5	1368	U	C2-N3-C4	-5.07	123.96	127.00
36	5	1400	G	N3-C4-C5	-5.07	126.06	128.60
36	1	805	G	C6-N1-C2	-5.07	122.06	125.10
36	1	1136	A	C6-N1-C2	-5.07	115.56	118.60
1	2	1773	C	C2-N1-C1'	5.07	124.37	118.80
36	1	1000	C	N3-C4-C5	5.07	123.93	121.90
1	6	1781	A	C8-N9-C4	-5.07	103.77	105.80
36	5	291	C	N3-C4-N4	-5.07	114.45	118.00
36	5	2829	U	N3-C2-O2	-5.07	118.65	122.20
36	5	3309	G	N7-C8-N9	5.07	115.63	113.10
1	2	551	G	C5-N7-C8	-5.07	101.77	104.30
1	2	704	C	N3-C2-O2	-5.07	118.36	121.90
36	1	712	G	N7-C8-N9	-5.07	110.57	113.10
36	1	934	G	C6-C5-N7	-5.07	127.36	130.40
37	3	81	U	C6-N1-C1'	-5.07	114.11	121.20
1	6	782	U	N1-C2-O2	5.07	126.35	122.80
1	6	1000	C	C2-N3-C4	-5.07	117.37	119.90
1	2	6	G	N3-C4-C5	-5.06	126.07	128.60
1	2	1339	C	OP1-P-O3'	5.06	116.34	105.20
36	1	908	G	C8-N9-C1'	-5.06	120.42	127.00
36	1	1183	C	N3-C4-C5	5.06	123.93	121.90
45	L8	65	LEU	CA-CB-CG	5.06	126.95	115.30
1	6	1	U	N3-C2-O2	-5.06	118.66	122.20
1	6	1473	U	N1-C2-O2	5.06	126.34	122.80
1	2	1536	G	C4-N9-C1'	5.06	133.08	126.50
36	1	3302	U	C6-N1-C2	5.06	124.04	121.00
36	5	85	A	N1-C6-N6	5.06	121.64	118.60
36	5	682	U	C5-C6-N1	-5.06	120.17	122.70
36	5	952	A	C4-C5-N7	5.06	113.23	110.70
36	5	1047	A	N1-C6-N6	5.06	121.64	118.60
36	5	1284	C	P-O3'-C3'	5.06	125.78	119.70
36	5	2179	C	O5'-P-OP1	-5.06	101.14	105.70
36	5	2307	G	N3-C2-N2	5.06	123.44	119.90
1	2	98	U	C6-N1-C2	5.06	124.04	121.00
1	2	1399	C	C2-N1-C1'	5.06	124.37	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2369	G	C2-N3-C4	5.06	114.43	111.90
1	6	1164	G	N3-C4-N9	5.06	129.04	126.00
36	5	361	A	N9-C4-C5	5.06	107.82	105.80
36	5	648	C	C5-C4-N4	-5.06	116.66	120.20
36	1	42	C	O5'-P-OP2	5.06	116.77	110.70
36	1	1380	G	N3-C4-C5	5.06	131.13	128.60
36	1	2405	C	N3-C2-O2	-5.06	118.36	121.90
36	5	1239	C	C5-C6-N1	5.06	123.53	121.00
36	5	1319	G	N1-C2-N2	-5.06	111.65	116.20
36	5	2250	G	N1-C6-O6	-5.06	116.86	119.90
36	5	3218	A	C2-N3-C4	-5.06	108.07	110.60
37	7	71	G	OP2-P-O3'	5.06	116.33	105.20
38	8	132	G	N9-C4-C5	5.06	107.42	105.40
38	8	132	G	N1-C6-O6	-5.06	116.86	119.90
36	1	835	G	N9-C4-C5	-5.06	103.38	105.40
36	1	1163	A	O5'-P-OP2	-5.06	101.15	105.70
36	1	2759	U	N1-C2-N3	5.06	117.94	114.90
1	6	1755	A	C5-N7-C8	-5.06	101.37	103.90
36	5	911	C	N3-C4-N4	5.06	121.54	118.00
36	5	1786	G	C5-C6-O6	-5.06	125.56	128.60
36	5	2852	C	O5'-P-OP1	5.06	116.77	110.70
36	1	1409	G	N9-C4-C5	5.06	107.42	105.40
36	1	2964	G	C5-C6-O6	-5.06	125.57	128.60
36	5	2167	A	N9-C4-C5	5.06	107.82	105.80
1	2	15	U	C6-N1-C2	-5.05	117.97	121.00
1	2	30	G	N1-C6-O6	5.05	122.93	119.90
36	1	1346	G	O5'-P-OP2	-5.05	101.15	105.70
36	1	2182	A	O5'-P-OP1	-5.05	101.15	105.70
36	1	2403	G	N3-C4-N9	5.05	129.03	126.00
36	1	2794	G	N1-C6-O6	-5.05	116.87	119.90
1	6	639	U	O4'-C1'-N1	5.05	112.24	108.20
1	6	993	A	O5'-P-OP2	-5.05	101.15	105.70
1	6	1114	G	C5-C6-N1	5.05	114.03	111.50
1	6	1456	C	N3-C2-O2	-5.05	118.36	121.90
1	6	1673	G	N3-C4-C5	-5.05	126.07	128.60
36	5	2191	U	N3-C4-O4	-5.05	115.86	119.40
36	5	3095	U	N3-C4-C5	5.05	117.63	114.60
36	5	3333	G	N1-C6-O6	5.05	122.93	119.90
36	1	2752	U	C5-C6-N1	-5.05	120.17	122.70
36	5	528	U	N3-C2-O2	-5.05	118.66	122.20
36	5	2954	U	C5-C4-O4	-5.05	122.87	125.90
36	1	1444	G	C5-C6-O6	-5.05	125.57	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1520	G	C5-N7-C8	5.05	106.83	104.30
36	1	2305	G	N1-C6-O6	5.05	122.93	119.90
36	1	2698	G	OP1-P-OP2	5.05	127.18	119.60
1	6	17	C	N1-C2-O2	5.05	121.93	118.90
36	1	190	U	C5-C6-N1	-5.05	120.18	122.70
36	1	2144	A	C5-C6-N1	5.05	120.22	117.70
36	1	3078	U	N3-C2-O2	-5.05	118.67	122.20
1	6	142	G	C6-C5-N7	-5.05	127.37	130.40
36	5	2816	G	C2-N3-C4	5.05	114.42	111.90
36	1	54	C	C6-N1-C2	5.05	122.32	120.30
36	1	1131	G	OP1-P-OP2	5.05	127.17	119.60
36	1	2222	A	N1-C6-N6	-5.05	115.57	118.60
36	5	2877	G	N3-C2-N2	5.05	123.43	119.90
38	8	25	G	O5'-P-OP1	5.05	116.76	110.70
36	1	1349	G	N3-C2-N2	5.05	123.43	119.90
36	1	1855	U	N3-C2-O2	-5.05	118.67	122.20
36	1	2424	A	C4-C5-N7	5.05	113.22	110.70
36	1	2522	G	N7-C8-N9	5.05	115.62	113.10
36	1	2598	G	C2-N3-C4	5.05	114.42	111.90
36	1	2875	U	N3-C4-O4	5.05	122.93	119.40
36	1	2950	G	N7-C8-N9	5.05	115.62	113.10
36	1	3362	A	C8-N9-C4	-5.05	103.78	105.80
38	4	25	G	C5-C6-O6	5.05	131.63	128.60
36	5	1116	G	OP2-P-O3'	5.05	116.30	105.20
36	5	2364	G	N9-C4-C5	5.05	107.42	105.40
37	7	70	U	OP2-P-O3'	5.05	116.30	105.20
36	1	939	U	N3-C4-O4	5.04	122.93	119.40
36	1	1895	A	OP1-P-O3'	5.04	116.30	105.20
36	1	1911	A	N9-C4-C5	-5.04	103.78	105.80
36	5	112	U	O4'-C1'-N1	5.04	112.24	108.20
36	5	1399	A	N1-C6-N6	5.04	121.63	118.60
36	1	934	G	O5'-P-OP1	-5.04	101.16	105.70
36	1	1520	G	C2-N3-C4	5.04	114.42	111.90
36	5	295	A	C2-N3-C4	-5.04	108.08	110.60
36	5	1306	G	N3-C4-N9	5.04	129.03	126.00
36	5	1435	A	P-O3'-C3'	5.04	125.75	119.70
36	5	2257	C	P-O3'-C3'	5.04	125.75	119.70
36	1	90	C	N1-C2-O2	5.04	121.92	118.90
36	1	295	A	C8-N9-C4	-5.04	103.78	105.80
36	1	780	A	N1-C6-N6	-5.04	115.58	118.60
36	5	280	U	N3-C4-C5	5.04	117.62	114.60
36	5	1858	A	C8-N9-C4	-5.04	103.78	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2301	U	O5'-P-OP2	-5.04	101.16	105.70
1	6	1092	A	N9-C4-C5	-5.04	103.78	105.80
36	5	2297	U	O5'-P-OP2	-5.04	101.16	105.70
37	7	47	C	N3-C2-O2	-5.04	118.37	121.90
1	2	1291	G	N1-C6-O6	5.04	122.92	119.90
36	1	422	A	N1-C6-N6	-5.04	115.58	118.60
36	1	2349	U	C2-N1-C1'	5.04	123.75	117.70
36	1	2651	G	C4-C5-N7	-5.04	108.78	110.80
36	5	419	G	N3-C4-N9	5.04	129.02	126.00
36	5	1177	G	N3-C4-N9	-5.04	122.98	126.00
36	5	1902	G	C5-C6-N1	5.04	114.02	111.50
36	5	2296	A	C8-N9-C4	-5.04	103.78	105.80
36	5	2393	G	O5'-P-OP1	5.04	116.75	110.70
38	8	25	G	N3-C4-C5	-5.04	126.08	128.60
1	6	308	C	C6-N1-C1'	5.04	126.84	120.80
1	2	970	A	OP2-P-O3'	5.04	116.28	105.20
36	1	88	A	N1-C6-N6	5.04	121.62	118.60
36	1	2537	U	P-O3'-C3'	5.04	125.74	119.70
1	6	609	U	C4-C5-C6	5.04	122.72	119.70
36	5	692	A	N1-C2-N3	-5.04	126.78	129.30
36	1	227	G	N1-C6-O6	5.03	122.92	119.90
36	1	1145	G	C5-C6-N1	5.03	114.02	111.50
36	1	1407	A	N1-C2-N3	-5.03	126.78	129.30
36	1	2249	G	C5-C6-N1	5.03	114.02	111.50
36	1	2954	U	N3-C2-O2	5.03	125.72	122.20
36	1	3214	U	O5'-P-OP2	-5.03	101.17	105.70
1	6	331	A	OP1-P-O3'	5.03	116.28	105.20
1	6	1399	C	C5-C6-N1	5.03	123.52	121.00
1	6	1771	U	C2-N3-C4	-5.03	123.98	127.00
36	5	3010	U	N3-C2-O2	-5.03	118.68	122.20
36	1	990	U	C5-C4-O4	-5.03	122.88	125.90
36	1	3200	G	C4-C5-N7	-5.03	108.79	110.80
36	5	2608	G	OP2-P-O3'	5.03	116.27	105.20
36	1	1420	C	N3-C4-N4	-5.03	114.48	118.00
36	1	2916	U	C5-C4-O4	-5.03	122.88	125.90
36	1	3268	A	C2-N3-C4	-5.03	108.08	110.60
38	4	28	C	C6-N1-C1'	-5.03	114.76	120.80
1	6	163	G	C4-N9-C1'	-5.03	119.96	126.50
1	6	1187	U	N3-C2-O2	-5.03	118.68	122.20
36	5	2990	G	N3-C4-N9	5.03	129.02	126.00
61	n5	115	ARG	NE-CZ-NH1	5.03	122.81	120.30
36	1	2152	A	C5-C6-N6	5.03	127.72	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1421	G	N3-C4-N9	-5.03	122.98	126.00
36	1	681	U	N3-C2-O2	5.03	125.72	122.20
36	1	2818	U	C4-C5-C6	-5.03	116.68	119.70
36	1	3057	U	N1-C2-N3	5.03	117.92	114.90
1	6	403	G	N9-C4-C5	-5.03	103.39	105.40
36	5	1440	G	N1-C6-O6	-5.03	116.88	119.90
36	5	2288	G	C6-N1-C2	-5.03	122.08	125.10
36	5	2399	A	O5'-P-OP2	-5.03	101.17	105.70
36	5	2945	G	C8-N9-C4	5.03	108.41	106.40
1	2	736	C	C2-N1-C1'	5.03	124.33	118.80
36	1	2885	C	C5-C6-N1	-5.03	118.49	121.00
1	6	926	A	C8-N9-C4	5.03	107.81	105.80
1	2	1035	G	N1-C6-O6	-5.02	116.89	119.90
36	1	2957	G	N7-C8-N9	-5.02	110.59	113.10
36	1	57	A	C8-N9-C4	5.02	107.81	105.80
36	1	1507	G	C4-C5-N7	-5.02	108.79	110.80
36	1	1911	A	C4-C5-N7	5.02	113.21	110.70
1	6	96	G	C8-N9-C4	-5.02	104.39	106.40
1	2	1783	C	O5'-P-OP1	5.02	116.72	110.70
36	1	200	C	C6-N1-C1'	-5.02	114.78	120.80
36	1	2323	G	N1-C6-O6	-5.02	116.89	119.90
36	1	2799	A	C4-C5-C6	5.02	119.51	117.00
36	1	3047	U	N3-C2-O2	-5.02	118.69	122.20
38	4	30	C	OP1-P-OP2	5.02	127.13	119.60
43	L6	77	ARG	NE-CZ-NH2	-5.02	117.79	120.30
36	5	368	G	N3-C2-N2	-5.02	116.39	119.90
36	5	3197	G	N1-C6-O6	5.02	122.91	119.90
36	1	93	C	C6-N1-C2	-5.02	118.29	120.30
36	1	874	U	C4-C5-C6	-5.02	116.69	119.70
36	1	1048	A	C4-C5-C6	-5.02	114.49	117.00
36	1	1555	U	N1-C2-O2	-5.02	119.29	122.80
36	1	2953	U	N1-C2-N3	5.02	117.91	114.90
36	5	74	G	N1-C6-O6	-5.02	116.89	119.90
36	5	1174	G	OP2-P-O3'	5.02	116.24	105.20
36	5	1335	C	N1-C2-O2	-5.02	115.89	118.90
36	5	3172	A	C8-N9-C4	5.02	107.81	105.80
37	7	81	U	N1-C2-O2	5.02	126.31	122.80
36	1	280	U	N3-C4-O4	5.02	122.91	119.40
1	6	378	A	N1-C6-N6	5.02	121.61	118.60
1	6	1032	G	N7-C8-N9	-5.02	110.59	113.10
36	5	26	A	N7-C8-N9	-5.02	111.29	113.80
36	5	103	G	N3-C4-N9	-5.02	122.99	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3188	G	N1-C6-O6	-5.02	116.89	119.90
1	2	469	C	N1-C2-O2	-5.01	115.89	118.90
36	1	2309	A	C5-C6-N6	-5.01	119.69	123.70
39	L2	207	VAL	CB-CA-C	-5.01	101.87	111.40
1	6	454	U	O5'-P-OP2	-5.01	101.19	105.70
36	5	2179	C	C6-N1-C2	5.01	122.31	120.30
36	5	2383	C	N3-C4-C5	-5.01	119.89	121.90
36	5	2426	U	N1-C2-O2	5.01	126.31	122.80
36	5	3308	C	N1-C2-N3	5.01	122.71	119.20
36	1	2932	U	O5'-P-OP2	-5.01	101.19	105.70
36	5	1655	G	N1-C6-O6	5.01	122.91	119.90
1	2	1758	U	N3-C2-O2	-5.01	118.69	122.20
36	1	347	G	C2-N3-C4	5.01	114.41	111.90
36	1	896	A	C8-N9-C4	-5.01	103.80	105.80
36	1	944	C	C2-N3-C4	5.01	122.41	119.90
36	1	2865	U	N3-C4-C5	5.01	117.61	114.60
36	5	1604	G	C8-N9-C1'	-5.01	120.49	127.00
1	2	1291	G	C6-C5-N7	-5.01	127.39	130.40
1	2	1324	G	N3-C2-N2	-5.01	116.39	119.90
36	1	421	G	N3-C2-N2	5.01	123.41	119.90
36	1	1117	G	N1-C6-O6	5.01	122.91	119.90
36	1	1362	G	C8-N9-C4	5.01	108.40	106.40
36	5	641	C	O5'-P-OP1	-5.01	101.19	105.70
36	5	1478	C	N1-C2-O2	-5.01	115.89	118.90
36	5	1520	G	O5'-P-OP2	5.01	116.71	110.70
36	5	3102	G	N3-C4-N9	5.01	129.00	126.00
1	2	767	U	N3-C2-O2	-5.01	118.69	122.20
36	1	110	G	N9-C1'-C2'	-5.01	106.49	112.00
36	1	660	A	C2-N3-C4	5.01	113.10	110.60
36	1	1166	G	C5-C6-O6	-5.01	125.60	128.60
36	1	2797	C	C6-N1-C2	5.01	122.30	120.30
1	6	1436	A	C8-N9-C4	-5.01	103.80	105.80
36	5	1454	A	O5'-P-OP2	-5.01	101.19	105.70
36	5	1685	C	N3-C2-O2	-5.01	118.39	121.90
36	1	1336	U	N1-C2-N3	5.00	117.90	114.90
1	6	1034	C	N1-C2-O2	-5.00	115.90	118.90
1	2	1782	A	N1-C6-N6	-5.00	115.60	118.60
36	1	2189	U	N1-C2-N3	5.00	117.90	114.90
36	5	220	G	OP1-P-O3'	5.00	116.21	105.20
36	5	1412	G	C8-N9-C1'	5.00	133.50	127.00
36	5	2816	G	C4-C5-N7	-5.00	108.80	110.80
36	5	2968	G	C5-C6-O6	5.00	131.60	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	706	A	N3-C4-N9	-5.00	123.40	127.40
36	1	814	U	O5'-P-OP2	5.00	116.70	110.70
36	1	826	G	O5'-P-OP1	-5.00	101.20	105.70
36	1	2184	U	C5-C6-N1	5.00	125.20	122.70
36	1	3040	A	OP2-P-O3'	5.00	116.20	105.20
36	1	3309	G	C6-C5-N7	-5.00	127.40	130.40
1	6	1019	A	N7-C8-N9	-5.00	111.30	113.80
1	6	1789	G	C5-N7-C8	5.00	106.80	104.30
36	5	1121	U	N1-C2-O2	-5.00	119.30	122.80
36	5	1484	U	C6-N1-C2	5.00	124.00	121.00
36	5	1889	G	N3-C4-C5	-5.00	126.10	128.60
36	5	2800	G	N3-C4-C5	5.00	131.10	128.60
36	5	2905	U	N3-C4-O4	-5.00	115.90	119.40

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	C1	88	ARG	Peptide
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
27	D5	54	VAL	Peptide
27	D5	94	LYS	Peptide
27	D5	96	SER	Peptide
28	D6	84	VAL	Peptide
28	D6	85	ARG	Peptide
28	D6	97	PRO	Peptide
39	L2	19	HIS	Peptide
43	L6	89	THR	Peptide
44	L7	157	ASN	Peptide
52	M6	110	PRO	Peptide
53	M7	120	ASN	Peptide
64	N8	30	GLY	Peptide
64	N8	93	SER	Peptide
65	N9	19	ASN	Peptide
67	O1	5	LYS	Peptide
78	Q2	29	LYS	Peptide
9	S7	31	SER	Peptide
10	S8	79	ALA	Peptide
34	SR	160	GLU	Mainchain

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Mol	Chain	Res	Type	Group
34	SR	161	LYS	Mainchain
17	c5	52	LYS	Peptide
19	c7	96	SER	Peptide
20	c8	144	ARG	Peptide
22	d0	70	THR	Peptide
25	d3	44	GLY	Peptide
81	e1	146	SER	Peptide
39	l2	143	GLU	Peptide
39	l2	171	GLY	Peptide
42	l5	271	LYS	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
52	m6	110	PRO	Peptide
53	m7	66	SER	Peptide
56	n0	133	ALA	Peptide
59	n3	33	ASN	Peptide
62	n6	111	LEU	Peptide
64	n8	66	ALA	Peptide
65	n9	19	ASN	Peptide
67	o1	64	VAL	Peptide
75	o9	50	ASN	Peptide
2	s0	165	ARG	Peptide
3	s1	130	SER	Peptide
6	s4	77	ARG	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%)	151 (74%)	36 (18%)	17 (8%)	1	2
2	s0	204/251 (81%)	157 (77%)	30 (15%)	17 (8%)	1	2
3	S1	212/254 (84%)	145 (68%)	35 (16%)	32 (15%)	0	0
3	s1	214/254 (84%)	179 (84%)	21 (10%)	14 (6%)	1	3
4	S2	215/253 (85%)	190 (88%)	17 (8%)	8 (4%)	3	13
4	s2	215/253 (85%)	184 (86%)	20 (9%)	11 (5%)	2	7
5	S3	221/239 (92%)	194 (88%)	19 (9%)	8 (4%)	3	14
5	s3	221/239 (92%)	182 (82%)	24 (11%)	15 (7%)	1	3
6	S4	258/260 (99%)	213 (83%)	34 (13%)	11 (4%)	2	10
6	s4	258/260 (99%)	224 (87%)	19 (7%)	15 (6%)	1	5
7	S5	204/224 (91%)	166 (81%)	20 (10%)	18 (9%)	1	2
7	s5	204/224 (91%)	167 (82%)	18 (9%)	19 (9%)	0	1
8	S6	224/236 (95%)	194 (87%)	19 (8%)	11 (5%)	2	8
8	s6	216/236 (92%)	189 (88%)	20 (9%)	7 (3%)	4	16
9	S7	182/189 (96%)	137 (75%)	26 (14%)	19 (10%)	0	1
9	s7	184/189 (97%)	154 (84%)	21 (11%)	9 (5%)	2	8
10	S8	184/200 (92%)	156 (85%)	13 (7%)	15 (8%)	1	2
10	s8	184/200 (92%)	163 (89%)	15 (8%)	6 (3%)	4	15
11	S9	183/196 (93%)	153 (84%)	21 (12%)	9 (5%)	2	8
11	s9	183/196 (93%)	154 (84%)	19 (10%)	10 (6%)	2	5
12	C0	94/105 (90%)	74 (79%)	13 (14%)	7 (7%)	1	2
12	c0	92/105 (88%)	65 (71%)	15 (16%)	12 (13%)	0	0
13	C1	153/155 (99%)	125 (82%)	14 (9%)	14 (9%)	1	1
13	c1	144/155 (93%)	123 (85%)	14 (10%)	7 (5%)	2	8
14	C2	122/142 (86%)	76 (62%)	24 (20%)	22 (18%)	0	0
14	c2	122/142 (86%)	74 (61%)	30 (25%)	18 (15%)	0	0
15	C3	148/150 (99%)	129 (87%)	13 (9%)	6 (4%)	3	11
15	c3	148/150 (99%)	124 (84%)	14 (10%)	10 (7%)	1	3
16	C4	125/136 (92%)	98 (78%)	16 (13%)	11 (9%)	1	2
16	c4	126/136 (93%)	102 (81%)	12 (10%)	12 (10%)	0	1
17	C5	122/141 (86%)	91 (75%)	21 (17%)	10 (8%)	1	2
17	c5	133/141 (94%)	97 (73%)	22 (16%)	14 (10%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C6	139/142 (98%)	122 (88%)	11 (8%)	6 (4%)	2	10
18	c6	140/142 (99%)	124 (89%)	10 (7%)	6 (4%)	2	10
19	C7	116/136 (85%)	87 (75%)	20 (17%)	9 (8%)	1	2
19	c7	113/136 (83%)	92 (81%)	10 (9%)	11 (10%)	0	1
20	C8	143/145 (99%)	117 (82%)	14 (10%)	12 (8%)	1	2
20	c8	143/145 (99%)	120 (84%)	16 (11%)	7 (5%)	2	8
21	C9	141/143 (99%)	121 (86%)	14 (10%)	6 (4%)	2	10
21	c9	141/143 (99%)	117 (83%)	17 (12%)	7 (5%)	2	7
22	D0	105/120 (88%)	87 (83%)	14 (13%)	4 (4%)	3	13
22	d0	108/120 (90%)	86 (80%)	13 (12%)	9 (8%)	1	2
23	D1	85/87 (98%)	67 (79%)	11 (13%)	7 (8%)	1	2
23	d1	85/87 (98%)	76 (89%)	8 (9%)	1 (1%)	13	40
24	D2	127/129 (98%)	113 (89%)	11 (9%)	3 (2%)	6	22
24	d2	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	51
25	D3	142/144 (99%)	109 (77%)	17 (12%)	16 (11%)	0	1
25	d3	142/144 (99%)	124 (87%)	17 (12%)	1 (1%)	22	54
26	D4	132/134 (98%)	111 (84%)	14 (11%)	7 (5%)	2	6
26	d4	132/134 (98%)	109 (83%)	18 (14%)	5 (4%)	3	13
27	D5	68/107 (64%)	48 (71%)	10 (15%)	10 (15%)	0	0
27	d5	67/107 (63%)	52 (78%)	10 (15%)	5 (8%)	1	2
28	D6	95/97 (98%)	66 (70%)	10 (10%)	19 (20%)	0	0
28	d6	95/97 (98%)	74 (78%)	13 (14%)	8 (8%)	1	2
29	D7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	3	13
29	d7	79/81 (98%)	62 (78%)	12 (15%)	5 (6%)	1	4
30	D8	61/66 (92%)	51 (84%)	6 (10%)	4 (7%)	1	3
30	d8	61/66 (92%)	46 (75%)	13 (21%)	2 (3%)	4	15
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	3	12
31	d9	51/55 (93%)	43 (84%)	4 (8%)	4 (8%)	1	2
32	E0	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	2	6
33	E1	69/76 (91%)	35 (51%)	19 (28%)	15 (22%)	0	0
34	SR	316/318 (99%)	252 (80%)	36 (11%)	28 (9%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	sR	316/318 (99%)	274 (87%)	30 (10%)	12 (4%)	3	13
35	SM	155/273 (57%)	112 (72%)	22 (14%)	21 (14%)	0	0
35	sM	98/273 (36%)	65 (66%)	18 (18%)	15 (15%)	0	0
39	L2	250/253 (99%)	222 (89%)	25 (10%)	3 (1%)	13	40
39	l2	250/253 (99%)	219 (88%)	25 (10%)	6 (2%)	6	22
40	L3	384/386 (100%)	339 (88%)	31 (8%)	14 (4%)	3	14
40	l3	384/386 (100%)	343 (89%)	31 (8%)	10 (3%)	5	20
41	L4	359/361 (99%)	303 (84%)	37 (10%)	19 (5%)	2	6
41	l4	359/361 (99%)	309 (86%)	31 (9%)	19 (5%)	2	6
42	L5	294/296 (99%)	249 (85%)	27 (9%)	18 (6%)	1	4
42	l5	292/296 (99%)	256 (88%)	32 (11%)	4 (1%)	11	36
43	L6	152/175 (87%)	140 (92%)	10 (7%)	2 (1%)	12	37
43	l6	153/175 (87%)	130 (85%)	19 (12%)	4 (3%)	5	20
44	L7	220/243 (90%)	202 (92%)	11 (5%)	7 (3%)	4	16
44	l7	221/243 (91%)	204 (92%)	14 (6%)	3 (1%)	11	36
45	L8	231/255 (91%)	189 (82%)	30 (13%)	12 (5%)	2	6
45	l8	229/255 (90%)	185 (81%)	23 (10%)	21 (9%)	1	1
46	L9	189/191 (99%)	170 (90%)	15 (8%)	4 (2%)	7	26
46	l9	189/191 (99%)	173 (92%)	13 (7%)	3 (2%)	9	32
47	M0	207/220 (94%)	182 (88%)	18 (9%)	7 (3%)	3	15
47	m0	209/220 (95%)	175 (84%)	25 (12%)	9 (4%)	2	10
48	M1	167/173 (96%)	127 (76%)	26 (16%)	14 (8%)	1	2
48	m1	167/173 (96%)	143 (86%)	15 (9%)	9 (5%)	2	6
49	M3	191/198 (96%)	170 (89%)	17 (9%)	4 (2%)	7	26
49	m3	192/198 (97%)	162 (84%)	18 (9%)	12 (6%)	1	4
50	M4	134/137 (98%)	116 (87%)	11 (8%)	7 (5%)	2	6
50	m4	135/137 (98%)	126 (93%)	7 (5%)	2 (2%)	10	34
51	M5	201/203 (99%)	186 (92%)	8 (4%)	7 (4%)	3	14
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	4	17
52	M6	195/198 (98%)	183 (94%)	7 (4%)	5 (3%)	5	20
52	m6	195/198 (98%)	184 (94%)	8 (4%)	3 (2%)	10	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	M7	181/183 (99%)	156 (86%)	17 (9%)	8 (4%)	2	10
53	m7	153/183 (84%)	136 (89%)	16 (10%)	1 (1%)	22	54
54	M8	183/185 (99%)	166 (91%)	12 (7%)	5 (3%)	5	19
54	m8	183/185 (99%)	161 (88%)	15 (8%)	7 (4%)	3	13
55	M9	186/188 (99%)	177 (95%)	7 (4%)	2 (1%)	14	42
55	m9	186/188 (99%)	169 (91%)	14 (8%)	3 (2%)	9	32
56	N0	170/172 (99%)	156 (92%)	10 (6%)	4 (2%)	6	22
56	n0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	25	58
57	N1	157/159 (99%)	137 (87%)	14 (9%)	6 (4%)	3	13
57	n1	157/159 (99%)	142 (90%)	12 (8%)	3 (2%)	8	28
58	N2	98/120 (82%)	73 (74%)	19 (19%)	6 (6%)	1	4
58	n2	96/120 (80%)	79 (82%)	13 (14%)	4 (4%)	3	10
59	N3	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	22	54
59	n3	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	10	34
60	N4	96/155 (62%)	72 (75%)	15 (16%)	9 (9%)	0	1
60	n4	133/155 (86%)	113 (85%)	11 (8%)	9 (7%)	1	3
61	N5	119/141 (84%)	108 (91%)	9 (8%)	2 (2%)	9	31
61	n5	118/141 (84%)	97 (82%)	15 (13%)	6 (5%)	2	7
62	N6	124/126 (98%)	111 (90%)	7 (6%)	6 (5%)	2	8
62	n6	124/126 (98%)	109 (88%)	10 (8%)	5 (4%)	3	11
63	N7	133/135 (98%)	115 (86%)	11 (8%)	7 (5%)	2	6
63	n7	133/135 (98%)	109 (82%)	11 (8%)	13 (10%)	0	1
64	N8	146/148 (99%)	120 (82%)	18 (12%)	8 (6%)	2	5
64	n8	146/148 (99%)	129 (88%)	16 (11%)	1 (1%)	22	54
65	N9	56/58 (97%)	50 (89%)	4 (7%)	2 (4%)	3	14
65	n9	56/58 (97%)	44 (79%)	9 (16%)	3 (5%)	2	6
66	O0	95/104 (91%)	89 (94%)	4 (4%)	2 (2%)	7	26
66	o0	98/104 (94%)	88 (90%)	8 (8%)	2 (2%)	7	27
67	O1	107/112 (96%)	96 (90%)	7 (6%)	4 (4%)	3	13
67	o1	107/112 (96%)	89 (83%)	10 (9%)	8 (8%)	1	2
68	O2	125/129 (97%)	113 (90%)	11 (9%)	1 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	o2	125/129 (97%)	108 (86%)	14 (11%)	3 (2%)	6	22
69	O3	104/106 (98%)	99 (95%)	4 (4%)	1 (1%)	15	45
69	o3	104/106 (98%)	95 (91%)	6 (6%)	3 (3%)	4	18
70	O4	110/119 (92%)	102 (93%)	7 (6%)	1 (1%)	17	48
70	o4	110/119 (92%)	102 (93%)	5 (4%)	3 (3%)	5	19
71	O5	117/119 (98%)	104 (89%)	9 (8%)	4 (3%)	3	15
71	o5	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	9	31
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	1	4
72	o6	97/99 (98%)	84 (87%)	5 (5%)	8 (8%)	1	2
73	O7	85/87 (98%)	74 (87%)	11 (13%)	0	100	100
73	o7	85/87 (98%)	74 (87%)	9 (11%)	2 (2%)	6	22
74	O8	75/77 (97%)	65 (87%)	8 (11%)	2 (3%)	5	19
74	o8	75/77 (97%)	67 (89%)	5 (7%)	3 (4%)	3	11
75	O9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	7	26
76	Q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3	11
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	7	27
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	89 (86%)	9 (9%)	5 (5%)	2	8
78	q2	103/105 (98%)	94 (91%)	7 (7%)	2 (2%)	8	28
79	Q3	89/91 (98%)	81 (91%)	6 (7%)	2 (2%)	6	24
79	q3	89/91 (98%)	81 (91%)	6 (7%)	2 (2%)	6	24
80	e0	60/62 (97%)	51 (85%)	5 (8%)	4 (7%)	1	3
81	e1	74/76 (97%)	37 (50%)	18 (24%)	19 (26%)	0	0
83	p0	139/311 (45%)	114 (82%)	21 (15%)	4 (3%)	4	18
All	All	22333/24141 (92%)	18964 (85%)	2226 (10%)	1143 (5%)	2	7

All (1143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	30	GLN

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Mol	Chain	Res	Type
2	S0	39	ASN
2	S0	95	ALA
2	S0	158	VAL
2	S0	191	ARG
3	S1	49	ASN
3	S1	81	PHE
3	S1	206	PRO
3	S1	221	PRO
5	S3	62	ASN
5	S3	93	ASP
5	S3	216	PRO
5	S3	220	PRO
6	S4	80	THR
6	S4	104	ASP
7	S5	26	ALA
7	S5	39	GLU
7	S5	43	PHE
7	S5	63	GLN
8	S6	122	GLU
8	S6	154	ARG
8	S6	173	PRO
8	S6	174	LYS
9	S7	31	SER
9	S7	64	VAL
9	S7	111	LYS
9	S7	112	ARG
9	S7	131	PHE
9	S7	155	ASP
10	S8	22	ARG
10	S8	81	VAL
10	S8	120	THR
10	S8	149	SER
10	S8	152	ILE
11	S9	134	ILE
11	S9	150	LEU
12	C0	54	TYR
12	C0	85	HIS
12	C0	87	VAL
12	C0	88	PRO
13	C1	7	VAL
13	C1	29	LYS
13	C1	139	VAL

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Mol	Chain	Res	Type
14	C2	101	ALA
14	C2	115	VAL
14	C2	126	TRP
14	C2	130	THR
15	C3	22	ALA
15	C3	27	LYS
16	C4	42	VAL
16	C4	50	ALA
16	C4	124	ASP
16	C4	125	SER
16	C4	126	THR
18	C6	58	ASP
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	124	VAL
20	C8	14	ILE
20	C8	60	GLU
20	C8	61	LEU
20	C8	82	PRO
20	C8	83	ALA
20	C8	91	ASP
20	C8	92	ILE
21	C9	53	TRP
22	D0	17	GLN
24	D2	66	ASN
24	D2	127	GLY
25	D3	5	LYS
25	D3	92	CYS
25	D3	114	LYS
25	D3	125	VAL
25	D3	131	SER
25	D3	137	LYS
25	D3	144	ARG
26	D4	35	VAL
27	D5	43	ASP
27	D5	44	GLN
27	D5	56	THR
27	D5	71	ILE
28	D6	45	VAL
28	D6	82	ARG
28	D6	84	VAL

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Mol	Chain	Res	Type
28	D6	85	ARG
29	D7	38	PRO
31	D9	8	PHE
32	E0	47	VAL
33	E1	98	VAL
33	E1	102	VAL
33	E1	103	LEU
33	E1	138	ARG
34	SR	24	ALA
34	SR	114	ASP
34	SR	155	ARG
34	SR	161	LYS
34	SR	203	THR
35	SM	52	PRO
35	SM	87	THR
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
39	L2	144	ASN
40	L3	3	HIS
40	L3	5	LYS
40	L3	140	ASP
40	L3	347	SER
41	L4	4	PRO
41	L4	130	ALA
41	L4	268	ALA
41	L4	269	SER
41	L4	270	SER
41	L4	311	HIS
41	L4	320	ASN
42	L5	215	ASP
42	L5	233	ALA
42	L5	234	ASP
42	L5	258	LYS
44	L7	24	GLU
44	L7	26	VAL
44	L7	164	SER
45	L8	25	PRO
45	L8	36	ILE
45	L8	157	VAL
46	L9	50	ASN
47	M0	211	ARG

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Mol	Chain	Res	Type
47	M0	219	ALA
47	M0	220	GLN
48	M1	9	MET
48	M1	24	GLY
48	M1	74	PRO
48	M1	165	GLN
49	M3	47	ALA
50	M4	8	LYS
50	M4	9	ALA
50	M4	136	ALA
51	M5	74	PRO
51	M5	144	ARG
52	M6	111	PRO
52	M6	182	ASN
53	M7	157	VAL
54	M8	99	THR
56	N0	167	ARG
57	N1	124	VAL
57	N1	159	PHE
58	N2	31	ALA
58	N2	51	GLY
58	N2	60	GLY
59	N3	82	ALA
60	N4	81	PRO
60	N4	97	LYS
61	N5	44	PRO
61	N5	45	LYS
62	N6	52	ARG
62	N6	84	LYS
63	N7	3	LYS
63	N7	125	GLY
63	N7	128	GLN
64	N8	57	GLY
64	N8	76	ASP
64	N8	93	SER
67	O1	84	ASP
71	O5	119	LYS
72	O6	33	ALA
72	O6	98	ARG
74	O8	8	ILE
76	Q0	78	ILE
78	Q2	94	GLY

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Mol	Chain	Res	Type
78	Q2	100	LYS
2	s0	4	PRO
2	s0	158	VAL
2	s0	186	GLY
2	s0	189	VAL
2	s0	206	ASP
3	s1	206	PRO
4	s2	91	ARG
4	s2	92	ALA
4	s2	107	SER
5	s3	61	GLU
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	24	SER
6	s4	195	ILE
6	s4	196	VAL
7	s5	28	PRO
7	s5	36	ALA
7	s5	43	PHE
7	s5	184	PHE
8	s6	25	ARG
8	s6	122	GLU
8	s6	173	PRO
9	s7	30	SER
9	s7	64	VAL
9	s7	67	LEU
9	s7	131	PHE
9	s7	185	ILE
11	s9	117	GLY
12	c0	2	LEU
12	c0	83	PRO
12	c0	88	PRO
12	c0	92	ILE
12	c0	97	PRO
13	c1	28	SER
13	c1	114	ALA
13	c1	144	ALA
14	c2	22	VAL
15	c3	19	SER
15	c3	66	ILE

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Mol	Chain	Res	Type
15	c3	87	ASP
16	c4	50	ALA
16	c4	124	ASP
16	c4	126	THR
16	c4	132	ARG
17	c5	51	SER
17	c5	52	LYS
17	c5	68	PRO
17	c5	125	PRO
17	c5	126	VAL
17	c5	127	ARG
18	c6	42	GLU
18	c6	116	LEU
19	c7	67	ARG
19	c7	88	VAL
20	c8	91	ASP
20	c8	92	ILE
20	c8	145	ARG
21	c9	29	GLU
21	c9	34	VAL
21	c9	142	GLU
22	d0	15	GLN
22	d0	49	ASN
22	d0	51	VAL
22	d0	52	LYS
22	d0	119	ALA
22	d0	120	SER
25	d3	131	SER
26	d4	30	PRO
26	d4	33	ALA
27	d5	85	LYS
27	d5	104	ALA
28	d6	63	ALA
29	d7	38	PRO
29	d7	59	CYS
30	d8	33	LEU
30	d8	61	ARG
31	d9	6	VAL
31	d9	7	TRP
80	e0	60	PRO
81	e1	83	LYS
81	e1	84	VAL

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Mol	Chain	Res	Type
81	e1	87	THR
81	e1	92	LYS
81	e1	98	VAL
81	e1	102	VAL
81	e1	103	LEU
81	e1	106	TYR
34	sR	4	ASN
34	sR	163	ASP
34	sR	165	ASP
35	sM	47	ALA
39	l2	194	ASN
40	l3	140	ASP
40	l3	347	SER
41	l4	90	PHE
41	l4	302	ALA
41	l4	311	HIS
41	l4	329	PRO
41	l4	330	TYR
41	l4	338	LYS
41	l4	339	LEU
42	l5	260	PHE
42	l5	270	LYS
43	l6	97	ASN
43	l6	98	VAL
45	l8	25	PRO
45	l8	34	PHE
45	l8	79	GLN
45	l8	120	LYS
45	l8	122	LYS
47	m0	3	ARG
47	m0	195	ALA
47	m0	219	ALA
48	m1	8	PRO
48	m1	10	ARG
48	m1	39	GLN
48	m1	108	GLU
49	m3	47	ALA
49	m3	51	LEU
49	m3	129	ASN
49	m3	134	GLU
49	m3	152	THR
50	m4	136	ALA

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Mol	Chain	Res	Type
51	m5	184	LYS
52	m6	16	VAL
52	m6	110	PRO
54	m8	41	ASP
54	m8	99	THR
56	n0	2	ALA
57	n1	122	GLN
57	n1	135	PRO
59	n3	42	SER
60	n4	26	SER
60	n4	76	VAL
61	n5	24	LEU
62	n6	45	ILE
62	n6	83	ASP
62	n6	126	LEU
63	n7	5	LEU
65	n9	21	ILE
65	n9	23	LYS
65	n9	39	PHE
67	o1	7	VAL
67	o1	45	GLY
68	o2	5	PRO
69	o3	88	ASN
70	o4	79	SER
72	o6	30	LYS
72	o6	33	ALA
72	o6	98	ARG
2	S0	5	ALA
2	S0	195	TRP
3	S1	35	PRO
3	S1	51	SER
3	S1	58	SER
3	S1	63	GLY
3	S1	79	HIS
3	S1	82	ARG
3	S1	116	LYS
3	S1	117	TRP
3	S1	148	ASN
3	S1	154	SER
3	S1	177	GLN
3	S1	179	SER
3	S1	209	ASN

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Mol	Chain	Res	Type
3	S1	218	LEU
4	S2	91	ARG
4	S2	107	SER
5	S3	143	ARG
6	S4	12	LEU
6	S4	26	CYS
6	S4	164	LEU
6	S4	195	ILE
7	S5	35	GLN
7	S5	45	LYS
7	S5	101	GLY
7	S5	127	GLN
7	S5	150	GLY
7	S5	153	GLY
7	S5	154	ALA
8	S6	146	GLY
8	S6	165	GLY
9	S7	5	GLN
9	S7	73	VAL
9	S7	98	ILE
9	S7	156	SER
10	S8	82	VAL
10	S8	105	ASP
10	S8	153	GLU
11	S9	121	SER
12	C0	60	SER
13	C1	55	ASP
13	C1	89	ALA
13	C1	140	VAL
13	C1	145	ALA
14	C2	54	ARG
14	C2	55	GLY
14	C2	91	VAL
14	C2	93	ASP
14	C2	106	ILE
16	C4	51	ASP
16	C4	123	SER
17	C5	54	ALA
18	C6	97	VAL
19	C7	115	LEU
20	C8	7	GLU
20	C8	25	ASN

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Mol	Chain	Res	Type
20	C8	145	ARG
21	C9	69	LYS
23	D1	49	GLU
24	D2	83	ILE
25	D3	8	GLY
25	D3	112	LYS
25	D3	124	VAL
26	D4	4	ALA
26	D4	5	VAL
27	D5	55	PRO
28	D6	10	ARG
28	D6	18	VAL
28	D6	47	ALA
28	D6	61	GLU
28	D6	63	ALA
28	D6	75	VAL
28	D6	86	VAL
29	D7	62	ILE
33	E1	110	ALA
33	E1	111	GLU
33	E1	128	ALA
34	SR	201	THR
34	SR	231	MET
35	SM	86	ASN
35	SM	89	ARG
35	SM	102	THR
35	SM	139	GLU
35	SM	172	VAL
39	L2	250	GLN
40	L3	138	ALA
40	L3	139	GLN
40	L3	155	ALA
40	L3	351	LEU
41	L4	15	ALA
41	L4	190	GLY
41	L4	291	ASN
42	L5	57	ASN
42	L5	253	PHE
42	L5	260	PHE
43	L6	98	VAL
44	L7	160	ARG
45	L8	39	ALA

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Mol	Chain	Res	Type
45	L8	78	PHE
45	L8	120	LYS
46	L9	190	ASP
49	M3	76	THR
50	M4	135	LEU
51	M5	75	VAL
51	M5	184	LYS
52	M6	16	VAL
52	M6	183	ALA
53	M7	179	GLN
53	M7	182	ILE
54	M8	147	ARG
55	M9	53	LYS
58	N2	11	ILE
58	N2	32	SER
60	N4	16	GLY
60	N4	64	THR
62	N6	53	ASP
62	N6	126	LEU
63	N7	35	SER
64	N8	47	LYS
64	N8	66	ALA
67	O1	6	ASP
68	O2	127	ALA
70	O4	77	GLY
71	O5	97	ALA
72	O6	28	TYR
74	O8	35	GLY
78	Q2	15	LYS
2	s0	44	GLY
2	s0	68	PRO
2	s0	95	ALA
2	s0	103	THR
3	s1	93	GLY
3	s1	106	THR
3	s1	147	ALA
3	s1	179	SER
3	s1	223	PHE
4	s2	93	GLY
4	s2	163	GLY
5	s3	180	GLY
5	s3	203	PRO

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Mol	Chain	Res	Type
6	s4	12	LEU
6	s4	57	ASN
6	s4	95	THR
6	s4	163	ASP
6	s4	164	LEU
7	s5	37	GLN
7	s5	39	GLU
7	s5	54	LYS
7	s5	58	LEU
7	s5	153	GLY
7	s5	204	GLY
8	s6	68	LEU
10	s8	62	THR
11	s9	134	ILE
11	s9	167	ALA
11	s9	183	ALA
12	c0	23	ALA
14	c2	45	LEU
14	c2	58	LEU
14	c2	89	ILE
14	c2	115	VAL
14	c2	118	ALA
14	c2	119	SER
15	c3	22	ALA
15	c3	29	SER
15	c3	139	TRP
16	c4	108	SER
16	c4	131	GLY
17	c5	11	VAL
17	c5	50	THR
19	c7	96	SER
19	c7	99	VAL
19	c7	116	LYS
20	c8	14	ILE
20	c8	60	GLU
20	c8	61	LEU
21	c9	33	TYR
22	d0	17	GLN
22	d0	118	VAL
26	d4	35	VAL
26	d4	58	PHE
27	d5	87	GLY

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Mol	Chain	Res	Type
29	d7	3	LEU
29	d7	75	GLU
31	d9	5	ASN
34	sR	161	LYS
35	sM	42	ALA
35	sM	50	ASN
39	l2	250	GLN
40	l3	3	HIS
40	l3	129	ALA
40	l3	333	LYS
41	l4	24	ALA
45	l8	119	ALA
45	l8	133	LYS
45	l8	237	ILE
46	l9	144	ILE
47	m0	193	ASP
48	m1	167	TYR
49	m3	50	PRO
49	m3	135	ALA
51	m5	183	THR
53	m7	67	ILE
54	m8	91	ALA
55	m9	35	ALA
55	m9	156	ASN
58	n2	50	LEU
58	n2	51	GLY
60	n4	63	ILE
60	n4	77	LYS
61	n5	38	LEU
61	n5	40	LEU
62	n6	84	LYS
62	n6	125	LYS
63	n7	16	GLY
63	n7	129	TRP
63	n7	130	PHE
63	n7	134	LEU
66	o0	46	ALA
67	o1	83	GLU
67	o1	84	ASP
68	o2	6	HIS
69	o3	91	ALA
71	o5	119	LYS

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Mol	Chain	Res	Type
72	o6	63	ASN
74	o8	18	ALA
76	q0	78	ILE
83	p0	47	GLY
83	p0	93	LEU
2	S0	49	ASN
2	S0	72	ASP
2	S0	189	VAL
2	S0	192	THR
2	S0	205	ARG
3	S1	26	ARG
3	S1	93	GLY
4	S2	147	ASN
4	S2	148	LEU
5	S3	218	LEU
6	S4	77	ARG
7	S5	58	LEU
7	S5	64	VAL
7	S5	156	ARG
8	S6	148	SER
9	S7	32	PRO
9	S7	36	ALA
9	S7	85	PHE
10	S8	40	ALA
10	S8	41	LYS
10	S8	52	ASN
11	S9	164	PHE
11	S9	169	PRO
12	C0	81	ASN
13	C1	4	GLU
13	C1	30	ARG
13	C1	75	VAL
13	C1	154	ALA
14	C2	21	GLU
14	C2	22	VAL
14	C2	107	ASP
14	C2	119	SER
14	C2	129	GLU
14	C2	131	ASP
15	C3	3	ARG
15	C3	10	GLY
16	C4	18	ARG

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Mol	Chain	Res	Type
16	C4	40	ALA
16	C4	114	ARG
17	C5	24	LYS
17	C5	25	LEU
17	C5	51	SER
17	C5	101	ALA
17	C5	125	PRO
20	C8	144	ARG
21	C9	50	ALA
23	D1	6	GLY
25	D3	41	SER
25	D3	109	ARG
25	D3	138	GLU
26	D4	34	ASN
26	D4	58	PHE
27	D5	39	ALA
27	D5	42	LEU
27	D5	97	LYS
28	D6	46	GLU
28	D6	65	PRO
28	D6	97	PRO
30	D8	14	LYS
30	D8	36	THR
32	E0	51	ASN
33	E1	87	THR
34	SR	98	GLU
34	SR	117	LYS
34	SR	160	GLU
34	SR	242	SER
34	SR	318	ALA
35	SM	42	ALA
35	SM	88	ARG
35	SM	101	ASP
35	SM	153	ASP
35	SM	174	LEU
40	L3	136	LYS
40	L3	142	ALA
40	L3	385	LYS
41	L4	16	THR
41	L4	233	LEU
41	L4	339	LEU
41	L4	361	HIS

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Mol	Chain	Res	Type
42	L5	58	LYS
42	L5	137	ASP
42	L5	252	ALA
42	L5	259	LYS
42	L5	295	GLY
44	L7	25	GLN
45	L8	112	GLU
46	L9	42	ASP
47	M0	113	GLN
47	M0	187	ALA
48	M1	8	PRO
48	M1	94	ARG
48	M1	114	ILE
48	M1	167	TYR
50	M4	10	SER
51	M5	145	ASP
53	M7	160	ALA
53	M7	161	ALA
53	M7	164	LYS
54	M8	98	LYS
56	N0	142	GLN
57	N1	114	ALA
57	N1	123	GLY
58	N2	44	GLU
60	N4	76	VAL
62	N6	83	ASP
65	N9	25	LYS
67	O1	82	GLU
71	O5	96	GLU
72	O6	3	VAL
72	O6	34	SER
79	Q3	51	ALA
2	s0	8	ASP
2	s0	14	ALA
2	s0	94	GLY
2	s0	185	ARG
3	s1	26	ARG
3	s1	129	THR
3	s1	154	SER
3	s1	232	HIS
5	s3	45	LYS
5	s3	60	GLY

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Mol	Chain	Res	Type
5	s3	90	ARG
5	s3	93	ASP
6	s4	245	LYS
7	s5	29	ILE
7	s5	60	ASP
7	s5	100	ASN
8	s6	70	PRO
9	s7	32	PRO
10	s8	101	ILE
11	s9	121	SER
11	s9	162	SER
12	c0	3	MET
12	c0	24	LYS
12	c0	82	LEU
13	c1	55	ASP
14	c2	87	PRO
14	c2	90	LYS
14	c2	101	ALA
14	c2	108	ARG
17	c5	8	LYS
17	c5	17	TYR
19	c7	63	LYS
19	c7	97	ASN
19	c7	98	GLY
19	c7	120	SER
22	d0	96	PRO
26	d4	53	ASP
28	d6	34	LYS
28	d6	46	GLU
80	e0	54	ARG
81	e1	107	LYS
81	e1	127	GLY
81	e1	128	ALA
81	e1	136	LYS
34	sR	96	THR
35	sM	46	LYS
35	sM	63	ASP
35	sM	78	ASP
35	sM	172	VAL
39	l2	56	ALA
39	l2	80	GLU
39	l2	142	ASP

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Mol	Chain	Res	Type
40	l3	155	ALA
40	l3	293	ASN
41	l4	5	GLN
41	l4	145	ILE
41	l4	232	SER
44	l7	191	VAL
45	l8	81	THR
45	l8	121	SER
45	l8	203	VAL
47	m0	175	ASN
47	m0	207	GLU
49	m3	60	ALA
49	m3	193	ALA
51	m5	81	TYR
54	m8	183	GLY
60	n4	127	LYS
61	n5	44	PRO
61	n5	47	ALA
63	n7	6	LYS
63	n7	125	GLY
67	o1	85	ALA
67	o1	86	LYS
70	o4	82	ALA
72	o6	34	SER
73	o7	85	LYS
73	o7	86	ALA
2	S0	103	THR
2	S0	185	ARG
2	S0	194	PRO
3	S1	54	LEU
3	S1	132	ASP
3	S1	147	ALA
3	S1	158	SER
3	S1	224	ASP
4	S2	150	GLN
5	S3	217	ILE
6	S4	245	LYS
7	S5	21	THR
7	S5	51	VAL
7	S5	65	ARG
7	S5	204	GLY
8	S6	152	ASP

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Mol	Chain	Res	Type
9	S7	30	SER
9	S7	84	LYS
9	S7	133	THR
9	S7	134	GLU
9	S7	186	PRO
10	S8	9	HIS
10	S8	199	LYS
11	S9	98	ALA
11	S9	120	LYS
11	S9	163	PRO
13	C1	72	THR
14	C2	25	GLU
14	C2	66	VAL
14	C2	87	PRO
14	C2	108	ARG
14	C2	112	ALA
15	C3	28	LEU
17	C5	52	LYS
17	C5	69	GLU
18	C6	113	ASP
19	C7	6	THR
19	C7	83	GLN
19	C7	113	LEU
20	C8	8	GLN
21	C9	35	ASP
22	D0	18	GLN
22	D0	21	LYS
23	D1	12	TYR
23	D1	81	ASN
27	D5	41	ILE
28	D6	64	LEU
33	E1	118	ARG
33	E1	137	ASP
33	E1	148	TYR
34	SR	4	ASN
34	SR	22	SER
34	SR	51	ASP
34	SR	112	SER
34	SR	163	ASP
34	SR	237	GLN
34	SR	244	ALA
34	SR	270	LEU

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Mol	Chain	Res	Type
35	SM	53	ARG
41	L4	232	SER
42	L5	93	THR
42	L5	115	LEU
42	L5	230	ASP
42	L5	296	GLN
45	L8	117	ALA
45	L8	169	LEU
47	M0	194	GLY
48	M1	73	GLY
48	M1	117	ASP
48	M1	148	VAL
49	M3	134	GLU
49	M3	136	GLU
50	M4	28	SER
51	M5	94	TYR
56	N0	2	ALA
57	N1	125	ALA
60	N4	87	LEU
60	N4	96	LEU
62	N6	92	GLY
63	N7	102	GLU
63	N7	103	GLN
64	N8	96	LYS
72	O6	21	THR
76	Q0	79	GLU
79	Q3	7	LYS
2	s0	10	THR
2	s0	139	VAL
3	s1	82	ARG
4	s2	95	ARG
4	s2	106	ASP
4	s2	150	GLN
4	s2	235	LEU
4	s2	238	SER
5	s3	59	LEU
6	s4	90	ILE
6	s4	202	ASP
7	s5	35	GLN
7	s5	57	SER
8	s6	165	GLY
9	s7	11	GLN

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Mol	Chain	Res	Type
10	s8	137	LYS
10	s8	199	LYS
11	s9	168	ARG
12	c0	35	ILE
13	c1	7	VAL
13	c1	61	THR
14	c2	103	LEU
14	c2	106	ILE
15	c3	140	LYS
16	c4	12	GLN
16	c4	37	GLU
16	c4	92	LYS
16	c4	114	ARG
16	c4	125	SER
17	c5	10	ARG
18	c6	4	VAL
19	c7	62	GLN
19	c7	86	PRO
21	c9	119	LYS
28	d6	59	TYR
31	d9	11	PRO
80	e0	47	VAL
80	e0	61	SER
81	e1	85	TYR
81	e1	100	LEU
34	sR	149	ASP
34	sR	318	ALA
35	sM	43	ASP
35	sM	77	THR
35	sM	121	LYS
39	l2	215	ASN
41	l4	15	ALA
41	l4	146	PRO
41	l4	304	GLN
42	l5	123	GLU
43	l6	10	TYR
44	l7	28	ALA
45	l8	39	ALA
45	l8	69	LEU
45	l8	82	LEU
45	l8	114	ALA
45	l8	115	ALA

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Mol	Chain	Res	Type
45	l8	117	ALA
45	l8	123	GLN
46	l9	2	LYS
47	m0	187	ALA
48	m1	153	LYS
49	m3	93	ILE
50	m4	3	THR
54	m8	98	LYS
54	m8	171	LYS
57	n1	121	ALA
59	n3	41	GLY
60	n4	72	SER
63	n7	56	LYS
63	n7	127	ASN
68	o2	124	GLY
71	o5	99	GLN
74	o8	17	ARG
75	o9	3	ALA
78	q2	78	LYS
79	q3	4	ARG
83	p0	198	PRO
3	S1	176	VAL
3	S1	202	LYS
4	S2	92	ALA
4	S2	248	SER
8	S6	69	LEU
10	S8	10	LYS
10	S8	59	ARG
12	C0	92	ILE
13	C1	3	THR
14	C2	53	THR
15	C3	12	SER
18	C6	59	LYS
19	C7	23	LYS
23	D1	10	GLU
25	D3	37	ALA
25	D3	40	SER
25	D3	97	ASP
28	D6	36	ILE
28	D6	62	TYR
29	D7	57	GLU
30	D8	61	ARG

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Mol	Chain	Res	Type
33	E1	84	VAL
33	E1	93	HIS
33	E1	94	LYS
33	E1	127	GLY
34	SR	3	SER
34	SR	153	GLN
35	SM	12	VAL
35	SM	17	VAL
35	SM	155	LEU
40	L3	4	ARG
40	L3	317	ILE
41	L4	5	GLN
41	L4	146	PRO
41	L4	338	LYS
42	L5	6	ASP
43	L6	132	ALA
44	L7	178	ILE
45	L8	79	GLN
47	M0	218	ALA
48	M1	11	ASP
48	M1	95	ASN
50	M4	6	ILE
53	M7	163	LYS
54	M8	162	ALA
55	M9	130	ASN
56	N0	50	LYS
57	N1	18	ASP
63	N7	36	HIS
64	N8	56	VAL
64	N8	117	ARG
65	N9	21	ILE
69	O3	59	VAL
78	Q2	34	SER
3	s1	22	ASP
3	s1	233	GLY
4	s2	83	ILE
5	s3	44	THR
6	s4	104	ASP
6	s4	168	LYS
7	s5	56	ALA
7	s5	127	GLN
9	s7	13	PRO

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Mol	Chain	Res	Type
9	s7	111	LYS
12	c0	20	VAL
12	c0	30	ALA
14	c2	39	ASP
14	c2	82	PRO
14	c2	107	ASP
15	c3	60	VAL
17	c5	69	GLU
17	c5	132	GLY
18	c6	97	VAL
23	d1	10	GLU
27	d5	44	GLN
27	d5	103	ARG
28	d6	13	LYS
81	e1	81	LYS
81	e1	131	PHE
81	e1	148	TYR
34	sR	281	TYR
35	sM	36	ASP
35	sM	64	LYS
35	sM	120	GLU
41	l4	328	ASN
41	l4	342	LYS
45	l8	112	GLU
45	l8	124	ASP
46	l9	167	VAL
47	m0	101	LYS
48	m1	114	ILE
48	m1	117	ASP
49	m3	76	THR
49	m3	150	PRO
51	m5	68	ARG
52	m6	111	PRO
55	m9	155	LEU
60	n4	71	ARG
60	n4	83	THR
61	n5	25	LYS
63	n7	36	HIS
63	n7	91	ALA
64	n8	120	ASN
67	o1	47	ASP
67	o1	82	GLU

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Mol	Chain	Res	Type
70	o4	78	GLY
79	q3	51	ALA
83	p0	33	VAL
3	S1	21	VAL
3	S1	55	LYS
3	S1	210	ILE
4	S2	235	LEU
5	S3	64	ARG
6	S4	200	ARG
11	S9	167	ALA
14	C2	128	ALA
16	C4	75	GLY
21	C9	31	PRO
21	C9	39	THR
26	D4	60	PHE
26	D4	97	ALA
28	D6	15	ARG
28	D6	59	TYR
34	SR	113	VAL
34	SR	162	ALA
34	SR	229	LYS
35	SM	82	THR
35	SM	154	TYR
41	L4	131	VAL
44	L7	91	GLY
54	M8	183	GLY
66	O0	96	GLY
67	O1	7	VAL
71	O5	75	TYR
78	Q2	17	CYS
3	s1	207	LEU
5	s3	219	ALA
6	s4	30	ARG
6	s4	171	ASP
7	s5	21	THR
10	s8	78	ILE
10	s8	136	SER
11	s9	110	GLN
13	c1	129	ARG
18	c6	40	GLU
20	c8	7	GLU
28	d6	8	ASN

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Mol	Chain	Res	Type
28	d6	35	ALA
29	d7	62	ILE
81	e1	137	ASP
34	sR	15	GLY
34	sR	146	GLY
35	sM	84	LYS
35	sM	166	VAL
40	l3	141	GLY
40	l3	187	SER
40	l3	386	ASP
41	l4	71	VAL
41	l4	190	GLY
42	l5	125	VAL
45	l8	196	ALA
51	m5	74	PRO
58	n2	48	GLY
60	n4	64	THR
63	n7	28	PRO
63	n7	103	GLN
72	o6	3	VAL
72	o6	64	SER
78	q2	33	ALA
6	S4	193	GLY
6	S4	204	GLY
17	C5	11	VAL
18	C6	40	GLU
23	D1	46	ILE
34	SR	271	VAL
39	L2	98	VAL
51	M5	89	VAL
2	s0	31	VAL
5	s3	115	ILE
17	c5	48	GLY
18	c6	39	VAL
21	c9	100	ILE
81	e1	112	GLY
44	l7	178	ILE
48	m1	7	ASN
51	m5	76	PRO
58	n2	27	VAL
72	o6	31	GLY
23	D1	82	VAL

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Mol	Chain	Res	Type
32	E0	50	VAL
42	L5	125	VAL
45	L8	163	VAL
46	L9	13	PRO
52	M6	110	PRO
53	M7	84	PRO
60	N4	24	GLY
60	N4	80	ARG
21	c9	3	GLY
28	d6	58	VAL
34	sR	194	GLY
41	l4	301	PRO
74	o8	37	PRO
2	S0	139	VAL
8	S6	70	PRO
8	S6	123	GLY
9	S7	13	PRO
31	D9	6	VAL
34	SR	28	GLY
45	L8	135	GLY
11	s9	5	PRO
14	c2	66	VAL
15	c3	65	VAL
47	m0	204	GLY
69	o3	59	VAL
3	S1	48	VAL
13	C1	113	PRO
17	C5	68	PRO
34	SR	105	GLY
66	O0	100	ILE
8	s6	69	LEU
14	c2	91	VAL
15	c3	37	ILE
16	c4	48	VAL
24	d2	6	VAL
34	sR	49	GLY
43	l6	171	PRO
54	m8	84	VAL
66	o0	10	ILE
3	S1	22	ASP
22	D0	51	VAL
27	D5	88	ILE

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Mol	Chain	Res	Type
30	D8	20	GLY
40	L3	185	GLY
48	M1	23	VAL
2	s0	111	ILE
7	s5	59	VAL
11	s9	185	GLY
18	C6	41	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	130 (79%)	34 (21%)	1	3
2	s0	165/209 (79%)	138 (84%)	27 (16%)	2	7
3	S1	191/223 (86%)	159 (83%)	32 (17%)	2	6
3	s1	192/223 (86%)	162 (84%)	30 (16%)	2	8
4	S2	176/204 (86%)	140 (80%)	36 (20%)	1	3
4	s2	176/204 (86%)	137 (78%)	39 (22%)	1	3
5	S3	182/194 (94%)	142 (78%)	40 (22%)	1	3
5	s3	182/194 (94%)	145 (80%)	37 (20%)	1	3
6	S4	221/221 (100%)	178 (80%)	43 (20%)	1	4
6	s4	221/221 (100%)	179 (81%)	42 (19%)	1	4
7	S5	173/190 (91%)	148 (86%)	25 (14%)	3	9
7	s5	173/190 (91%)	144 (83%)	29 (17%)	2	6
8	S6	188/201 (94%)	150 (80%)	38 (20%)	1	4
8	s6	187/201 (93%)	155 (83%)	32 (17%)	2	6
9	S7	165/169 (98%)	127 (77%)	38 (23%)	1	2
9	s7	165/169 (98%)	136 (82%)	29 (18%)	2	5
10	S8	150/161 (93%)	128 (85%)	22 (15%)	3	9
10	s8	150/161 (93%)	126 (84%)	24 (16%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	S9	158/165 (96%)	122 (77%)	36 (23%)	1	2
11	s9	158/165 (96%)	123 (78%)	35 (22%)	1	3
12	C0	77/98 (79%)	62 (80%)	15 (20%)	1	4
12	c0	73/98 (74%)	63 (86%)	10 (14%)	3	11
13	C1	129/136 (95%)	108 (84%)	21 (16%)	2	7
13	c1	129/136 (95%)	105 (81%)	24 (19%)	1	5
14	C2	88/118 (75%)	67 (76%)	21 (24%)	0	2
14	c2	88/118 (75%)	70 (80%)	18 (20%)	1	3
15	C3	127/127 (100%)	106 (84%)	21 (16%)	2	7
15	c3	127/127 (100%)	103 (81%)	24 (19%)	1	4
16	C4	81/104 (78%)	58 (72%)	23 (28%)	0	1
16	c4	97/104 (93%)	75 (77%)	22 (23%)	1	2
17	C5	101/117 (86%)	86 (85%)	15 (15%)	3	9
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	6
18	C6	117/118 (99%)	97 (83%)	20 (17%)	2	6
18	c6	118/118 (100%)	95 (80%)	23 (20%)	1	4
19	C7	94/124 (76%)	73 (78%)	21 (22%)	1	3
19	c7	92/124 (74%)	77 (84%)	15 (16%)	2	7
20	C8	128/128 (100%)	102 (80%)	26 (20%)	1	3
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	2
21	C9	115/115 (100%)	95 (83%)	20 (17%)	2	6
21	c9	115/115 (100%)	96 (84%)	19 (16%)	2	7
22	D0	100/113 (88%)	76 (76%)	24 (24%)	0	2
22	d0	103/113 (91%)	81 (79%)	22 (21%)	1	3
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	5
23	d1	74/74 (100%)	60 (81%)	14 (19%)	1	4
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1	4
24	d2	110/110 (100%)	96 (87%)	14 (13%)	4	13
25	D3	119/119 (100%)	96 (81%)	23 (19%)	1	4
25	d3	119/119 (100%)	102 (86%)	17 (14%)	3	10
26	D4	112/112 (100%)	95 (85%)	17 (15%)	3	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	d4	112/112 (100%)	98 (88%)	14 (12%)	4	14
27	D5	61/88 (69%)	47 (77%)	14 (23%)	1	2
27	d5	61/88 (69%)	52 (85%)	9 (15%)	3	9
28	D6	83/83 (100%)	68 (82%)	15 (18%)	1	5
28	d6	83/83 (100%)	72 (87%)	11 (13%)	4	11
29	D7	70/70 (100%)	59 (84%)	11 (16%)	2	8
29	d7	70/70 (100%)	63 (90%)	7 (10%)	7	23
30	D8	56/59 (95%)	42 (75%)	14 (25%)	0	2
30	d8	56/59 (95%)	47 (84%)	9 (16%)	2	7
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	6
31	d9	47/48 (98%)	41 (87%)	6 (13%)	4	13
32	E0	51/51 (100%)	44 (86%)	7 (14%)	3	11
33	E1	62/66 (94%)	51 (82%)	11 (18%)	2	5
34	SR	260/261 (100%)	223 (86%)	37 (14%)	3	10
34	sR	260/261 (100%)	230 (88%)	30 (12%)	5	17
35	SM	97/228 (42%)	79 (81%)	18 (19%)	1	5
35	sM	54/228 (24%)	39 (72%)	15 (28%)	0	1
39	L2	193/195 (99%)	156 (81%)	37 (19%)	1	4
39	l2	192/195 (98%)	160 (83%)	32 (17%)	2	6
40	L3	321/322 (100%)	250 (78%)	71 (22%)	1	3
40	l3	319/322 (99%)	250 (78%)	69 (22%)	1	3
41	L4	288/288 (100%)	241 (84%)	47 (16%)	2	7
41	l4	288/288 (100%)	239 (83%)	49 (17%)	2	6
42	L5	244/244 (100%)	206 (84%)	38 (16%)	2	8
42	l5	243/244 (100%)	198 (82%)	45 (18%)	1	5
43	L6	134/152 (88%)	115 (86%)	19 (14%)	3	10
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	5
44	L7	186/204 (91%)	169 (91%)	17 (9%)	9	28
44	l7	187/204 (92%)	160 (86%)	27 (14%)	3	9
45	L8	187/207 (90%)	152 (81%)	35 (19%)	1	5
45	l8	177/207 (86%)	146 (82%)	31 (18%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	L9	171/171 (100%)	140 (82%)	31 (18%)	1	5
46	l9	171/171 (100%)	141 (82%)	30 (18%)	2	6
47	M0	177/186 (95%)	139 (78%)	38 (22%)	1	3
47	m0	179/186 (96%)	140 (78%)	39 (22%)	1	3
48	M1	147/150 (98%)	117 (80%)	30 (20%)	1	3
48	m1	147/150 (98%)	123 (84%)	24 (16%)	2	7
49	M3	154/158 (98%)	124 (80%)	30 (20%)	1	4
49	m3	154/158 (98%)	132 (86%)	22 (14%)	3	10
50	M4	107/108 (99%)	89 (83%)	18 (17%)	2	6
50	m4	108/108 (100%)	88 (82%)	20 (18%)	1	5
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	6
51	m5	175/175 (100%)	146 (83%)	29 (17%)	2	7
52	M6	160/161 (99%)	138 (86%)	22 (14%)	3	10
52	m6	160/161 (99%)	127 (79%)	33 (21%)	1	3
53	M7	140/145 (97%)	112 (80%)	28 (20%)	1	4
53	m7	125/145 (86%)	106 (85%)	19 (15%)	3	8
54	M8	150/150 (100%)	126 (84%)	24 (16%)	2	7
54	m8	150/150 (100%)	120 (80%)	30 (20%)	1	4
55	M9	153/153 (100%)	128 (84%)	25 (16%)	2	7
55	m9	153/153 (100%)	123 (80%)	30 (20%)	1	4
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1	4
56	n0	156/156 (100%)	125 (80%)	31 (20%)	1	4
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1	2
57	n1	136/136 (100%)	109 (80%)	27 (20%)	1	4
58	N2	87/106 (82%)	79 (91%)	8 (9%)	9	27
58	n2	85/106 (80%)	72 (85%)	13 (15%)	2	8
59	N3	104/104 (100%)	91 (88%)	13 (12%)	4	14
59	n3	104/104 (100%)	96 (92%)	8 (8%)	13	35
60	N4	57/129 (44%)	52 (91%)	5 (9%)	10	30
60	n4	100/129 (78%)	84 (84%)	16 (16%)	2	7
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	n5	104/117 (89%)	82 (79%)	22 (21%)	1	3
62	N6	109/109 (100%)	86 (79%)	23 (21%)	1	3
62	n6	109/109 (100%)	82 (75%)	27 (25%)	0	2
63	N7	115/115 (100%)	93 (81%)	22 (19%)	1	4
63	n7	115/115 (100%)	96 (84%)	19 (16%)	2	7
64	N8	118/118 (100%)	101 (86%)	17 (14%)	3	9
64	n8	118/118 (100%)	96 (81%)	22 (19%)	1	5
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1	3
65	n9	46/46 (100%)	36 (78%)	10 (22%)	1	3
66	O0	81/87 (93%)	70 (86%)	11 (14%)	3	11
66	o0	84/87 (97%)	68 (81%)	16 (19%)	1	4
67	O1	92/96 (96%)	75 (82%)	17 (18%)	1	5
67	o1	94/96 (98%)	73 (78%)	21 (22%)	1	3
68	O2	109/110 (99%)	91 (84%)	18 (16%)	2	7
68	o2	109/110 (99%)	88 (81%)	21 (19%)	1	4
69	O3	90/90 (100%)	78 (87%)	12 (13%)	4	11
69	o3	90/90 (100%)	76 (84%)	14 (16%)	2	8
70	O4	95/101 (94%)	75 (79%)	20 (21%)	1	3
70	o4	95/101 (94%)	82 (86%)	13 (14%)	3	11
71	O5	104/104 (100%)	82 (79%)	22 (21%)	1	3
71	o5	103/104 (99%)	83 (81%)	20 (19%)	1	4
72	O6	81/81 (100%)	63 (78%)	18 (22%)	1	3
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	6
73	o7	70/70 (100%)	55 (79%)	15 (21%)	1	3
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	3
74	o8	67/68 (98%)	56 (84%)	11 (16%)	2	7
75	O9	45/45 (100%)	39 (87%)	6 (13%)	4	11
75	o9	45/45 (100%)	40 (89%)	5 (11%)	6	19
76	Q0	47/47 (100%)	42 (89%)	5 (11%)	6	20
76	q0	47/47 (100%)	38 (81%)	9 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0	1
78	Q2	90/90 (100%)	74 (82%)	16 (18%)	2	5
78	q2	90/90 (100%)	72 (80%)	18 (20%)	1	4
79	Q3	71/71 (100%)	57 (80%)	14 (20%)	1	4
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	3
80	e0	53/53 (100%)	42 (79%)	11 (21%)	1	3
81	e1	66/66 (100%)	48 (73%)	18 (27%)	0	1
83	p0	105/253 (42%)	83 (79%)	22 (21%)	1	3
All	All	18728/20239 (92%)	15327 (82%)	3401 (18%)	1	5

All (3401) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	6	THR
2	S0	9	LEU
2	S0	27	ARG
2	S0	34	GLU
2	S0	37	VAL
2	S0	43	ASP
2	S0	47	VAL
2	S0	49	ASN
2	S0	50	VAL
2	S0	52	LYS
2	S0	62	ARG
2	S0	72	ASP
2	S0	76	ILE
2	S0	84	ARG
2	S0	87	LEU
2	S0	88	LYS
2	S0	96	THR
2	S0	101	ARG
2	S0	108	THR
2	S0	111	ILE
2	S0	112	THR
2	S0	119	ARG
2	S0	122	ILE
2	S0	135	GLU
2	S0	153	SER

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Mol	Chain	Res	Type
2	S0	154	GLU
2	S0	156	VAL
2	S0	157	ASP
2	S0	172	LEU
2	S0	177	LEU
2	S0	188	LEU
2	S0	196	SER
2	S0	198	MET
2	S0	203	PHE
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	61	LEU
3	S1	67	GLU
3	S1	70	LEU
3	S1	77	GLU
3	S1	79	HIS
3	S1	81	PHE
3	S1	89	ASP
3	S1	97	LEU
3	S1	104	ASP
3	S1	105	PHE
3	S1	111	ARG
3	S1	127	VAL
3	S1	137	ILE
3	S1	154	SER
3	S1	176	VAL
3	S1	179	SER
3	S1	180	THR
3	S1	181	LEU
3	S1	193	ILE
3	S1	202	LYS
3	S1	214	LYS
3	S1	215	VAL
3	S1	218	LEU
3	S1	220	GLN
3	S1	223	PHE
3	S1	231	LEU
4	S2	39	THR

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Mol	Chain	Res	Type
4	S2	53	ILE
4	S2	55	GLU
4	S2	58	LEU
4	S2	64	LYS
4	S2	68	ILE
4	S2	69	ILE
4	S2	76	LEU
4	S2	80	VAL
4	S2	87	GLN
4	S2	89	GLN
4	S2	90	THR
4	S2	91	ARG
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	111	VAL
4	S2	117	THR
4	S2	134	LEU
4	S2	137	ILE
4	S2	140	ARG
4	S2	141	ARG
4	S2	146	THR
4	S2	148	LEU
4	S2	166	THR
4	S2	174	ARG
4	S2	206	THR
4	S2	207	LEU
4	S2	208	GLU
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	237	VAL
4	S2	240	LEU
4	S2	245	ASP
4	S2	246	GLU
5	S3	4	LEU
5	S3	6	SER
5	S3	9	ARG
5	S3	21	LEU
5	S3	23	GLU
5	S3	37	VAL
5	S3	39	VAL

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Mol	Chain	Res	Type
5	S3	41	VAL
5	S3	65	ARG
5	S3	67	ASN
5	S3	70	THR
5	S3	76	ARG
5	S3	84	ILE
5	S3	92	GLN
5	S3	93	ASP
5	S3	103	GLU
5	S3	105	MET
5	S3	111	ASN
5	S3	127	MET
5	S3	134	CYS
5	S3	135	GLU
5	S3	142	LEU
5	S3	146	ARG
5	S3	151	LYS
5	S3	158	ILE
5	S3	164	VAL
5	S3	170	THR
5	S3	172	THR
5	S3	175	VAL
5	S3	176	LEU
5	S3	178	ARG
5	S3	182	LEU
5	S3	185	LYS
5	S3	209	ILE
5	S3	212	LYS
5	S3	215	GLU
5	S3	217	ILE
5	S3	220	PRO
5	S3	221	SER
5	S3	222	VAL
6	S4	7	LYS
6	S4	9	LEU
6	S4	11	ARG
6	S4	12	LEU
6	S4	21	ASP
6	S4	38	LEU
6	S4	39	ARG
6	S4	42	LEU
6	S4	45	ILE

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Mol	Chain	Res	Type
6	S4	48	LEU
6	S4	62	LYS
6	S4	67	GLN
6	S4	68	ARG
6	S4	70	VAL
6	S4	77	ARG
6	S4	78	THR
6	S4	92	LEU
6	S4	95	THR
6	S4	102	VAL
6	S4	113	ARG
6	S4	116	ASP
6	S4	117	GLU
6	S4	120	SER
6	S4	123	LEU
6	S4	126	VAL
6	S4	131	LEU
6	S4	166	SER
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	206	ASP
6	S4	215	ASP
6	S4	217	THR
6	S4	220	THR
6	S4	221	ARG
6	S4	222	LEU
6	S4	226	PHE
6	S4	227	VAL
6	S4	237	SER
6	S4	240	LYS
6	S4	242	LYS
6	S4	247	SER
6	S4	258	GLN
7	S5	25	LEU
7	S5	38	THR
7	S5	41	LYS
7	S5	43	PHE
7	S5	45	LYS
7	S5	53	VAL
7	S5	65	ARG
7	S5	76	ARG

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Mol	Chain	Res	Type
7	S5	79	ASN
7	S5	84	LYS
7	S5	93	LEU
7	S5	94	THR
7	S5	119	ASP
7	S5	130	ILE
7	S5	146	THR
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	162	VAL
7	S5	163	SER
7	S5	166	ARG
7	S5	186	ASN
7	S5	190	ILE
7	S5	193	THR
7	S5	194	LEU
8	S6	5	ILE
8	S6	6	SER
8	S6	12	SER
8	S6	13	GLN
8	S6	25	ARG
8	S6	30	LYS
8	S6	32	ILE
8	S6	58	LYS
8	S6	65	GLN
8	S6	68	LEU
8	S6	69	LEU
8	S6	72	ARG
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	89	ASP
8	S6	97	VAL
8	S6	98	ARG
8	S6	105	ASP
8	S6	109	LEU
8	S6	115	LYS
8	S6	120	GLU
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR

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Mol	Chain	Res	Type
8	S6	129	VAL
8	S6	132	ARG
8	S6	133	LEU
8	S6	143	LYS
8	S6	154	ARG
8	S6	155	ASP
8	S6	158	ILE
8	S6	170	THR
8	S6	174	LYS
8	S6	176	GLN
8	S6	179	VAL
8	S6	216	LEU
8	S6	223	LYS
9	S7	9	LEU
9	S7	14	THR
9	S7	15	GLU
9	S7	16	LEU
9	S7	38	LEU
9	S7	49	ILE
9	S7	50	ASP
9	S7	51	VAL
9	S7	55	LYS
9	S7	60	ILE
9	S7	62	VAL
9	S7	67	LEU
9	S7	70	PHE
9	S7	77	LEU
9	S7	80	GLU
9	S7	85	PHE
9	S7	87	ASP
9	S7	92	PHE
9	S7	95	GLU
9	S7	97	ARG
9	S7	99	LEU
9	S7	104	ARG
9	S7	107	ARG
9	S7	108	GLN
9	S7	114	ARG
9	S7	116	ARG
9	S7	117	THR
9	S7	119	THR
9	S7	126	LEU

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Mol	Chain	Res	Type
9	S7	130	VAL
9	S7	143	LEU
9	S7	144	VAL
9	S7	149	ILE
9	S7	161	GLN
9	S7	165	LYS
9	S7	166	LEU
9	S7	167	GLU
9	S7	185	ILE
10	S8	8	ARG
10	S8	12	SER
10	S8	14	THR
10	S8	20	GLN
10	S8	21	PHE
10	S8	29	LEU
10	S8	36	THR
10	S8	45	SER
10	S8	58	LEU
10	S8	60	ILE
10	S8	73	SER
10	S8	77	ARG
10	S8	81	VAL
10	S8	88	ASN
10	S8	107	THR
10	S8	120	THR
10	S8	138	ASN
10	S8	151	LYS
10	S8	152	ILE
10	S8	185	GLU
10	S8	193	LEU
10	S8	196	LEU
11	S9	3	ARG
11	S9	7	THR
11	S9	14	THR
11	S9	21	SER
11	S9	28	LEU
11	S9	49	LEU
11	S9	54	ARG
11	S9	60	LEU
11	S9	61	THR
11	S9	79	ARG
11	S9	82	ARG

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Mol	Chain	Res	Type
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	94	ASP
11	S9	96	VAL
11	S9	97	LEU
11	S9	99	LEU
11	S9	102	GLU
11	S9	105	LEU
11	S9	106	GLU
11	S9	109	LEU
11	S9	110	GLN
11	S9	118	LEU
11	S9	120	LYS
11	S9	126	ARG
11	S9	130	THR
11	S9	134	ILE
11	S9	138	LYS
11	S9	149	ARG
11	S9	150	LEU
11	S9	161	THR
11	S9	171	ARG
11	S9	172	VAL
11	S9	175	ARG
11	S9	182	GLU
12	C0	5	LYS
12	C0	20	VAL
12	C0	27	PHE
12	C0	29	GLN
12	C0	31	LYS
12	C0	32	HIS
12	C0	46	LEU
12	C0	47	GLN
12	C0	49	LEU
12	C0	51	SER
12	C0	55	VAL
12	C0	56	LYS
12	C0	76	LEU
12	C0	81	ASN
12	C0	82	LEU
13	C1	7	VAL
13	C1	8	GLN

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Mol	Chain	Res	Type
13	C1	21	ASN
13	C1	27	THR
13	C1	29	LYS
13	C1	40	LEU
13	C1	44	THR
13	C1	56	LYS
13	C1	67	ARG
13	C1	69	LYS
13	C1	70	ILE
13	C1	83	THR
13	C1	90	TYR
13	C1	91	LEU
13	C1	99	ARG
13	C1	109	VAL
13	C1	118	GLN
13	C1	136	ARG
13	C1	140	VAL
13	C1	141	LYS
13	C1	143	SER
14	C2	28	LEU
14	C2	36	LEU
14	C2	43	ARG
14	C2	45	LEU
14	C2	50	LYS
14	C2	52	LEU
14	C2	54	ARG
14	C2	59	LEU
14	C2	61	VAL
14	C2	66	VAL
14	C2	71	ILE
14	C2	73	LYS
14	C2	74	LEU
14	C2	89	ILE
14	C2	97	LEU
14	C2	103	LEU
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	139	HIS
14	C2	140	PHE
15	C3	3	ARG
15	C3	16	ILE

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Mol	Chain	Res	Type
15	C3	27	LYS
15	C3	30	SER
15	C3	39	LYS
15	C3	40	TYR
15	C3	42	ARG
15	C3	50	ILE
15	C3	64	ARG
15	C3	66	ILE
15	C3	76	LYS
15	C3	88	LEU
15	C3	97	SER
15	C3	102	LEU
15	C3	114	ARG
15	C3	115	LEU
15	C3	125	LEU
15	C3	130	ARG
15	C3	134	VAL
15	C3	149	LEU
15	C3	151	ASN
16	C4	14	PHE
16	C4	16	VAL
16	C4	20	TYR
16	C4	29	HIS
16	C4	30	VAL
16	C4	38	THR
16	C4	41	ARG
16	C4	42	VAL
16	C4	48	VAL
16	C4	51	ASP
16	C4	56	SER
16	C4	79	VAL
16	C4	81	VAL
16	C4	90	ARG
16	C4	92	LYS
16	C4	99	GLN
16	C4	102	LEU
16	C4	103	ARG
16	C4	117	ASP
16	C4	123	SER
16	C4	125	SER
16	C4	136	ARG
16	C4	137	LEU

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Mol	Chain	Res	Type
17	C5	11	VAL
17	C5	21	ASP
17	C5	22	LEU
17	C5	34	VAL
17	C5	36	LEU
17	C5	43	ARG
17	C5	44	ARG
17	C5	47	ARG
17	C5	52	LYS
17	C5	60	LEU
17	C5	89	MET
17	C5	110	GLU
17	C5	121	ILE
17	C5	124	THR
17	C5	125	PRO
18	C6	17	THR
18	C6	23	LYS
18	C6	26	LYS
18	C6	43	ILE
18	C6	53	LEU
18	C6	54	LEU
18	C6	57	LEU
18	C6	66	ARG
18	C6	68	ARG
18	C6	69	VAL
18	C6	94	GLN
18	C6	98	ASP
18	C6	101	SER
18	C6	106	LYS
18	C6	114	ARG
18	C6	118	ILE
18	C6	123	ARG
18	C6	128	LYS
18	C6	137	ARG
18	C6	143	ARG
19	C7	25	THR
19	C7	26	LEU
19	C7	30	THR
19	C7	34	LEU
19	C7	38	ILE
19	C7	40	THR
19	C7	45	ARG

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Mol	Chain	Res	Type
19	C7	46	LEU
19	C7	49	LYS
19	C7	54	THR
19	C7	62	GLN
19	C7	69	ILE
19	C7	72	LYS
19	C7	76	GLU
19	C7	78	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	88	VAL
19	C7	105	GLN
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	11	PHE
20	C8	13	HIS
20	C8	14	ILE
20	C8	15	LEU
20	C8	18	LEU
20	C8	20	THR
20	C8	25	ASN
20	C8	26	ILE
20	C8	28	ILE
20	C8	54	LEU
20	C8	61	LEU
20	C8	67	GLU
20	C8	73	MET
20	C8	80	LYS
20	C8	88	ARG
20	C8	92	ILE
20	C8	93	THR
20	C8	108	LYS
20	C8	110	ARG
20	C8	119	ILE
20	C8	133	VAL
20	C8	136	GLN
20	C8	143	ARG
20	C8	145	ARG
21	C9	4	VAL
21	C9	6	VAL

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Mol	Chain	Res	Type
21	C9	18	TYR
21	C9	22	LEU
21	C9	28	LEU
21	C9	35	ASP
21	C9	36	ILE
21	C9	48	GLN
21	C9	57	ARG
21	C9	60	SER
21	C9	67	MET
21	C9	68	ARG
21	C9	88	VAL
21	C9	111	ILE
21	C9	125	SER
21	C9	126	GLU
21	C9	130	ARG
21	C9	131	ASP
21	C9	133	ASP
21	C9	134	ARG
22	D0	15	GLN
22	D0	17	GLN
22	D0	23	ARG
22	D0	25	THR
22	D0	27	THR
22	D0	30	LYS
22	D0	34	LEU
22	D0	39	SER
22	D0	52	LYS
22	D0	57	ARG
22	D0	58	LEU
22	D0	60	THR
22	D0	61	LYS
22	D0	66	SER
22	D0	67	THR
22	D0	74	GLU
22	D0	76	SER
22	D0	81	THR
22	D0	88	LYS
22	D0	89	ARG
22	D0	97	VAL
22	D0	99	ILE
22	D0	103	ILE
22	D0	117	VAL

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Mol	Chain	Res	Type
23	D1	7	GLN
23	D1	9	VAL
23	D1	11	LEU
23	D1	18	SER
23	D1	32	VAL
23	D1	34	ILE
23	D1	41	GLU
23	D1	42	GLU
23	D1	52	THR
23	D1	62	ARG
23	D1	69	LEU
23	D1	78	LEU
23	D1	80	LYS
24	D2	6	VAL
24	D2	7	LEU
24	D2	22	LYS
24	D2	23	ARG
24	D2	24	GLN
24	D2	26	LEU
24	D2	27	ILE
24	D2	29	PRO
24	D2	42	GLN
24	D2	53	ILE
24	D2	65	LEU
24	D2	68	ARG
24	D2	70	ASN
24	D2	76	SER
24	D2	83	ILE
24	D2	93	LEU
24	D2	97	ARG
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR
24	D2	129	VAL
25	D3	7	ARG
25	D3	9	LEU
25	D3	16	ARG
25	D3	19	ARG
25	D3	23	ARG
25	D3	26	GLU
25	D3	28	ASN

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Mol	Chain	Res	Type
25	D3	40	SER
25	D3	73	ARG
25	D3	78	LYS
25	D3	79	ASN
25	D3	82	LYS
25	D3	83	VAL
25	D3	84	THR
25	D3	100	ASP
25	D3	103	LEU
25	D3	107	PHE
25	D3	109	ARG
25	D3	114	LYS
25	D3	131	SER
25	D3	138	GLU
25	D3	139	LYS
25	D3	144	ARG
26	D4	17	LEU
26	D4	28	LEU
26	D4	32	ARG
26	D4	34	ASN
26	D4	51	GLU
26	D4	52	LYS
26	D4	57	VAL
26	D4	61	ARG
26	D4	62	THR
26	D4	79	VAL
26	D4	96	LEU
26	D4	99	LYS
26	D4	102	LYS
26	D4	105	ARG
26	D4	124	ARG
26	D4	127	LYS
26	D4	128	LYS
27	D5	42	LEU
27	D5	50	ILE
27	D5	58	ARG
27	D5	59	TYR
27	D5	60	VAL
27	D5	67	ASP
27	D5	68	ARG
27	D5	69	LEU
27	D5	71	ILE

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Mol	Chain	Res	Type
27	D5	75	LEU
27	D5	78	ILE
27	D5	85	LYS
27	D5	96	SER
27	D5	100	ILE
28	D6	12	LYS
28	D6	30	ILE
28	D6	36	ILE
28	D6	41	ILE
28	D6	45	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	70	LYS
28	D6	82	ARG
28	D6	83	ILE
28	D6	84	VAL
28	D6	85	ARG
28	D6	88	SER
28	D6	90	GLU
28	D6	91	ASP
29	D7	2	VAL
29	D7	3	LEU
29	D7	17	ARG
29	D7	20	LYS
29	D7	26	GLN
29	D7	29	ARG
29	D7	33	LEU
29	D7	34	ASP
29	D7	56	CYS
29	D7	60	SER
29	D7	72	LYS
30	D8	13	ILE
30	D8	15	VAL
30	D8	19	THR
30	D8	28	VAL
30	D8	32	PHE
30	D8	33	LEU
30	D8	34	GLU
30	D8	35	ASP
30	D8	38	ARG
30	D8	39	THR
30	D8	49	ARG

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Mol	Chain	Res	Type
30	D8	58	GLU
30	D8	59	SER
30	D8	64	ARG
31	D9	6	VAL
31	D9	8	PHE
31	D9	9	SER
31	D9	19	ARG
31	D9	30	LEU
31	D9	39	CYS
31	D9	44	ARG
31	D9	48	ASN
32	E0	8	LEU
32	E0	20	LYS
32	E0	37	ARG
32	E0	39	LEU
32	E0	47	VAL
32	E0	48	THR
32	E0	50	VAL
33	E1	82	LYS
33	E1	89	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	97	LYS
33	E1	108	VAL
33	E1	109	ASP
33	E1	113	LYS
33	E1	120	GLU
33	E1	130	VAL
33	E1	137	ASP
34	SR	6	VAL
34	SR	7	LEU
34	SR	10	ARG
34	SR	29	GLN
34	SR	37	SER
34	SR	48	THR
34	SR	50	ASP
34	SR	52	GLN
34	SR	59	ARG
34	SR	76	ASP
34	SR	96	THR
34	SR	106	HIS
34	SR	116	ASP

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Mol	Chain	Res	Type
34	SR	117	LYS
34	SR	118	LYS
34	SR	134	TRP
34	SR	136	ILE
34	SR	141	LEU
34	SR	153	GLN
34	SR	159	ASN
34	SR	165	ASP
34	SR	185	GLN
34	SR	195	HIS
34	SR	199	ILE
34	SR	200	ASN
34	SR	201	THR
34	SR	211	ILE
34	SR	231	MET
34	SR	238	ASP
34	SR	241	PHE
34	SR	265	LEU
34	SR	268	GLN
34	SR	277	GLU
34	SR	288	HIS
34	SR	312	VAL
34	SR	317	THR
34	SR	319	ASN
35	SM	33	LYS
35	SM	41	SER
35	SM	46	LYS
35	SM	51	ARG
35	SM	53	ARG
35	SM	61	ILE
35	SM	64	LYS
35	SM	77	THR
35	SM	84	LYS
35	SM	89	ARG
35	SM	94	HIS
35	SM	96	ARG
35	SM	97	THR
35	SM	100	THR
35	SM	103	LYS
35	SM	105	LYS
35	SM	116	GLU
35	SM	117	LEU

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Mol	Chain	Res	Type
39	L2	10	LYS
39	L2	20	THR
39	L2	32	LEU
39	L2	44	ILE
39	L2	45	VAL
39	L2	46	LYS
39	L2	48	ILE
39	L2	62	VAL
39	L2	70	ARG
39	L2	71	LEU
39	L2	73	GLU
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	114	SER
39	L2	119	LYS
39	L2	134	VAL
39	L2	137	ILE
39	L2	141	PRO
39	L2	143	GLU
39	L2	157	VAL
39	L2	165	VAL
39	L2	177	LYS
39	L2	179	LEU
39	L2	181	LYS
39	L2	190	ARG
39	L2	191	LEU
39	L2	193	ARG
39	L2	202	VAL
39	L2	204	MET
39	L2	207	VAL
39	L2	227	ARG
39	L2	230	VAL
40	L3	3	HIS
40	L3	7	GLU
40	L3	10	ARG
40	L3	17	LEU
40	L3	19	ARG

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Mol	Chain	Res	Type
40	L3	21	ARG
40	L3	24	SER
40	L3	25	ILE
40	L3	37	ARG
40	L3	38	SER
40	L3	39	LYS
40	L3	43	LEU
40	L3	47	LEU
40	L3	50	LYS
40	L3	56	ILE
40	L3	67	PHE
40	L3	70	ARG
40	L3	73	VAL
40	L3	79	VAL
40	L3	84	VAL
40	L3	85	VAL
40	L3	100	ARG
40	L3	103	THR
40	L3	110	LEU
40	L3	114	VAL
40	L3	116	ARG
40	L3	121	ASN
40	L3	134	SER
40	L3	139	GLN
40	L3	146	ARG
40	L3	148	LEU
40	L3	150	ARG
40	L3	156	SER
40	L3	160	VAL
40	L3	169	THR
40	L3	173	GLN
40	L3	183	LEU
40	L3	188	ILE
40	L3	189	SER
40	L3	192	VAL
40	L3	196	ARG
40	L3	200	GLU
40	L3	202	THR
40	L3	205	VAL
40	L3	206	ASP
40	L3	210	GLU
40	L3	229	VAL

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Mol	Chain	Res	Type
40	L3	232	ARG
40	L3	235	THR
40	L3	238	LEU
40	L3	241	LYS
40	L3	242	THR
40	L3	247	ARG
40	L3	252	ILE
40	L3	264	VAL
40	L3	277	SER
40	L3	281	LYS
40	L3	284	ARG
40	L3	305	ILE
40	L3	308	MET
40	L3	324	VAL
40	L3	328	ILE
40	L3	332	ARG
40	L3	336	VAL
40	L3	338	LEU
40	L3	341	SER
40	L3	347	SER
40	L3	348	ARG
40	L3	361	THR
40	L3	364	LYS
40	L3	382	THR
41	L4	4	PRO
41	L4	12	THR
41	L4	25	VAL
41	L4	40	THR
41	L4	52	VAL
41	L4	53	SER
41	L4	60	THR
41	L4	71	VAL
41	L4	74	ILE
41	L4	93	MET
41	L4	99	MET
41	L4	122	THR
41	L4	124	SER
41	L4	131	VAL
41	L4	133	SER
41	L4	138	ARG
41	L4	152	VAL
41	L4	156	LEU

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Mol	Chain	Res	Type
41	L4	170	LYS
41	L4	172	VAL
41	L4	179	LEU
41	L4	188	ARG
41	L4	193	LYS
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	232	SER
41	L4	233	LEU
41	L4	246	ARG
41	L4	258	LEU
41	L4	289	ILE
41	L4	292	SER
41	L4	293	SER
41	L4	295	ILE
41	L4	306	THR
41	L4	319	LYS
41	L4	322	GLN
41	L4	323	VAL
41	L4	327	LEU
41	L4	332	LYS
41	L4	349	THR
41	L4	350	LYS
41	L4	357	GLU
41	L4	358	THR
42	L5	5	LYS
42	L5	22	ARG
42	L5	23	ARG
42	L5	35	ARG
42	L5	38	THR
42	L5	41	LYS
42	L5	63	GLN
42	L5	68	THR
42	L5	69	ILE
42	L5	93	THR
42	L5	105	ILE
42	L5	112	LYS
42	L5	115	LEU

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Mol	Chain	Res	Type
42	L5	118	THR
42	L5	120	LYS
42	L5	131	LEU
42	L5	140	ARG
42	L5	144	VAL
42	L5	146	LEU
42	L5	148	ILE
42	L5	151	GLN
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	194	LEU
42	L5	216	GLU
42	L5	232	ASP
42	L5	234	ASP
42	L5	242	SER
42	L5	254	LYS
42	L5	257	GLU
42	L5	259	LYS
42	L5	263	GLU
42	L5	273	ARG
42	L5	290	ILE
43	L6	5	LYS
43	L6	9	TRP
43	L6	21	THR
43	L6	35	VAL
43	L6	46	ARG
43	L6	52	VAL
43	L6	64	LEU
43	L6	65	ILE
43	L6	70	LYS
43	L6	78	ARG
43	L6	79	VAL
43	L6	84	VAL
43	L6	89	THR
43	L6	93	VAL
43	L6	129	GLU
43	L6	134	ARG
43	L6	155	LEU

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Mol	Chain	Res	Type
43	L6	160	SER
43	L6	162	SER
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	40	LYS
44	L7	82	LYS
44	L7	83	LEU
44	L7	89	ILE
44	L7	98	LYS
44	L7	100	ARG
44	L7	110	ARG
44	L7	121	LYS
44	L7	124	LEU
44	L7	143	THR
44	L7	179	LEU
44	L7	184	LEU
44	L7	239	LEU
44	L7	244	ASN
45	L8	26	LEU
45	L8	27	THR
45	L8	41	GLN
45	L8	57	ARG
45	L8	63	LYS
45	L8	67	ILE
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	81	THR
45	L8	82	LEU
45	L8	83	ASP
45	L8	84	ARG
45	L8	92	LYS
45	L8	95	ASN
45	L8	101	THR
45	L8	106	LYS
45	L8	110	THR
45	L8	132	VAL
45	L8	136	LEU
45	L8	145	ASN
45	L8	150	LEU
45	L8	156	ASP

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Mol	Chain	Res	Type
45	L8	160	ILE
45	L8	163	VAL
45	L8	169	LEU
45	L8	181	LYS
45	L8	185	ARG
45	L8	189	LEU
45	L8	204	ARG
45	L8	214	LEU
45	L8	238	LEU
45	L8	241	LYS
45	L8	248	LYS
45	L8	251	LYS
46	L9	4	ILE
46	L9	5	GLN
46	L9	9	GLN
46	L9	14	GLU
46	L9	18	VAL
46	L9	19	SER
46	L9	20	ILE
46	L9	22	SER
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	82	VAL
46	L9	121	LYS
46	L9	132	VAL
46	L9	133	THR
46	L9	138	THR
46	L9	139	ASN
46	L9	151	VAL
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	177	ASP

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Mol	Chain	Res	Type
46	L9	189	GLU
47	M0	3	ARG
47	M0	7	ARG
47	M0	18	PRO
47	M0	21	ARG
47	M0	24	ARG
47	M0	30	LYS
47	M0	32	ARG
47	M0	33	ILE
47	M0	39	LYS
47	M0	40	LYS
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	57	LEU
47	M0	63	GLU
47	M0	69	ARG
47	M0	74	LYS
47	M0	77	THR
47	M0	87	LEU
47	M0	91	VAL
47	M0	99	ILE
47	M0	102	MET
47	M0	128	ARG
47	M0	129	VAL
47	M0	130	ASP
47	M0	139	ARG
47	M0	140	THR
47	M0	146	ASP
47	M0	163	GLN
47	M0	165	ILE
47	M0	169	LYS
47	M0	174	THR
47	M0	178	ARG
47	M0	185	ARG
47	M0	191	LYS
47	M0	197	VAL
47	M0	201	SER
47	M0	203	LYS
48	M1	6	GLN
48	M1	7	ASN
48	M1	9	MET

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Mol	Chain	Res	Type
48	M1	10	ARG
48	M1	12	LEU
48	M1	13	LYS
48	M1	23	VAL
48	M1	31	THR
48	M1	40	LEU
48	M1	44	THR
48	M1	46	VAL
48	M1	65	ILE
48	M1	68	HIS
48	M1	80	LEU
48	M1	82	ARG
48	M1	88	GLU
48	M1	94	ARG
48	M1	99	THR
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	115	LYS
48	M1	119	SER
48	M1	130	VAL
48	M1	140	ARG
48	M1	142	LYS
48	M1	147	THR
48	M1	158	ASP
48	M1	166	LYS
48	M1	171	VAL
49	M3	21	ARG
49	M3	23	LYS
49	M3	24	VAL
49	M3	34	SER
49	M3	35	ARG
49	M3	46	ILE
49	M3	54	LEU
49	M3	55	ARG
49	M3	57	VAL
49	M3	58	VAL
49	M3	59	ARG
49	M3	63	VAL
49	M3	67	ARG
49	M3	69	VAL
49	M3	100	ARG

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Mol	Chain	Res	Type
49	M3	107	GLU
49	M3	114	GLN
49	M3	115	ARG
49	M3	124	ILE
49	M3	131	LYS
49	M3	136	GLU
49	M3	164	GLU
49	M3	165	SER
49	M3	168	ARG
49	M3	171	ARG
49	M3	174	ARG
49	M3	182	ILE
49	M3	186	ARG
49	M3	190	LYS
49	M3	194	GLU
50	M4	8	LYS
50	M4	27	GLN
50	M4	50	LYS
50	M4	53	VAL
50	M4	58	ILE
50	M4	63	VAL
50	M4	66	THR
50	M4	72	LEU
50	M4	82	SER
50	M4	90	VAL
50	M4	93	LYS
50	M4	102	LYS
50	M4	106	ARG
50	M4	108	ARG
50	M4	126	GLN
50	M4	130	THR
50	M4	135	LEU
50	M4	137	LYS
51	M5	7	LEU
51	M5	10	LEU
51	M5	18	VAL
51	M5	19	LEU
51	M5	20	ARG
51	M5	22	LEU
51	M5	24	ARG
51	M5	27	VAL
51	M5	46	ASP

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Mol	Chain	Res	Type
51	M5	49	ARG
51	M5	50	ARG
51	M5	68	ARG
51	M5	71	ARG
51	M5	80	THR
51	M5	83	LYS
51	M5	85	THR
51	M5	92	LEU
51	M5	96	ARG
51	M5	97	SER
51	M5	98	LEU
51	M5	109	ARG
51	M5	117	ASN
51	M5	133	ILE
51	M5	138	GLN
51	M5	142	ILE
51	M5	151	ILE
51	M5	182	ASN
51	M5	190	THR
51	M5	196	THR
51	M5	204	LYS
52	M6	22	VAL
52	M6	25	LYS
52	M6	33	ILE
52	M6	41	LEU
52	M6	58	LEU
52	M6	59	ARG
52	M6	67	THR
52	M6	78	ARG
52	M6	84	LEU
52	M6	85	ARG
52	M6	106	GLU
52	M6	110	PRO
52	M6	116	LYS
52	M6	117	ARG
52	M6	124	LEU
52	M6	128	ARG
52	M6	143	THR
52	M6	152	VAL
52	M6	159	LYS
52	M6	160	ARG
52	M6	184	THR

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Mol	Chain	Res	Type
52	M6	192	LYS
53	M7	9	THR
53	M7	14	SER
53	M7	24	VAL
53	M7	25	SER
53	M7	29	THR
53	M7	32	THR
53	M7	36	ILE
53	M7	42	THR
53	M7	43	LYS
53	M7	52	LEU
53	M7	53	ASP
53	M7	56	ARG
53	M7	67	ILE
53	M7	75	GLU
53	M7	78	VAL
53	M7	91	VAL
53	M7	94	LEU
53	M7	112	LEU
53	M7	117	ILE
53	M7	119	VAL
53	M7	126	ARG
53	M7	136	ILE
53	M7	138	LYS
53	M7	144	SER
53	M7	157	VAL
53	M7	173	ARG
53	M7	180	LYS
53	M7	181	ARG
54	M8	7	SER
54	M8	17	THR
54	M8	22	ASP
54	M8	24	VAL
54	M8	26	LEU
54	M8	32	LEU
54	M8	34	THR
54	M8	49	LEU
54	M8	57	ILE
54	M8	63	SER
54	M8	64	VAL
54	M8	69	ARG
54	M8	73	GLN

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Mol	Chain	Res	Type
54	M8	80	THR
54	M8	95	GLU
54	M8	122	ILE
54	M8	135	GLN
54	M8	141	ARG
54	M8	147	ARG
54	M8	150	VAL
54	M8	159	LYS
54	M8	168	THR
54	M8	178	ARG
54	M8	180	ARG
55	M9	8	LYS
55	M9	10	LEU
55	M9	20	ARG
55	M9	22	VAL
55	M9	28	GLU
55	M9	30	SER
55	M9	41	ILE
55	M9	44	LEU
55	M9	51	VAL
55	M9	71	ARG
55	M9	74	ARG
55	M9	86	GLU
55	M9	98	ARG
55	M9	99	LEU
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	108	LYS
55	M9	110	ARG
55	M9	116	ASP
55	M9	138	LEU
55	M9	144	GLN
55	M9	173	ARG
55	M9	175	GLN
55	M9	180	LYS
56	N0	1	MET
56	N0	8	GLN
56	N0	21	GLU
56	N0	45	LEU
56	N0	50	LYS
56	N0	51	VAL

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Mol	Chain	Res	Type
56	N0	61	ILE
56	N0	80	ARG
56	N0	87	THR
56	N0	100	VAL
56	N0	104	GLU
56	N0	105	THR
56	N0	113	ARG
56	N0	115	ARG
56	N0	117	ARG
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	144	LEU
56	N0	155	ARG
56	N0	156	VAL
56	N0	160	THR
56	N0	161	LYS
56	N0	166	LYS
56	N0	167	ARG
56	N0	169	SER
56	N0	171	PHE
56	N0	172	TYR
57	N1	9	SER
57	N1	12	ARG
57	N1	25	VAL
57	N1	26	HIS
57	N1	27	LEU
57	N1	32	LYS
57	N1	43	LYS
57	N1	55	LYS
57	N1	68	THR
57	N1	69	LYS
57	N1	71	SER
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	80	VAL
57	N1	83	ARG
57	N1	87	LYS

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Mol	Chain	Res	Type
57	N1	88	ARG
57	N1	96	ILE
57	N1	102	ARG
57	N1	103	GLN
57	N1	104	GLU
57	N1	106	LEU
57	N1	118	GLU
57	N1	124	VAL
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	139	ARG
57	N1	143	THR
57	N1	146	ASN
57	N1	149	GLN
58	N2	10	LYS
58	N2	43	VAL
58	N2	52	ASN
58	N2	54	VAL
58	N2	87	ASN
58	N2	88	GLN
58	N2	93	ILE
58	N2	100	THR
59	N3	13	ILE
59	N3	32	ARG
59	N3	42	SER
59	N3	44	SER
59	N3	64	LYS
59	N3	69	LEU
59	N3	72	LYS
59	N3	73	VAL
59	N3	74	MET
59	N3	83	LYS
59	N3	84	SER
59	N3	102	ILE
59	N3	115	THR
60	N4	4	GLU
60	N4	5	ILE
60	N4	19	THR
60	N4	39	LEU
60	N4	54	LEU
61	N5	27	ARG

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Mol	Chain	Res	Type
61	N5	36	LYS
61	N5	37	THR
61	N5	38	LEU
61	N5	40	LEU
61	N5	45	LYS
61	N5	63	ILE
61	N5	69	SER
61	N5	71	THR
61	N5	73	MET
61	N5	77	GLU
61	N5	85	GLN
61	N5	86	VAL
61	N5	92	LYS
61	N5	108	LEU
61	N5	109	LYS
61	N5	115	ARG
61	N5	125	ARG
61	N5	133	LEU
61	N5	135	ILE
61	N5	138	ARG
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS
62	N6	6	LEU
62	N6	13	ARG
62	N6	17	LYS
62	N6	26	GLN
62	N6	37	LYS
62	N6	39	LEU
62	N6	45	ILE
62	N6	50	ILE
62	N6	51	ARG
62	N6	55	GLU
62	N6	56	VAL
62	N6	57	LEU
62	N6	59	VAL
62	N6	70	ILE
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	88	GLU
62	N6	89	LYS

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Mol	Chain	Res	Type
62	N6	105	VAL
62	N6	115	ARG
62	N6	125	LYS
63	N7	14	VAL
63	N7	17	ARG
63	N7	24	VAL
63	N7	30	ASP
63	N7	34	LYS
63	N7	46	ILE
63	N7	54	THR
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	90	GLU
63	N7	99	GLU
63	N7	102	GLU
63	N7	103	GLN
63	N7	109	GLU
63	N7	121	ARG
63	N7	132	SER
63	N7	134	LEU
64	N8	4	ARG
64	N8	6	THR
64	N8	8	THR
64	N8	10	LYS
64	N8	12	ARG
64	N8	16	SER
64	N8	42	ARG
64	N8	58	MET
64	N8	60	TYR
64	N8	76	ASP
64	N8	78	LEU
64	N8	91	LEU
64	N8	115	LYS
64	N8	117	ARG
64	N8	123	VAL
64	N8	130	VAL
64	N8	133	LEU

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Mol	Chain	Res	Type
65	N9	4	SER
65	N9	14	ARG
65	N9	25	LYS
65	N9	28	LYS
65	N9	35	VAL
65	N9	40	ARG
65	N9	50	THR
65	N9	52	LYS
65	N9	58	LYS
65	N9	59	LYS
66	O0	16	LEU
66	O0	18	ILE
66	O0	30	THR
66	O0	34	LEU
66	O0	48	THR
66	O0	61	MET
66	O0	65	THR
66	O0	66	LYS
66	O0	76	GLU
66	O0	83	LYS
66	O0	100	ILE
67	O1	8	VAL
67	O1	13	THR
67	O1	16	LEU
67	O1	26	LYS
67	O1	31	ARG
67	O1	55	LEU
67	O1	64	VAL
67	O1	73	LEU
67	O1	76	SER
67	O1	79	ARG
67	O1	84	ASP
67	O1	86	LYS
67	O1	89	LEU
67	O1	94	GLU
67	O1	102	LYS
67	O1	105	GLN
67	O1	106	THR
68	O2	3	SER
68	O2	15	LYS
68	O2	19	ARG
68	O2	30	GLU

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Mol	Chain	Res	Type
68	O2	33	ARG
68	O2	41	VAL
68	O2	54	LYS
68	O2	62	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	76	VAL
68	O2	84	THR
68	O2	106	VAL
68	O2	109	LEU
68	O2	111	ARG
68	O2	125	ARG
68	O2	126	LEU
68	O2	128	LEU
69	O3	20	LYS
69	O3	28	SER
69	O3	31	LYS
69	O3	48	ARG
69	O3	49	ILE
69	O3	59	VAL
69	O3	60	ARG
69	O3	80	VAL
69	O3	82	ARG
69	O3	86	ARG
69	O3	98	VAL
69	O3	106	ASN
70	O4	5	VAL
70	O4	8	ARG
70	O4	16	ARG
70	O4	20	ILE
70	O4	23	VAL
70	O4	24	LYS
70	O4	29	ILE
70	O4	35	VAL
70	O4	38	LEU
70	O4	51	LEU
70	O4	56	THR
70	O4	58	ARG
70	O4	61	GLN
70	O4	68	THR
70	O4	71	THR
70	O4	80	ARG

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Mol	Chain	Res	Type
70	O4	86	LYS
70	O4	87	GLU
70	O4	103	LYS
70	O4	104	VAL
71	O5	15	GLU
71	O5	27	GLU
71	O5	28	LEU
71	O5	31	LEU
71	O5	44	ILE
71	O5	46	THR
71	O5	48	ARG
71	O5	49	LYS
71	O5	50	SER
71	O5	71	LYS
71	O5	84	LYS
71	O5	85	THR
71	O5	86	ARG
71	O5	89	ARG
71	O5	94	LYS
71	O5	96	GLU
71	O5	100	VAL
71	O5	101	THR
71	O5	102	GLU
71	O5	104	GLN
71	O5	107	LYS
71	O5	119	LYS
72	O6	11	LEU
72	O6	18	THR
72	O6	21	THR
72	O6	26	ILE
72	O6	34	SER
72	O6	36	ARG
72	O6	37	THR
72	O6	45	ARG
72	O6	57	LEU
72	O6	58	ILE
72	O6	62	ARG
72	O6	66	GLU
72	O6	68	ARG
72	O6	76	ARG
72	O6	81	THR
72	O6	88	GLU

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Mol	Chain	Res	Type
72	O6	98	ARG
72	O6	99	ARG
73	O7	5	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	26	SER
73	O7	33	THR
73	O7	45	ARG
73	O7	58	THR
73	O7	59	THR
73	O7	64	MET
73	O7	65	ARG
73	O7	67	LEU
73	O7	79	GLN
74	O8	5	ILE
74	O8	8	ILE
74	O8	24	THR
74	O8	31	LEU
74	O8	32	ASN
74	O8	41	THR
74	O8	45	VAL
74	O8	46	ARG
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
75	O9	5	LYS
75	O9	21	ARG
75	O9	34	THR
75	O9	36	ARG
75	O9	45	ARG
75	O9	51	ILE
76	Q0	78	ILE
76	Q0	83	LYS
76	Q0	85	LEU
76	Q0	112	LYS
76	Q0	113	ARG
77	Q1	4	LYS
77	Q1	6	ARG

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Mol	Chain	Res	Type
77	Q1	9	ARG
77	Q1	10	THR
77	Q1	11	ARG
77	Q1	19	LYS
77	Q1	20	VAL
77	Q1	21	ARG
78	Q2	3	ASN
78	Q2	4	VAL
78	Q2	6	LYS
78	Q2	8	ARG
78	Q2	17	CYS
78	Q2	21	THR
78	Q2	26	THR
78	Q2	35	LEU
78	Q2	47	GLN
78	Q2	48	SER
78	Q2	55	LYS
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	93	LEU
78	Q2	99	GLN
78	Q2	104	LEU
79	Q3	5	THR
79	Q3	11	THR
79	Q3	16	VAL
79	Q3	24	ARG
79	Q3	25	GLN
79	Q3	36	ARG
79	Q3	45	LYS
79	Q3	49	ARG
79	Q3	58	SER
79	Q3	60	CYS
79	Q3	73	THR
79	Q3	78	THR
79	Q3	84	ARG
79	Q3	91	GLU
2	s0	6	THR
2	s0	12	GLU
2	s0	18	LEU
2	s0	30	GLN
2	s0	41	ARG
2	s0	43	ASP

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Mol	Chain	Res	Type
2	s0	45	VAL
2	s0	55	GLU
2	s0	57	LEU
2	s0	62	ARG
2	s0	80	THR
2	s0	87	LEU
2	s0	93	THR
2	s0	111	ILE
2	s0	112	THR
2	s0	124	THR
2	s0	144	ILE
2	s0	146	LEU
2	s0	151	SER
2	s0	157	ASP
2	s0	164	ASN
2	s0	172	LEU
2	s0	183	ARG
2	s0	185	ARG
2	s0	188	LEU
2	s0	189	VAL
2	s0	198	MET
3	s1	21	VAL
3	s1	25	THR
3	s1	37	THR
3	s1	47	LEU
3	s1	51	SER
3	s1	54	LEU
3	s1	55	LYS
3	s1	62	LYS
3	s1	65	VAL
3	s1	70	LEU
3	s1	73	LEU
3	s1	83	LYS
3	s1	97	LEU
3	s1	105	PHE
3	s1	106	THR
3	s1	116	LYS
3	s1	122	GLU
3	s1	126	THR
3	s1	131	ASP
3	s1	169	SER
3	s1	173	THR

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Mol	Chain	Res	Type
3	s1	181	LEU
3	s1	183	GLN
3	s1	184	LEU
3	s1	192	VAL
3	s1	203	ASP
3	s1	206	PRO
3	s1	219	LYS
3	s1	222	LYS
3	s1	228	LEU
4	s2	41	LEU
4	s2	53	ILE
4	s2	55	GLU
4	s2	58	LEU
4	s2	69	ILE
4	s2	71	THR
4	s2	73	LEU
4	s2	83	ILE
4	s2	84	LYS
4	s2	89	GLN
4	s2	91	ARG
4	s2	94	GLN
4	s2	95	ARG
4	s2	97	ARG
4	s2	106	ASP
4	s2	111	VAL
4	s2	113	LEU
4	s2	117	THR
4	s2	137	ILE
4	s2	139	ILE
4	s2	141	ARG
4	s2	146	THR
4	s2	148	LEU
4	s2	159	THR
4	s2	164	SER
4	s2	166	THR
4	s2	170	ILE
4	s2	185	LYS
4	s2	186	LYS
4	s2	194	GLU
4	s2	206	THR
4	s2	207	LEU
4	s2	218	ILE

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Mol	Chain	Res	Type
4	s2	222	TYR
4	s2	225	LEU
4	s2	229	LEU
4	s2	233	GLN
4	s2	245	ASP
4	s2	248	SER
5	s3	4	LEU
5	s3	7	LYS
5	s3	10	LYS
5	s3	11	LEU
5	s3	21	LEU
5	s3	40	ARG
5	s3	41	VAL
5	s3	44	THR
5	s3	61	GLU
5	s3	66	ILE
5	s3	67	ASN
5	s3	69	LEU
5	s3	84	ILE
5	s3	86	LEU
5	s3	93	ASP
5	s3	94	ARG
5	s3	103	GLU
5	s3	111	ASN
5	s3	115	ILE
5	s3	124	ARG
5	s3	127	MET
5	s3	128	GLU
5	s3	134	CYS
5	s3	142	LEU
5	s3	143	ARG
5	s3	146	ARG
5	s3	158	ILE
5	s3	168	ILE
5	s3	169	ASP
5	s3	172	THR
5	s3	176	LEU
5	s3	189	MET
5	s3	202	LEU
5	s3	207	THR
5	s3	212	LYS
5	s3	223	LYS

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Mol	Chain	Res	Type
5	s3	225	TYR
6	s4	6	LYS
6	s4	7	LYS
6	s4	9	LEU
6	s4	12	LEU
6	s4	23	LEU
6	s4	38	LEU
6	s4	42	LEU
6	s4	45	ILE
6	s4	48	LEU
6	s4	49	ARG
6	s4	50	ASN
6	s4	51	ARG
6	s4	67	GLN
6	s4	68	ARG
6	s4	70	VAL
6	s4	78	THR
6	s4	95	THR
6	s4	105	VAL
6	s4	113	ARG
6	s4	117	GLU
6	s4	118	GLU
6	s4	123	LEU
6	s4	127	LYS
6	s4	147	ILE
6	s4	148	ARG
6	s4	159	THR
6	s4	160	VAL
6	s4	180	LEU
6	s4	182	TYR
6	s4	187	ARG
6	s4	194	THR
6	s4	210	ILE
6	s4	219	VAL
6	s4	221	ARG
6	s4	222	LEU
6	s4	233	LYS
6	s4	236	ILE
6	s4	237	SER
6	s4	245	LYS
6	s4	246	LEU
6	s4	254	ARG

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Mol	Chain	Res	Type
6	s4	256	ARG
7	s5	23	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	38	THR
7	s5	39	GLU
7	s5	45	LYS
7	s5	63	GLN
7	s5	66	GLN
7	s5	68	ILE
7	s5	76	ARG
7	s5	89	ILE
7	s5	93	LEU
7	s5	109	LYS
7	s5	119	ASP
7	s5	125	THR
7	s5	130	ILE
7	s5	146	THR
7	s5	147	THR
7	s5	148	ARG
7	s5	157	ARG
7	s5	163	SER
7	s5	167	ARG
7	s5	186	ASN
7	s5	187	ILE
7	s5	190	ILE
7	s5	192	GLU
7	s5	194	LEU
7	s5	203	LYS
7	s5	205	SER
8	s6	22	HIS
8	s6	25	ARG
8	s6	30	LYS
8	s6	34	GLN
8	s6	44	GLU
8	s6	69	LEU
8	s6	71	THR
8	s6	76	LEU
8	s6	89	ASP
8	s6	97	VAL
8	s6	108	VAL
8	s6	109	LEU

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Mol	Chain	Res	Type
8	s6	114	VAL
8	s6	115	LYS
8	s6	116	LYS
8	s6	120	GLU
8	s6	121	LEU
8	s6	126	ASP
8	s6	128	THR
8	s6	129	VAL
8	s6	133	LEU
8	s6	137	ARG
8	s6	143	LYS
8	s6	151	ASP
8	s6	155	ASP
8	s6	168	THR
8	s6	177	ARG
8	s6	179	VAL
8	s6	193	LEU
8	s6	215	ARG
8	s6	216	LEU
8	s6	217	SER
9	s7	11	GLN
9	s7	16	LEU
9	s7	18	LEU
9	s7	28	GLU
9	s7	33	GLU
9	s7	49	ILE
9	s7	50	ASP
9	s7	55	LYS
9	s7	67	LEU
9	s7	73	VAL
9	s7	77	LEU
9	s7	79	ARG
9	s7	97	ARG
9	s7	105	THR
9	s7	106	SER
9	s7	110	GLN
9	s7	114	ARG
9	s7	116	ARG
9	s7	117	THR
9	s7	126	LEU
9	s7	136	VAL
9	s7	143	LEU

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Mol	Chain	Res	Type
9	s7	144	VAL
9	s7	148	LYS
9	s7	150	GLN
9	s7	159	VAL
9	s7	163	ASP
9	s7	166	LEU
9	s7	185	ILE
10	s8	18	ARG
10	s8	25	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	46	VAL
10	s8	61	GLU
10	s8	64	ASN
10	s8	76	THR
10	s8	77	ARG
10	s8	82	VAL
10	s8	89	GLU
10	s8	110	ARG
10	s8	111	GLN
10	s8	119	GLN
10	s8	120	THR
10	s8	121	LEU
10	s8	135	LYS
10	s8	138	ASN
10	s8	153	GLU
10	s8	155	SER
10	s8	176	SER
10	s8	183	ILE
10	s8	184	LEU
10	s8	199	LYS
11	s9	3	ARG
11	s9	6	ARG
11	s9	7	THR
11	s9	20	GLU
11	s9	21	SER
11	s9	28	LEU
11	s9	37	LYS
11	s9	39	LYS
11	s9	49	LEU
11	s9	50	SER
11	s9	54	ARG

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Mol	Chain	Res	Type
11	s9	77	ILE
11	s9	78	ARG
11	s9	82	ARG
11	s9	89	ASP
11	s9	90	LYS
11	s9	91	LYS
11	s9	93	LEU
11	s9	101	VAL
11	s9	105	LEU
11	s9	109	LEU
11	s9	110	GLN
11	s9	111	THR
11	s9	115	LYS
11	s9	126	ARG
11	s9	130	THR
11	s9	133	HIS
11	s9	134	ILE
11	s9	140	ILE
11	s9	149	ARG
11	s9	162	SER
11	s9	168	ARG
11	s9	172	VAL
11	s9	180	LYS
11	s9	182	GLU
12	c0	2	LEU
12	c0	12	HIS
12	c0	15	LEU
12	c0	20	VAL
12	c0	21	VAL
12	c0	55	VAL
12	c0	56	LYS
12	c0	57	THR
12	c0	67	THR
12	c0	71	GLU
13	c1	3	THR
13	c1	5	LEU
13	c1	10	GLU
13	c1	21	ASN
13	c1	26	LYS
13	c1	30	ARG
13	c1	31	THR
13	c1	33	ARG

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Mol	Chain	Res	Type
13	c1	40	LEU
13	c1	44	THR
13	c1	47	THR
13	c1	60	PHE
13	c1	67	ARG
13	c1	74	THR
13	c1	76	VAL
13	c1	80	MET
13	c1	83	THR
13	c1	86	ILE
13	c1	109	VAL
13	c1	123	VAL
13	c1	129	ARG
13	c1	138	ASN
13	c1	140	VAL
13	c1	143	SER
14	c2	38	HIS
14	c2	39	ASP
14	c2	45	LEU
14	c2	58	LEU
14	c2	61	VAL
14	c2	65	SER
14	c2	71	ILE
14	c2	83	GLU
14	c2	85	LYS
14	c2	89	ILE
14	c2	103	LEU
14	c2	120	VAL
14	c2	121	VAL
14	c2	125	ASN
14	c2	132	GLU
14	c2	136	ILE
14	c2	137	MET
14	c2	140	PHE
15	c3	12	SER
15	c3	13	SER
15	c3	16	ILE
15	c3	20	ARG
15	c3	27	LYS
15	c3	35	GLU
15	c3	39	LYS
15	c3	66	ILE

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Mol	Chain	Res	Type
15	c3	67	THR
15	c3	70	LYS
15	c3	80	LEU
15	c3	84	ILE
15	c3	87	ASP
15	c3	88	LEU
15	c3	93	LYS
15	c3	102	LEU
15	c3	104	ARG
15	c3	106	ARG
15	c3	115	LEU
15	c3	125	LEU
15	c3	127	ARG
15	c3	131	THR
15	c3	138	ASN
15	c3	147	SER
16	c4	18	ARG
16	c4	31	THR
16	c4	33	LEU
16	c4	36	LYS
16	c4	49	LYS
16	c4	51	ASP
16	c4	52	ARG
16	c4	61	MET
16	c4	70	LYS
16	c4	79	VAL
16	c4	81	VAL
16	c4	92	LYS
16	c4	102	LEU
16	c4	111	ARG
16	c4	114	ARG
16	c4	119	THR
16	c4	125	SER
16	c4	127	ARG
16	c4	129	LYS
16	c4	132	ARG
16	c4	133	ARG
16	c4	136	ARG
17	c5	12	PHE
17	c5	24	LYS
17	c5	29	SER
17	c5	36	LEU

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Mol	Chain	Res	Type
17	c5	40	ARG
17	c5	43	ARG
17	c5	44	ARG
17	c5	52	LYS
17	c5	57	MET
17	c5	69	GLU
17	c5	71	GLU
17	c5	72	LYS
17	c5	77	ARG
17	c5	107	ILE
17	c5	110	GLU
17	c5	122	THR
17	c5	124	THR
17	c5	127	ARG
18	c6	17	THR
18	c6	23	LYS
18	c6	28	LEU
18	c6	34	SER
18	c6	37	THR
18	c6	40	GLU
18	c6	43	ILE
18	c6	48	VAL
18	c6	53	LEU
18	c6	57	LEU
18	c6	68	ARG
18	c6	69	VAL
18	c6	70	THR
18	c6	81	ILE
18	c6	94	GLN
18	c6	107	LYS
18	c6	110	THR
18	c6	113	ASP
18	c6	114	ARG
18	c6	115	THR
18	c6	117	LEU
18	c6	137	ARG
18	c6	143	ARG
19	c7	8	THR
19	c7	19	ARG
19	c7	34	LEU
19	c7	43	SER
19	c7	46	LEU

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Mol	Chain	Res	Type
19	c7	60	ARG
19	c7	63	LYS
19	c7	69	ILE
19	c7	72	LYS
19	c7	74	GLN
19	c7	83	GLN
19	c7	85	VAL
19	c7	88	VAL
19	c7	104	ASN
19	c7	113	LEU
20	c8	2	SER
20	c8	3	LEU
20	c8	4	VAL
20	c8	6	GLN
20	c8	7	GLU
20	c8	8	GLN
20	c8	12	GLN
20	c8	15	LEU
20	c8	20	THR
20	c8	25	ASN
20	c8	28	ILE
20	c8	33	THR
20	c8	36	LYS
20	c8	40	ARG
20	c8	57	ARG
20	c8	61	LEU
20	c8	64	GLU
20	c8	86	LEU
20	c8	88	ARG
20	c8	93	THR
20	c8	105	VAL
20	c8	113	LEU
20	c8	116	LEU
20	c8	119	ILE
20	c8	120	ARG
20	c8	133	VAL
20	c8	136	GLN
20	c8	138	THR
20	c8	143	ARG
20	c8	145	ARG
21	c9	6	VAL
21	c9	28	LEU

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Mol	Chain	Res	Type
21	c9	34	VAL
21	c9	35	ASP
21	c9	36	ILE
21	c9	37	VAL
21	c9	46	PRO
21	c9	51	GLU
21	c9	57	ARG
21	c9	71	VAL
21	c9	84	LYS
21	c9	88	VAL
21	c9	111	ILE
21	c9	123	ARG
21	c9	134	ARG
21	c9	135	ILE
21	c9	139	THR
21	c9	142	GLU
21	c9	144	GLU
22	d0	13	GLU
22	d0	20	ILE
22	d0	27	THR
22	d0	31	VAL
22	d0	33	GLN
22	d0	44	ASN
22	d0	47	GLN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	67	THR
22	d0	70	THR
22	d0	74	GLU
22	d0	81	THR
22	d0	88	LYS
22	d0	89	ARG
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	107	THR
22	d0	108	ILE
22	d0	113	ASP
23	d1	2	GLU
23	d1	5	LYS
23	d1	8	LEU

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Mol	Chain	Res	Type
23	d1	10	GLU
23	d1	11	LEU
23	d1	12	TYR
23	d1	15	ARG
23	d1	32	VAL
23	d1	44	ARG
23	d1	52	THR
23	d1	68	SER
23	d1	78	LEU
23	d1	81	ASN
23	d1	86	SER
24	d2	6	VAL
24	d2	7	LEU
24	d2	15	ASN
24	d2	22	LYS
24	d2	25	VAL
24	d2	26	LEU
24	d2	43	LYS
24	d2	65	LEU
24	d2	74	VAL
24	d2	88	LYS
24	d2	93	LEU
24	d2	103	ILE
24	d2	105	THR
24	d2	129	VAL
25	d3	9	LEU
25	d3	14	LYS
25	d3	16	ARG
25	d3	19	ARG
25	d3	28	ASN
25	d3	33	LEU
25	d3	36	THR
25	d3	40	SER
25	d3	73	ARG
25	d3	83	VAL
25	d3	84	THR
25	d3	96	VAL
25	d3	103	LEU
25	d3	107	PHE
25	d3	121	ARG
25	d3	131	SER
25	d3	133	LEU

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Mol	Chain	Res	Type
26	d4	5	VAL
26	d4	10	ARG
26	d4	12	VAL
26	d4	26	ASP
26	d4	29	HIS
26	d4	42	GLU
26	d4	43	LYS
26	d4	46	GLU
26	d4	49	LYS
26	d4	62	THR
26	d4	88	THR
26	d4	100	VAL
26	d4	132	ARG
26	d4	133	ASN
27	d5	42	LEU
27	d5	43	ASP
27	d5	46	LYS
27	d5	51	LEU
27	d5	53	GLU
27	d5	57	TYR
27	d5	60	VAL
27	d5	81	ARG
27	d5	93	SER
28	d6	11	ASN
28	d6	24	VAL
28	d6	25	ASN
28	d6	34	LYS
28	d6	41	ILE
28	d6	44	ILE
28	d6	67	THR
28	d6	76	SER
28	d6	82	ARG
28	d6	85	ARG
28	d6	87	ARG
29	d7	3	LEU
29	d7	4	VAL
29	d7	17	ARG
29	d7	22	LYS
29	d7	43	ILE
29	d7	44	THR
29	d7	72	LYS
30	d8	22	ARG

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Mol	Chain	Res	Type
30	d8	28	VAL
30	d8	33	LEU
30	d8	36	THR
30	d8	48	VAL
30	d8	49	ARG
30	d8	54	LEU
30	d8	58	GLU
30	d8	64	ARG
31	d9	19	ARG
31	d9	30	LEU
31	d9	32	ARG
31	d9	36	LEU
31	d9	54	LYS
31	d9	56	ARG
80	e0	5	HIS
80	e0	23	LYS
80	e0	26	LYS
80	e0	29	LYS
80	e0	38	LEU
80	e0	41	THR
80	e0	43	ARG
80	e0	44	PHE
80	e0	46	ASN
80	e0	55	ARG
80	e0	56	MET
81	e1	86	THR
81	e1	90	LYS
81	e1	96	LYS
81	e1	100	LEU
81	e1	102	VAL
81	e1	106	TYR
81	e1	107	LYS
81	e1	109	ASP
81	e1	113	LYS
81	e1	119	ARG
81	e1	121	CYS
81	e1	122	SER
81	e1	130	VAL
81	e1	135	HIS
81	e1	137	ASP
81	e1	147	VAL
81	e1	148	TYR

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Mol	Chain	Res	Type
81	e1	150	VAL
34	sR	25	THR
34	sR	42	LEU
34	sR	56	VAL
34	sR	58	VAL
34	sR	59	ARG
34	sR	60	SER
34	sR	65	SER
34	sR	66	HIS
34	sR	76	ASP
34	sR	96	THR
34	sR	101	GLN
34	sR	108	SER
34	sR	136	ILE
34	sR	145	LEU
34	sR	166	SER
34	sR	168	THR
34	sR	184	ASN
34	sR	199	ILE
34	sR	203	THR
34	sR	228	LYS
34	sR	232	TYR
34	sR	245	PHE
34	sR	256	THR
34	sR	266	ASP
34	sR	275	ARG
34	sR	286	GLU
34	sR	295	SER
34	sR	297	ASP
34	sR	299	GLN
34	sR	317	THR
35	sM	23	LYS
35	sM	27	LYS
35	sM	28	SER
35	sM	33	LYS
35	sM	43	ASP
35	sM	45	SER
35	sM	48	ARG
35	sM	49	LYS
35	sM	53	ARG
35	sM	61	ILE
35	sM	64	LYS

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Mol	Chain	Res	Type
35	sM	74	LYS
35	sM	77	THR
35	sM	79	SER
35	sM	85	SER
39	l2	15	ILE
39	l2	23	ARG
39	l2	32	LEU
39	l2	44	ILE
39	l2	45	VAL
39	l2	46	LYS
39	l2	48	ILE
39	l2	62	VAL
39	l2	70	ARG
39	l2	74	GLU
39	l2	82	VAL
39	l2	96	LEU
39	l2	101	VAL
39	l2	113	VAL
39	l2	114	SER
39	l2	116	VAL
39	l2	137	ILE
39	l2	142	ASP
39	l2	147	ARG
39	l2	149	ARG
39	l2	155	LYS
39	l2	157	VAL
39	l2	158	ILE
39	l2	179	LEU
39	l2	181	LYS
39	l2	188	LYS
39	l2	193	ARG
39	l2	215	ASN
39	l2	227	ARG
39	l2	241	ARG
39	l2	243	THR
39	l2	246	LEU
40	l3	3	HIS
40	l3	4	ARG
40	l3	10	ARG
40	l3	17	LEU
40	l3	19	ARG
40	l3	21	ARG

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Mol	Chain	Res	Type
40	l3	34	LYS
40	l3	43	LEU
40	l3	47	LEU
40	l3	50	LYS
40	l3	67	PHE
40	l3	70	ARG
40	l3	77	THR
40	l3	79	VAL
40	l3	84	VAL
40	l3	85	VAL
40	l3	102	LEU
40	l3	103	THR
40	l3	104	THR
40	l3	114	VAL
40	l3	116	ARG
40	l3	134	SER
40	l3	139	GLN
40	l3	145	GLU
40	l3	146	ARG
40	l3	148	LEU
40	l3	150	ARG
40	l3	156	SER
40	l3	157	VAL
40	l3	169	THR
40	l3	178	LEU
40	l3	183	LEU
40	l3	192	VAL
40	l3	196	ARG
40	l3	202	THR
40	l3	205	VAL
40	l3	213	GLU
40	l3	221	THR
40	l3	222	LYS
40	l3	229	VAL
40	l3	232	ARG
40	l3	235	THR
40	l3	238	LEU
40	l3	242	THR
40	l3	248	LYS
40	l3	249	VAL
40	l3	252	ILE
40	l3	261	MET

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Mol	Chain	Res	Type
40	l3	264	VAL
40	l3	284	ARG
40	l3	297	SER
40	l3	304	THR
40	l3	308	MET
40	l3	317	ILE
40	l3	319	ASN
40	l3	320	ASP
40	l3	328	ILE
40	l3	332	ARG
40	l3	335	ILE
40	l3	338	LEU
40	l3	341	SER
40	l3	348	ARG
40	l3	349	LYS
40	l3	355	SER
40	l3	361	THR
40	l3	364	LYS
40	l3	369	ARG
40	l3	376	LYS
40	l3	382	THR
41	l4	3	ARG
41	l4	14	GLU
41	l4	16	THR
41	l4	25	VAL
41	l4	47	ARG
41	l4	52	VAL
41	l4	60	THR
41	l4	71	VAL
41	l4	93	MET
41	l4	99	MET
41	l4	112	LYS
41	l4	117	GLU
41	l4	120	TYR
41	l4	122	THR
41	l4	138	ARG
41	l4	144	LYS
41	l4	145	ILE
41	l4	150	LEU
41	l4	156	LEU
41	l4	170	LYS
41	l4	172	VAL

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Mol	Chain	Res	Type
41	14	179	LEU
41	14	186	LYS
41	14	187	LEU
41	14	203	ARG
41	14	206	LEU
41	14	217	LYS
41	14	220	ARG
41	14	230	VAL
41	14	246	ARG
41	14	258	LEU
41	14	289	ILE
41	14	290	ILE
41	14	293	SER
41	14	300	ARG
41	14	301	PRO
41	14	306	THR
41	14	307	GLN
41	14	308	LYS
41	14	313	LEU
41	14	319	LYS
41	14	323	VAL
41	14	327	LEU
41	14	339	LEU
41	14	342	LYS
41	14	345	GLU
41	14	347	THR
41	14	356	THR
41	14	359	LEU
42	15	4	GLN
42	15	5	LYS
42	15	34	LYS
42	15	35	ARG
42	15	51	LEU
42	15	65	ILE
42	15	68	THR
42	15	70	THR
42	15	74	VAL
42	15	75	LEU
42	15	89	THR
42	15	93	THR
42	15	110	LEU
42	15	112	LYS

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Mol	Chain	Res	Type
42	15	113	LEU
42	15	115	LEU
42	15	118	THR
42	15	120	LYS
42	15	133	GLU
42	15	136	GLU
42	15	144	VAL
42	15	146	LEU
42	15	148	ILE
42	15	152	ARG
42	15	155	THR
42	15	164	LYS
42	15	177	GLU
42	15	183	TRP
42	15	185	PHE
42	15	186	GLU
42	15	194	LEU
42	15	205	SER
42	15	211	LEU
42	15	227	LEU
42	15	241	THR
42	15	254	LYS
42	15	258	LYS
42	15	259	LYS
42	15	262	LYS
42	15	268	GLU
42	15	273	ARG
42	15	275	THR
42	15	276	LYS
42	15	282	ARG
42	15	297	GLN
43	16	8	LYS
43	16	20	LYS
43	16	21	THR
43	16	31	ARG
43	16	46	ARG
43	16	50	LYS
43	16	64	LEU
43	16	65	ILE
43	16	78	ARG
43	16	79	VAL
43	16	88	SER

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Mol	Chain	Res	Type
43	16	89	THR
43	16	93	VAL
43	16	98	VAL
43	16	99	GLU
43	16	108	LYS
43	16	109	GLU
43	16	131	LYS
43	16	133	GLU
43	16	151	LYS
43	16	152	THR
43	16	155	LEU
43	16	162	SER
43	16	175	LYS
44	17	22	THR
44	17	24	GLU
44	17	26	VAL
44	17	41	ARG
44	17	56	GLU
44	17	59	GLU
44	17	60	ARG
44	17	77	VAL
44	17	83	LEU
44	17	88	ARG
44	17	98	LYS
44	17	100	ARG
44	17	110	ARG
44	17	124	LEU
44	17	130	ILE
44	17	156	ILE
44	17	158	LYS
44	17	159	GLN
44	17	173	LEU
44	17	175	LYS
44	17	179	LEU
44	17	184	LEU
44	17	196	LYS
44	17	219	LYS
44	17	229	PHE
44	17	234	GLU
44	17	239	LEU
45	18	41	GLN
45	18	50	VAL

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Mol	Chain	Res	Type
45	18	65	LEU
45	18	67	ILE
45	18	71	VAL
45	18	74	THR
45	18	81	THR
45	18	93	LEU
45	18	95	ASN
45	18	109	LEU
45	18	111	LYS
45	18	136	LEU
45	18	145	ASN
45	18	149	LYS
45	18	160	ILE
45	18	163	VAL
45	18	164	VAL
45	18	169	LEU
45	18	172	LYS
45	18	183	LYS
45	18	185	ARG
45	18	191	ASN
45	18	192	GLN
45	18	200	LEU
45	18	211	LEU
45	18	214	LEU
45	18	217	THR
45	18	230	LYS
45	18	241	LYS
45	18	245	LYS
45	18	248	LYS
46	19	5	GLN
46	19	6	THR
46	19	16	VAL
46	19	18	VAL
46	19	31	ARG
46	19	33	THR
46	19	43	VAL
46	19	44	THR
46	19	46	THR
46	19	52	LEU
46	19	55	VAL
46	19	62	ARG
46	19	68	LEU

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Mol	Chain	Res	Type
46	l9	69	ARG
46	l9	70	THR
46	l9	80	THR
46	l9	82	VAL
46	l9	105	GLU
46	l9	124	ARG
46	l9	133	THR
46	l9	144	ILE
46	l9	151	VAL
46	l9	157	ASN
46	l9	161	LEU
46	l9	162	GLN
46	l9	166	ARG
46	l9	170	LYS
46	l9	179	ILE
46	l9	188	THR
46	l9	191	LEU
47	m0	4	ARG
47	m0	7	ARG
47	m0	24	ARG
47	m0	35	ASP
47	m0	36	LEU
47	m0	38	LYS
47	m0	39	LYS
47	m0	48	LEU
47	m0	52	LEU
47	m0	54	SER
47	m0	57	LEU
47	m0	58	GLU
47	m0	63	GLU
47	m0	74	LYS
47	m0	76	MET
47	m0	78	THR
47	m0	87	LEU
47	m0	91	VAL
47	m0	99	ILE
47	m0	101	LYS
47	m0	129	VAL
47	m0	130	ASP
47	m0	139	ARG
47	m0	140	THR
47	m0	143	SER

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Mol	Chain	Res	Type
47	m0	144	ASN
47	m0	153	ARG
47	m0	156	ARG
47	m0	167	LEU
47	m0	169	LYS
47	m0	185	ARG
47	m0	197	VAL
47	m0	203	LYS
47	m0	205	SER
47	m0	206	LEU
47	m0	209	ASN
47	m0	211	ARG
47	m0	212	GLU
47	m0	217	PHE
48	m1	10	ARG
48	m1	11	ASP
48	m1	12	LEU
48	m1	13	LYS
48	m1	31	THR
48	m1	34	SER
48	m1	44	THR
48	m1	54	VAL
48	m1	55	ARG
48	m1	56	THR
48	m1	80	LEU
48	m1	94	ARG
48	m1	106	ILE
48	m1	107	ASP
48	m1	112	LEU
48	m1	115	LYS
48	m1	129	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	142	LYS
48	m1	153	LYS
48	m1	158	ASP
48	m1	159	THR
48	m1	171	VAL
49	m3	54	LEU
49	m3	55	ARG
49	m3	58	VAL
49	m3	59	ARG

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Mol	Chain	Res	Type
49	m3	67	ARG
49	m3	69	VAL
49	m3	73	ARG
49	m3	107	GLU
49	m3	114	GLN
49	m3	121	SER
49	m3	123	ILE
49	m3	124	ILE
49	m3	128	ARG
49	m3	131	LYS
49	m3	149	GLN
49	m3	152	THR
49	m3	164	GLU
49	m3	165	SER
49	m3	168	ARG
49	m3	183	ARG
49	m3	184	GLU
49	m3	194	GLU
50	m4	3	THR
50	m4	4	ASP
50	m4	10	SER
50	m4	13	ARG
50	m4	20	VAL
50	m4	27	GLN
50	m4	42	LYS
50	m4	53	VAL
50	m4	62	GLN
50	m4	64	VAL
50	m4	72	LEU
50	m4	80	THR
50	m4	82	SER
50	m4	92	GLU
50	m4	105	GLN
50	m4	106	ARG
50	m4	113	THR
50	m4	126	GLN
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	8	GLU
51	m5	10	LEU
51	m5	12	ARG

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Mol	Chain	Res	Type
51	m5	20	ARG
51	m5	22	LEU
51	m5	24	ARG
51	m5	49	ARG
51	m5	66	VAL
51	m5	76	PRO
51	m5	80	THR
51	m5	85	THR
51	m5	91	GLU
51	m5	96	ARG
51	m5	97	SER
51	m5	98	LEU
51	m5	105	ARG
51	m5	138	GLN
51	m5	151	ILE
51	m5	153	ASP
51	m5	155	VAL
51	m5	159	ARG
51	m5	170	LYS
51	m5	171	SER
51	m5	175	ASN
51	m5	183	THR
51	m5	184	LYS
51	m5	190	THR
51	m5	204	LYS
52	m6	22	VAL
52	m6	25	LYS
52	m6	34	VAL
52	m6	41	LEU
52	m6	58	LEU
52	m6	59	ARG
52	m6	60	LYS
52	m6	66	LYS
52	m6	67	THR
52	m6	68	ARG
52	m6	74	ARG
52	m6	78	ARG
52	m6	85	ARG
52	m6	100	GLU
52	m6	106	GLU
52	m6	108	ILE
52	m6	110	PRO

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Mol	Chain	Res	Type
52	m6	117	ARG
52	m6	122	GLN
52	m6	124	LEU
52	m6	128	ARG
52	m6	129	LEU
52	m6	130	LYS
52	m6	144	SER
52	m6	152	VAL
52	m6	160	ARG
52	m6	166	GLU
52	m6	167	TYR
52	m6	171	LYS
52	m6	175	THR
52	m6	182	ASN
52	m6	190	VAL
52	m6	197	LEU
53	m7	9	THR
53	m7	24	VAL
53	m7	29	THR
53	m7	32	THR
53	m7	41	LEU
53	m7	52	LEU
53	m7	55	GLN
53	m7	56	ARG
53	m7	74	LYS
53	m7	79	THR
53	m7	94	LEU
53	m7	103	GLU
53	m7	112	LEU
53	m7	114	VAL
53	m7	119	VAL
53	m7	126	ARG
53	m7	127	ARG
53	m7	128	ARG
53	m7	144	SER
54	m8	3	ILE
54	m8	7	SER
54	m8	17	THR
54	m8	22	ASP
54	m8	24	VAL
54	m8	26	LEU
54	m8	32	LEU

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Mol	Chain	Res	Type
54	m8	34	THR
54	m8	49	LEU
54	m8	57	ILE
54	m8	63	SER
54	m8	64	VAL
54	m8	80	THR
54	m8	81	VAL
54	m8	86	THR
54	m8	93	ILE
54	m8	95	GLU
54	m8	100	THR
54	m8	104	LEU
54	m8	111	ARG
54	m8	113	LYS
54	m8	129	VAL
54	m8	135	GLN
54	m8	137	THR
54	m8	144	ARG
54	m8	165	ILE
54	m8	167	SER
54	m8	168	THR
54	m8	170	ARG
54	m8	171	LYS
55	m9	7	GLN
55	m9	10	LEU
55	m9	17	VAL
55	m9	20	ARG
55	m9	29	THR
55	m9	31	GLU
55	m9	36	ASN
55	m9	39	ASN
55	m9	43	LYS
55	m9	49	THR
55	m9	52	LYS
55	m9	56	THR
55	m9	57	VAL
55	m9	61	SER
55	m9	63	THR
55	m9	70	LYS
55	m9	74	ARG
55	m9	76	SER
55	m9	99	LEU

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Mol	Chain	Res	Type
55	m9	105	LEU
55	m9	106	LEU
55	m9	126	GLU
55	m9	138	LEU
55	m9	152	GLU
55	m9	153	LYS
55	m9	158	GLU
55	m9	164	LEU
55	m9	167	ARG
55	m9	170	ARG
55	m9	177	VAL
56	n0	1	MET
56	n0	13	ARG
56	n0	17	GLU
56	n0	21	GLU
56	n0	23	LYS
56	n0	39	SER
56	n0	49	HIS
56	n0	50	LYS
56	n0	52	LYS
56	n0	61	ILE
56	n0	70	THR
56	n0	73	LYS
56	n0	87	THR
56	n0	96	ASP
56	n0	97	VAL
56	n0	100	VAL
56	n0	104	GLU
56	n0	105	THR
56	n0	115	ARG
56	n0	117	ARG
56	n0	120	SER
56	n0	130	GLU
56	n0	132	THR
56	n0	136	LYS
56	n0	148	LEU
56	n0	161	LYS
56	n0	162	THR
56	n0	164	SER
56	n0	166	LYS
56	n0	169	SER
56	n0	172	TYR

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Mol	Chain	Res	Type
57	n1	3	LYS
57	n1	9	SER
57	n1	12	ARG
57	n1	25	VAL
57	n1	26	HIS
57	n1	55	LYS
57	n1	68	THR
57	n1	78	LYS
57	n1	80	VAL
57	n1	83	ARG
57	n1	86	GLU
57	n1	88	ARG
57	n1	89	LEU
57	n1	102	ARG
57	n1	104	GLU
57	n1	122	GLN
57	n1	126	VAL
57	n1	127	GLN
57	n1	130	ARG
57	n1	131	GLN
57	n1	135	PRO
57	n1	139	ARG
57	n1	140	ILE
57	n1	143	THR
57	n1	150	THR
57	n1	154	VAL
57	n1	160	ILE
58	n2	16	THR
58	n2	27	VAL
58	n2	28	PHE
58	n2	37	LEU
58	n2	43	VAL
58	n2	55	THR
58	n2	63	VAL
58	n2	66	VAL
58	n2	88	GLN
58	n2	90	ARG
58	n2	98	THR
58	n2	100	THR
58	n2	105	LEU
59	n3	7	GLN
59	n3	13	ILE

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Mol	Chain	Res	Type
59	n3	48	ARG
59	n3	69	LEU
59	n3	73	VAL
59	n3	88	ARG
59	n3	91	VAL
59	n3	120	LYS
60	n4	1	MET
60	n4	7	SER
60	n4	34	SER
60	n4	39	LEU
60	n4	43	ARG
60	n4	54	LEU
60	n4	63	ILE
60	n4	96	LEU
60	n4	97	LYS
60	n4	99	GLU
60	n4	100	VAL
60	n4	107	GLU
60	n4	119	GLU
60	n4	120	LYS
60	n4	127	LYS
60	n4	135	SER
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	37	THR
61	n5	38	LEU
61	n5	40	LEU
61	n5	45	LYS
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	71	THR
61	n5	74	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	129	ASP
61	n5	133	LEU

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Mol	Chain	Res	Type
61	n5	135	ILE
61	n5	142	ILE
62	n6	4	GLN
62	n6	10	SER
62	n6	12	ARG
62	n6	13	ARG
62	n6	14	LYS
62	n6	17	LYS
62	n6	37	LYS
62	n6	39	LEU
62	n6	40	ARG
62	n6	43	TYR
62	n6	45	ILE
62	n6	50	ILE
62	n6	55	GLU
62	n6	56	VAL
62	n6	57	LEU
62	n6	62	SER
62	n6	64	LYS
62	n6	66	GLN
62	n6	74	TYR
62	n6	76	LEU
62	n6	80	VAL
62	n6	83	ASP
62	n6	86	THR
62	n6	94	SER
62	n6	95	VAL
62	n6	115	ARG
62	n6	120	GLN
63	n7	3	LYS
63	n7	14	VAL
63	n7	17	ARG
63	n7	21	LYS
63	n7	24	VAL
63	n7	34	LYS
63	n7	46	ILE
63	n7	52	LYS
63	n7	81	LEU
63	n7	83	THR
63	n7	90	GLU
63	n7	94	SER
63	n7	99	GLU

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Mol	Chain	Res	Type
63	n7	103	GLN
63	n7	105	SER
63	n7	111	LYS
63	n7	126	LYS
63	n7	134	LEU
63	n7	135	ARG
64	n8	4	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	10	LYS
64	n8	26	ARG
64	n8	27	LYS
64	n8	34	MET
64	n8	47	LYS
64	n8	60	TYR
64	n8	65	GLN
64	n8	76	ASP
64	n8	80	THR
64	n8	82	ILE
64	n8	85	ASP
64	n8	91	LEU
64	n8	98	THR
64	n8	115	LYS
64	n8	117	ARG
64	n8	128	ARG
64	n8	132	LYS
64	n8	133	LEU
64	n8	139	ARG
65	n9	12	GLN
65	n9	14	ARG
65	n9	22	LYS
65	n9	23	LYS
65	n9	33	LYS
65	n9	35	VAL
65	n9	38	LYS
65	n9	52	LYS
65	n9	58	LYS
65	n9	59	LYS
66	o0	8	GLU
66	o0	9	SER
66	o0	10	ILE
66	o0	12	GLN

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Mol	Chain	Res	Type
66	o0	14	LEU
66	o0	19	LYS
66	o0	33	SER
66	o0	40	LYS
66	o0	41	LEU
66	o0	48	THR
66	o0	61	MET
66	o0	68	TYR
66	o0	81	VAL
66	o0	84	LEU
66	o0	86	ARG
66	o0	87	VAL
67	o1	6	ASP
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	26	LYS
67	o1	31	ARG
67	o1	34	LYS
67	o1	44	MET
67	o1	46	THR
67	o1	55	LEU
67	o1	61	LYS
67	o1	76	SER
67	o1	90	PHE
67	o1	91	SER
67	o1	93	VAL
67	o1	100	SER
67	o1	102	LYS
67	o1	104	LEU
67	o1	106	THR
67	o1	107	VAL
67	o1	110	GLU
68	o2	4	LEU
68	o2	16	LYS
68	o2	18	LYS
68	o2	19	ARG
68	o2	24	ARG
68	o2	31	ASN
68	o2	33	ARG
68	o2	41	VAL
68	o2	51	SER

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Mol	Chain	Res	Type
68	o2	54	LYS
68	o2	59	SER
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	87	MET
68	o2	106	VAL
68	o2	109	LEU
68	o2	111	ARG
68	o2	113	LYS
68	o2	125	ARG
68	o2	126	LEU
69	o3	10	LYS
69	o3	21	ARG
69	o3	28	SER
69	o3	31	LYS
69	o3	37	THR
69	o3	49	ILE
69	o3	57	LYS
69	o3	59	VAL
69	o3	81	VAL
69	o3	90	PRO
69	o3	92	LYS
69	o3	98	VAL
69	o3	105	SER
69	o3	107	ILE
70	o4	3	GLN
70	o4	9	ARG
70	o4	20	ILE
70	o4	24	LYS
70	o4	29	ILE
70	o4	30	LEU
70	o4	40	THR
70	o4	56	THR
70	o4	58	ARG
70	o4	65	VAL
70	o4	68	THR
70	o4	79	SER
70	o4	108	GLN
71	o5	21	LEU
71	o5	27	GLU
71	o5	28	LEU

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Mol	Chain	Res	Type
71	o5	31	LEU
71	o5	38	ARG
71	o5	43	LYS
71	o5	45	LYS
71	o5	47	VAL
71	o5	57	VAL
71	o5	62	GLN
71	o5	69	LEU
71	o5	79	ASP
71	o5	81	ARG
71	o5	84	LYS
71	o5	85	THR
71	o5	89	ARG
71	o5	98	SER
71	o5	101	THR
71	o5	107	LYS
71	o5	108	GLN
72	o6	3	VAL
72	o6	7	ILE
72	o6	9	ILE
72	o6	18	THR
72	o6	21	THR
72	o6	26	ILE
72	o6	29	LYS
72	o6	35	ASN
72	o6	36	ARG
72	o6	37	THR
72	o6	38	LYS
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	59	ASP
72	o6	63	ASN
72	o6	66	GLU
72	o6	68	ARG
72	o6	75	LYS
72	o6	76	ARG
72	o6	79	SER
72	o6	81	THR
72	o6	98	ARG
73	o7	17	THR

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Mol	Chain	Res	Type
73	o7	21	ARG
73	o7	24	ARG
73	o7	25	ARG
73	o7	31	LYS
73	o7	33	THR
73	o7	44	THR
73	o7	55	ARG
73	o7	58	THR
73	o7	59	THR
73	o7	67	LEU
73	o7	68	LYS
73	o7	75	LYS
73	o7	80	THR
73	o7	84	SER
74	o8	5	ILE
74	o8	6	THR
74	o8	8	ILE
74	o8	17	ARG
74	o8	24	THR
74	o8	41	THR
74	o8	46	ARG
74	o8	53	THR
74	o8	64	LYS
74	o8	65	LEU
74	o8	72	THR
75	o9	4	GLN
75	o9	21	ARG
75	o9	47	THR
75	o9	48	LYS
75	o9	51	ILE
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	120	GLN
76	q0	126	LYS
76	q0	127	LEU
77	q1	6	ARG
77	q1	9	ARG
77	q1	13	LEU

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Mol	Chain	Res	Type
77	q1	21	ARG
77	q1	23	ARG
77	q1	24	SER
78	q2	2	VAL
78	q2	4	VAL
78	q2	6	LYS
78	q2	7	THR
78	q2	8	ARG
78	q2	16	THR
78	q2	32	LYS
78	q2	46	LYS
78	q2	63	LYS
78	q2	73	GLU
78	q2	78	LYS
78	q2	79	THR
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	89	LYS
78	q2	93	LEU
78	q2	104	LEU
79	q3	3	LYS
79	q3	5	THR
79	q3	10	ILE
79	q3	20	SER
79	q3	22	LEU
79	q3	23	ARG
79	q3	24	ARG
79	q3	44	LYS
79	q3	45	LYS
79	q3	48	LYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	78	THR
79	q3	90	VAL
83	p0	4	ILE
83	p0	5	ARG
83	p0	15	LEU
83	p0	25	LEU
83	p0	30	VAL
83	p0	39	HIS

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Mol	Chain	Res	Type
83	p0	43	LYS
83	p0	50	VAL
83	p0	51	VAL
83	p0	57	THR
83	p0	60	ARG
83	p0	68	SER
83	p0	69	ASP
83	p0	70	LEU
83	p0	72	ASP
83	p0	76	LEU
83	p0	81	LYS
83	p0	84	VAL
83	p0	91	GLU
83	p0	93	LEU
83	p0	97	LYS
83	p0	103	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
9	S7	180	GLN
13	C1	110	HIS
23	D1	74	GLN
33	E1	135	HIS
34	SR	159	ASN
39	L2	83	HIS
39	L2	209	HIS
40	L3	256	HIS
42	L5	40	HIS
44	L7	244	ASN
59	N3	98	ASN
66	O0	11	ASN
3	s1	209	ASN
3	s1	211	HIS
6	s4	231	GLN
8	s6	197	ASN
8	s6	201	GLN
11	s9	110	GLN
12	c0	32	HIS
20	c8	55	HIS
22	d0	72	ASN
26	d4	22	GLN

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Mol	Chain	Res	Type
34	sR	184	ASN
46	l9	102	ASN
48	m1	95	ASN
51	m5	194	GLN
72	o6	63	ASN
78	q2	102	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	451 (25%)	57 (3%)
1	6	1792/1800 (99%)	435 (24%)	48 (2%)
36	1	3145/3396 (92%)	619 (19%)	91 (2%)
36	5	3146/3396 (92%)	623 (19%)	88 (2%)
37	3	120/121 (99%)	10 (8%)	2 (1%)
37	7	120/121 (99%)	17 (14%)	0
38	4	157/158 (99%)	33 (21%)	3 (1%)
38	8	157/158 (99%)	38 (24%)	2 (1%)
All	All	10384/10950 (94%)	2226 (21%)	291 (2%)

All (2226) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	8	U
1	2	17	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	39	A
1	2	40	A
1	2	45	U
1	2	46	A
1	2	47	A
1	2	50	C
1	2	57	G
1	2	60	U
1	2	67	A
1	2	68	A

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Mol	Chain	Res	Type
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	97	C
1	2	104	A
1	2	114	C
1	2	115	G
1	2	127	G
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	142	G
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	169	A
1	2	170	U
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
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	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	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	288	A
1	2	299	A
1	2	308	C
1	2	309	C
1	2	314	C
1	2	316	A
1	2	319	U
1	2	320	U
1	2	321	C
1	2	322	G
1	2	337	G

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Mol	Chain	Res	Type
1	2	338	C
1	2	341	A
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	387	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	403	G
1	2	404	G
1	2	414	C
1	2	416	A
1	2	417	A
1	2	418	G
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	444	C
1	2	445	A
1	2	448	C
1	2	475	A
1	2	484	C
1	2	485	A
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U

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Mol	Chain	Res	Type
1	2	508	U
1	2	510	G
1	2	511	A
1	2	512	A
1	2	513	U
1	2	514	G
1	2	515	A
1	2	525	A
1	2	527	A
1	2	532	U
1	2	536	C
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	548	G
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	569	C
1	2	570	A
1	2	579	A
1	2	580	A
1	2	582	U
1	2	585	A
1	2	594	A
1	2	595	G
1	2	609	U
1	2	611	U
1	2	617	U
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	639	U
1	2	640	U
1	2	645	C
1	2	650	U

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Mol	Chain	Res	Type
1	2	653	C
1	2	655	G
1	2	656	G
1	2	658	C
1	2	677	G
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C
1	2	690	G
1	2	694	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	709	C
1	2	710	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	729	G
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A

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Mol	Chain	Res	Type
1	2	738	G
1	2	742	U
1	2	743	U
1	2	745	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	758	U
1	2	759	U
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	780	A
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	794	U
1	2	812	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	823	G
1	2	824	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	833	U
1	2	835	U
1	2	837	G
1	2	840	U
1	2	846	G
1	2	856	A
1	2	862	A

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Mol	Chain	Res	Type
1	2	863	A
1	2	876	G
1	2	886	U
1	2	898	A
1	2	912	U
1	2	913	G
1	2	914	G
1	2	933	A
1	2	935	U
1	2	942	G
1	2	944	A
1	2	951	A
1	2	960	U
1	2	966	A
1	2	982	U
1	2	988	A
1	2	992	A
1	2	993	A
1	2	995	A
1	2	997	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1020	A
1	2	1021	C
1	2	1026	A
1	2	1028	C
1	2	1031	U
1	2	1039	A
1	2	1040	G
1	2	1044	U
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	1063	U
1	2	1074	G
1	2	1079	U
1	2	1080	U
1	2	1082	C

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Mol	Chain	Res	Type
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	1101	G
1	2	1111	G
1	2	1138	A
1	2	1146	G
1	2	1149	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	1176	G
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1203	A
1	2	1207	C
1	2	1208	A
1	2	1217	A
1	2	1218	G
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	1257	U
1	2	1258	U

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Mol	Chain	Res	Type
1	2	1274	C
1	2	1286	U
1	2	1314	U
1	2	1315	U
1	2	1321	A
1	2	1337	A
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1361	U
1	2	1363	U
1	2	1364	G
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	1414	U
1	2	1415	U
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1446	A
1	2	1448	G
1	2	1457	C
1	2	1459	C
1	2	1461	C
1	2	1462	G
1	2	1464	G
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1475	A
1	2	1482	C
1	2	1486	G

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Mol	Chain	Res	Type
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1499	G
1	2	1506	G
1	2	1514	U
1	2	1516	A
1	2	1521	G
1	2	1523	G
1	2	1524	A
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	1590	G
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1626	U
1	2	1631	A
1	2	1657	U
1	2	1658	G
1	2	1664	C
1	2	1680	G
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1728	A
1	2	1729	C
1	2	1731	A
1	2	1736	G
1	2	1756	A
1	2	1759	C

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Mol	Chain	Res	Type
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	13	A
36	1	14	U
36	1	26	A
36	1	40	A
36	1	43	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	74	G
36	1	75	G
36	1	83	U
36	1	92	G
36	1	93	C
36	1	99	A
36	1	109	A
36	1	110	G
36	1	113	C
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	156	G
36	1	157	A
36	1	160	G

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Mol	Chain	Res	Type
36	1	166	C
36	1	169	U
36	1	170	G
36	1	172	G
36	1	173	G
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C
36	1	210	U
36	1	218	G
36	1	219	A
36	1	224	C
36	1	230	U
36	1	234	G
36	1	240	U
36	1	241	G
36	1	243	G
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	269	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	323	A
36	1	329	U
36	1	338	A
36	1	339	C
36	1	349	A
36	1	350	C
36	1	376	G
36	1	397	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	424	G

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Mol	Chain	Res	Type
36	1	438	A
36	1	440	A
36	1	495	G
36	1	520	U
36	1	521	A
36	1	535	G
36	1	536	U
36	1	544	C
36	1	546	C
36	1	547	G
36	1	548	G
36	1	551	A
36	1	552	G
36	1	555	U
36	1	557	A
36	1	559	A
36	1	568	G
36	1	578	A
36	1	579	G
36	1	592	A
36	1	602	A
36	1	604	G
36	1	609	G
36	1	611	A
36	1	619	A
36	1	620	U
36	1	621	A
36	1	623	U
36	1	624	G
36	1	625	G
36	1	636	C
36	1	649	A
36	1	656	A
36	1	660	A
36	1	661	G
36	1	677	A
36	1	681	U
36	1	684	G
36	1	691	A
36	1	705	A
36	1	712	G
36	1	715	A

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Mol	Chain	Res	Type
36	1	716	A
36	1	719	U
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	780	A
36	1	781	G
36	1	785	G
36	1	799	G
36	1	801	A
36	1	806	A
36	1	815	G
36	1	817	A
36	1	830	A
36	1	849	C
36	1	861	C
36	1	874	U
36	1	879	U
36	1	883	A
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	923	C
36	1	924	G
36	1	937	G
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	980	A
36	1	981	U
36	1	982	C

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Mol	Chain	Res	Type
36	1	993	G
36	1	994	G
36	1	997	A
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1013	G
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1037	C
36	1	1047	A
36	1	1049	C
36	1	1063	G
36	1	1064	A
36	1	1065	A
36	1	1071	U
36	1	1072	G
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1131	G
36	1	1150	A
36	1	1153	A
36	1	1159	A
36	1	1160	C
36	1	1178	G
36	1	1179	A
36	1	1180	A

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Mol	Chain	Res	Type
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	1209	G
36	1	1213	G
36	1	1216	C
36	1	1218	U
36	1	1222	G
36	1	1226	G
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1235	U
36	1	1236	G
36	1	1237	G
36	1	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	1285	G
36	1	1287	A
36	1	1292	C
36	1	1307	G
36	1	1308	A

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Mol	Chain	Res	Type
36	1	1309	U
36	1	1313	G
36	1	1329	U
36	1	1330	A
36	1	1333	C
36	1	1348	U
36	1	1349	G
36	1	1350	A
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1366	A
36	1	1386	A
36	1	1399	A
36	1	1400	G
36	1	1419	A
36	1	1429	G
36	1	1434	G
36	1	1437	C
36	1	1446	A
36	1	1450	G
36	1	1454	A
36	1	1455	U
36	1	1467	A
36	1	1477	A
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1490	A
36	1	1496	C
36	1	1503	A
36	1	1508	C
36	1	1511	U
36	1	1526	U
36	1	1527	C
36	1	1528	G
36	1	1533	U
36	1	1538	G
36	1	1554	U

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Mol	Chain	Res	Type
36	1	1555	U
36	1	1556	C
36	1	1560	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1576	G
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	1620	U
36	1	1629	U
36	1	1643	A
36	1	1645	U
36	1	1657	C
36	1	1683	A
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1725	C
36	1	1741	A
36	1	1750	A
36	1	1751	G
36	1	1760	A
36	1	1762	C
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1770	G
36	1	1780	G
36	1	1781	C
36	1	1797	A
36	1	1809	A

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Mol	Chain	Res	Type
36	1	1810	A
36	1	1814	A
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1834	U
36	1	1839	A
36	1	1840	U
36	1	1841	A
36	1	1842	A
36	1	1846	C
36	1	1849	C
36	1	1855	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	1948	G
36	1	1951	C
36	1	1952	G
36	1	1954	G
36	1	2094	C
36	1	2101	C
36	1	2102	U
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2114	C
36	1	2116	G
36	1	2121	G
36	1	2122	G
36	1	2130	G
36	1	2131	A
36	1	2140	U
36	1	2158	A
36	1	2169	G
36	1	2170	U
36	1	2177	G

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Mol	Chain	Res	Type
36	1	2188	A
36	1	2201	G
36	1	2205	U
36	1	2208	A
36	1	2210	G
36	1	2223	A
36	1	2225	U
36	1	2228	A
36	1	2244	A
36	1	2248	C
36	1	2249	G
36	1	2250	G
36	1	2253	G
36	1	2255	A
36	1	2256	A
36	1	2272	G
36	1	2273	G
36	1	2279	A
36	1	2281	A
36	1	2282	U
36	1	2284	C
36	1	2299	A
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2334	U
36	1	2336	U
36	1	2366	C
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2375	G
36	1	2378	C
36	1	2379	U
36	1	2385	G
36	1	2388	U
36	1	2393	G
36	1	2397	A
36	1	2401	A
36	1	2402	A

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Mol	Chain	Res	Type
36	1	2403	G
36	1	2404	A
36	1	2411	U
36	1	2418	G
36	1	2419	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	2511	A
36	1	2513	U
36	1	2514	U
36	1	2515	A
36	1	2519	A
36	1	2522	G
36	1	2523	A
36	1	2529	A
36	1	2532	U
36	1	2533	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2548	C
36	1	2549	G
36	1	2551	U
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	2585	G

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Mol	Chain	Res	Type
36	1	2586	G
36	1	2593	A
36	1	2594	C
36	1	2595	A
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2626	A
36	1	2635	A
36	1	2637	A
36	1	2652	U
36	1	2656	A
36	1	2674	A
36	1	2677	G
36	1	2681	U
36	1	2689	A
36	1	2690	G
36	1	2691	A
36	1	2694	A
36	1	2696	A
36	1	2699	G
36	1	2714	G
36	1	2728	G
36	1	2729	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	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2802	A
36	1	2804	A
36	1	2810	C
36	1	2815	G

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Mol	Chain	Res	Type
36	1	2816	G
36	1	2817	A
36	1	2818	U
36	1	2825	C
36	1	2829	U
36	1	2830	G
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2847	A
36	1	2849	C
36	1	2860	U
36	1	2871	G
36	1	2872	A
36	1	2875	U
36	1	2876	C
36	1	2887	A
36	1	2889	C
36	1	2898	G
36	1	2899	C
36	1	2922	G
36	1	2923	U
36	1	2927	C
36	1	2935	U
36	1	2936	A
36	1	2937	G
36	1	2942	C
36	1	2945	G
36	1	2947	G
36	1	2971	A
36	1	2974	U
36	1	2983	C
36	1	2990	G
36	1	2997	G
36	1	3006	A
36	1	3012	A
36	1	3030	G
36	1	3039	C
36	1	3040	A
36	1	3049	A
36	1	3056	U
36	1	3057	U

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Mol	Chain	Res	Type
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	3092	C
36	1	3113	A
36	1	3122	A
36	1	3128	G
36	1	3130	A
36	1	3131	U
36	1	3134	A
36	1	3139	A
36	1	3142	A
36	1	3143	C
36	1	3151	U
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3164	C
36	1	3165	A
36	1	3167	A
36	1	3169	U
36	1	3170	A
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3187	A
36	1	3195	U
36	1	3196	U
36	1	3198	U
36	1	3207	U
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3228	C
36	1	3229	G

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Mol	Chain	Res	Type
36	1	3235	C
36	1	3243	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3259	U
36	1	3270	U
36	1	3272	C
36	1	3273	A
36	1	3276	G
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3289	G
36	1	3292	A
36	1	3294	A
36	1	3295	A
36	1	3304	U
36	1	3313	U
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3330	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3350	C
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3369	G
36	1	3375	A
36	1	3376	A
36	1	3378	C
36	1	3382	U
36	1	3383	G

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Mol	Chain	Res	Type
36	1	3389	U
36	1	3396	U
37	3	13	A
37	3	22	A
37	3	42	A
37	3	45	A
37	3	54	U
37	3	65	G
37	3	74	C
37	3	76	A
37	3	102	A
37	3	112	G
38	4	2	A
38	4	21	C
38	4	34	U
38	4	35	C
38	4	48	A
38	4	52	A
38	4	53	A
38	4	59	A
38	4	62	C
38	4	63	G
38	4	79	A
38	4	80	A
38	4	81	U
38	4	83	C
38	4	84	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	104	A
38	4	105	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	125	U
38	4	126	A
38	4	128	U
38	4	138	A
38	4	152	G

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Mol	Chain	Res	Type
38	4	155	A
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	44	U
1	6	47	A
1	6	49	C
1	6	57	G
1	6	66	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	78	A
1	6	103	A
1	6	104	A
1	6	114	C
1	6	115	G
1	6	116	U
1	6	127	G
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	144	U
1	6	145	A
1	6	158	U
1	6	159	U
1	6	166	C
1	6	178	U
1	6	179	A
1	6	181	A
1	6	182	A

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Mol	Chain	Res	Type
1	6	185	U
1	6	187	G
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	197	A
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	222	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	230	C
1	6	232	U
1	6	233	C
1	6	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	261	U
1	6	265	A
1	6	271	A
1	6	272	U
1	6	273	G
1	6	275	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	299	A
1	6	308	C
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U

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Mol	Chain	Res	Type
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	381	C
1	6	393	C
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	418	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	439	U
1	6	444	C
1	6	445	A
1	6	446	A
1	6	448	C
1	6	454	U
1	6	468	A
1	6	470	A
1	6	475	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
1	6	493	U
1	6	494	U
1	6	495	C

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Mol	Chain	Res	Type
1	6	496	G
1	6	497	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	514	G
1	6	519	C
1	6	527	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	555	A
1	6	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	600	U
1	6	606	A
1	6	610	G
1	6	611	U
1	6	616	G
1	6	617	U

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Mol	Chain	Res	Type
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	630	A
1	6	637	C
1	6	639	U
1	6	640	U
1	6	645	C
1	6	652	G
1	6	653	C
1	6	658	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	691	C
1	6	696	C
1	6	710	U
1	6	711	U
1	6	714	G
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	730	G
1	6	733	A
1	6	734	A
1	6	742	U
1	6	754	A
1	6	755	A

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Mol	Chain	Res	Type
1	6	756	A
1	6	765	G
1	6	768	C
1	6	774	A
1	6	775	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G
1	6	789	A
1	6	793	A
1	6	794	U
1	6	795	U
1	6	811	A
1	6	812	A
1	6	815	G
1	6	816	G
1	6	821	U
1	6	823	G
1	6	824	G
1	6	825	U
1	6	826	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	854	U
1	6	863	A
1	6	864	U
1	6	873	U
1	6	876	G
1	6	886	U
1	6	898	A
1	6	905	A
1	6	906	A
1	6	910	C
1	6	913	G
1	6	914	G
1	6	916	U

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Mol	Chain	Res	Type
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	969	C
1	6	970	A
1	6	971	A
1	6	976	G
1	6	991	G
1	6	992	A
1	6	993	A
1	6	997	G
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1021	C
1	6	1026	A
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	1061	A
1	6	1062	A
1	6	1066	C
1	6	1067	C
1	6	1071	U
1	6	1081	A
1	6	1082	C
1	6	1091	A
1	6	1092	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1100	G
1	6	1101	G

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Mol	Chain	Res	Type
1	6	1109	G
1	6	1138	A
1	6	1143	A
1	6	1146	G
1	6	1150	G
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1162	C
1	6	1167	G
1	6	1185	U
1	6	1193	A
1	6	1194	A
1	6	1196	A
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1208	A
1	6	1212	G
1	6	1217	A
1	6	1218	G
1	6	1220	C
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1231	U
1	6	1239	U
1	6	1241	G
1	6	1242	A
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1259	U
1	6	1262	U

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Mol	Chain	Res	Type
1	6	1275	A
1	6	1286	U
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1354	G
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1371	A
1	6	1372	U
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1413	U
1	6	1414	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1429	G
1	6	1433	G
1	6	1437	U
1	6	1445	G
1	6	1446	A
1	6	1448	G
1	6	1458	G
1	6	1459	C
1	6	1461	C
1	6	1471	A
1	6	1482	C
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A

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Mol	Chain	Res	Type
1	6	1493	A
1	6	1494	C
1	6	1506	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1569	A
1	6	1573	A
1	6	1574	G
1	6	1584	G
1	6	1600	A
1	6	1601	G
1	6	1616	G
1	6	1621	U
1	6	1634	C
1	6	1652	C
1	6	1657	U
1	6	1658	G
1	6	1664	C
1	6	1680	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1703	C
1	6	1712	A
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1731	A

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Mol	Chain	Res	Type
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	1792	G
1	6	1793	G
1	6	1794	A
1	6	1795	U
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	15	C
36	5	26	A
36	5	40	A
36	5	49	A
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	73	C
36	5	74	G
36	5	76	G
36	5	92	G
36	5	93	C
36	5	99	A
36	5	109	A
36	5	110	G
36	5	116	A
36	5	119	U
36	5	121	A
36	5	122	A
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G

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Mol	Chain	Res	Type
36	5	142	C
36	5	146	U
36	5	148	G
36	5	150	A
36	5	152	U
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	178	U
36	5	180	C
36	5	182	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	200	C
36	5	210	U
36	5	211	A
36	5	218	G
36	5	219	A
36	5	221	A
36	5	231	G
36	5	234	G
36	5	235	A
36	5	237	G
36	5	239	G
36	5	240	U
36	5	244	G
36	5	245	U
36	5	247	C
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	269	G

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Mol	Chain	Res	Type
36	5	283	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	311	C
36	5	323	A
36	5	329	U
36	5	330	G
36	5	338	A
36	5	339	C
36	5	349	A
36	5	350	C
36	5	370	U
36	5	376	G
36	5	390	G
36	5	395	A
36	5	397	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	407	A
36	5	421	G
36	5	422	A
36	5	436	A
36	5	437	G
36	5	438	A
36	5	439	C
36	5	440	A
36	5	441	U
36	5	442	G
36	5	443	G
36	5	492	U
36	5	495	G
36	5	520	U
36	5	521	A
36	5	531	G
36	5	534	U
36	5	535	G
36	5	546	C
36	5	547	G

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Mol	Chain	Res	Type
36	5	548	G
36	5	551	A
36	5	553	U
36	5	555	U
36	5	557	A
36	5	559	A
36	5	578	A
36	5	579	G
36	5	593	C
36	5	600	G
36	5	604	G
36	5	609	G
36	5	611	A
36	5	612	U
36	5	619	A
36	5	620	U
36	5	621	A
36	5	636	C
36	5	649	A
36	5	660	A
36	5	661	G
36	5	677	A
36	5	681	U
36	5	683	U
36	5	705	A
36	5	708	G
36	5	712	G
36	5	715	A
36	5	716	A
36	5	725	G
36	5	736	A
36	5	758	C
36	5	766	U
36	5	767	U
36	5	768	C
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

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Mol	Chain	Res	Type
36	5	806	A
36	5	817	A
36	5	830	A
36	5	861	C
36	5	874	U
36	5	879	U
36	5	881	C
36	5	891	G
36	5	896	A
36	5	897	U
36	5	907	G
36	5	908	G
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	923	C
36	5	937	G
36	5	944	C
36	5	959	C
36	5	960	U
36	5	963	G
36	5	974	G
36	5	979	U
36	5	980	A
36	5	981	U
36	5	983	A
36	5	994	G
36	5	1001	G
36	5	1002	A
36	5	1003	A
36	5	1010	G
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1019	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1028	U

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Mol	Chain	Res	Type
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	1071	U
36	5	1072	G
36	5	1081	U
36	5	1082	U
36	5	1087	G
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1117	G
36	5	1131	G
36	5	1153	A
36	5	1154	A
36	5	1155	C
36	5	1159	A
36	5	1160	C
36	5	1166	G
36	5	1174	G
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1192	C
36	5	1193	A
36	5	1199	C
36	5	1201	C
36	5	1208	U
36	5	1209	G
36	5	1222	G
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U

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Mol	Chain	Res	Type
36	5	1242	G
36	5	1245	A
36	5	1246	G
36	5	1258	U
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1285	G
36	5	1305	U
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1312	C
36	5	1313	G
36	5	1321	G
36	5	1330	A
36	5	1349	G
36	5	1351	U
36	5	1353	U
36	5	1356	U
36	5	1357	G
36	5	1379	G
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1431	G
36	5	1434	G
36	5	1437	C
36	5	1446	A
36	5	1450	G
36	5	1465	A
36	5	1481	A
36	5	1482	A
36	5	1490	A
36	5	1500	G
36	5	1508	C

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Mol	Chain	Res	Type
36	5	1522	U
36	5	1527	C
36	5	1536	G
36	5	1539	A
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1558	A
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1564	U
36	5	1565	G
36	5	1566	A
36	5	1567	U
36	5	1569	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1605	A
36	5	1620	U
36	5	1629	U
36	5	1639	C
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1657	C
36	5	1683	A
36	5	1716	U
36	5	1717	U
36	5	1724	U

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Mol	Chain	Res	Type
36	5	1725	C
36	5	1736	G
36	5	1741	A
36	5	1750	A
36	5	1751	G
36	5	1762	C
36	5	1765	U
36	5	1766	G
36	5	1769	G
36	5	1770	G
36	5	1778	G
36	5	1780	G
36	5	1781	C
36	5	1797	A
36	5	1810	A
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1821	U
36	5	1835	A
36	5	1839	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1849	C
36	5	1876	U
36	5	1879	A
36	5	1880	U
36	5	1893	A
36	5	1906	G
36	5	1920	U
36	5	1932	A
36	5	1953	G
36	5	2100	A
36	5	2101	C
36	5	2102	U
36	5	2111	G
36	5	2112	U
36	5	2113	A
36	5	2114	C

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Mol	Chain	Res	Type
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	2188	A
36	5	2201	G
36	5	2205	U
36	5	2207	A
36	5	2210	G
36	5	2222	A
36	5	2223	A
36	5	2228	A
36	5	2244	A
36	5	2250	G
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2258	U
36	5	2273	G
36	5	2278	C
36	5	2279	A
36	5	2281	A
36	5	2288	G
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2352	A
36	5	2362	C
36	5	2363	A
36	5	2366	C
36	5	2372	A
36	5	2373	A
36	5	2374	C

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Mol	Chain	Res	Type
36	5	2375	G
36	5	2385	G
36	5	2388	U
36	5	2393	G
36	5	2397	A
36	5	2401	A
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2435	G
36	5	2436	U
36	5	2438	A
36	5	2439	A
36	5	2440	G
36	5	2441	A
36	5	2443	A
36	5	2504	U
36	5	2505	U
36	5	2506	U
36	5	2507	C
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2514	U
36	5	2515	A
36	5	2518	C
36	5	2523	A
36	5	2526	C
36	5	2530	G
36	5	2531	C
36	5	2532	U
36	5	2534	G
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2545	C
36	5	2549	G

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Mol	Chain	Res	Type
36	5	2552	C
36	5	2555	G
36	5	2562	A
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2589	G
36	5	2593	A
36	5	2598	G
36	5	2606	G
36	5	2607	G
36	5	2610	G
36	5	2614	G
36	5	2625	C
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	2678	A
36	5	2689	A
36	5	2690	G
36	5	2691	A
36	5	2696	A
36	5	2714	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

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Mol	Chain	Res	Type
36	5	2796	G
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2805	G
36	5	2810	C
36	5	2817	A
36	5	2818	U
36	5	2819	A
36	5	2825	C
36	5	2829	U
36	5	2843	U
36	5	2845	A
36	5	2847	A
36	5	2853	A
36	5	2871	G
36	5	2872	A
36	5	2875	U
36	5	2876	C
36	5	2887	A
36	5	2889	C
36	5	2896	A
36	5	2897	A
36	5	2898	G
36	5	2899	C
36	5	2902	A
36	5	2904	U
36	5	2912	G
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2941	A
36	5	2942	C
36	5	2945	G
36	5	2947	G
36	5	2954	U
36	5	2971	A
36	5	2972	G
36	5	2979	U
36	5	2983	C
36	5	2990	G
36	5	2996	U

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Mol	Chain	Res	Type
36	5	2997	G
36	5	3006	A
36	5	3012	A
36	5	3018	C
36	5	3033	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	3119	U
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3150	A
36	5	3153	U
36	5	3154	C
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3159	C
36	5	3164	C
36	5	3165	A
36	5	3168	A
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3178	A
36	5	3179	U
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3207	U
36	5	3217	C
36	5	3218	A

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Mol	Chain	Res	Type
36	5	3219	G
36	5	3228	C
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	3260	G
36	5	3265	C
36	5	3270	U
36	5	3273	A
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3278	C
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	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3306	U
36	5	3307	A
36	5	3313	U
36	5	3316	A
36	5	3317	U
36	5	3319	U
36	5	3320	A
36	5	3332	U
36	5	3333	G
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3351	U

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Mol	Chain	Res	Type
36	5	3352	U
36	5	3354	U
36	5	3356	G
36	5	3358	U
36	5	3369	G
36	5	3378	C
36	5	3383	G
36	5	3389	U
36	5	3390	G
36	5	3393	U
36	5	3396	U
37	7	2	G
37	7	7	G
37	7	22	A
37	7	23	A
37	7	33	U
37	7	42	A
37	7	54	U
37	7	55	A
37	7	65	G
37	7	73	C
37	7	91	G
37	7	93	C
37	7	101	G
37	7	102	A
37	7	103	A
37	7	112	G
37	7	121	U
38	8	2	A
38	8	21	C
38	8	25	G
38	8	34	U
38	8	35	C
38	8	48	A
38	8	49	G
38	8	52	A
38	8	53	A
38	8	57	C
38	8	58	G
38	8	59	A
38	8	62	C
38	8	63	G

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Mol	Chain	Res	Type
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	104	A
38	8	105	A
38	8	106	C
38	8	108	C
38	8	111	A
38	8	113	U
38	8	122	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	148	G
38	8	155	A
38	8	156	U
38	8	157	U
38	8	158	U

All (291) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	73	U
1	2	74	U
1	2	126	A
1	2	130	C
1	2	131	C
1	2	132	U
1	2	139	C
1	2	144	U
1	2	158	U
1	2	187	G
1	2	218	A
1	2	240	U

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Mol	Chain	Res	Type
1	2	278	U
1	2	280	U
1	2	319	U
1	2	400	A
1	2	417	A
1	2	468	A
1	2	497	G
1	2	498	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	558	U
1	2	582	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	811	A
1	2	829	A
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	1244	A
1	2	1250	U
1	2	1339	C
1	2	1344	A
1	2	1370	U
1	2	1481	C
1	2	1489	U
1	2	1521	G
1	2	1568	C
1	2	1572	G
1	2	1573	A
1	2	1600	A
1	2	1615	C
1	2	1657	U

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Mol	Chain	Res	Type
1	2	1761	U
36	1	13	A
36	1	43	A
36	1	65	A
36	1	99	A
36	1	169	U
36	1	210	U
36	1	217	U
36	1	223	U
36	1	239	G
36	1	282	G
36	1	397	A
36	1	547	G
36	1	588	G
36	1	594	U
36	1	620	U
36	1	647	A
36	1	715	A
36	1	719	U
36	1	763	G
36	1	764	U
36	1	816	A
36	1	873	C
36	1	896	A
36	1	916	G
36	1	979	U
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1196	C
36	1	1273	A
36	1	1307	G
36	1	1317	A
36	1	1329	U
36	1	1352	A
36	1	1355	A
36	1	1419	A
36	1	1481	A
36	1	1484	U

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Mol	Chain	Res	Type
36	1	1507	G
36	1	1514	G
36	1	1554	U
36	1	1562	C
36	1	1716	U
36	1	1815	U
36	1	1816	A
36	1	1820	U
36	1	1841	A
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2227	C
36	1	2249	G
36	1	2281	A
36	1	2314	U
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2403	G
36	1	2418	G
36	1	2522	G
36	1	2537	U
36	1	2541	U
36	1	2585	G
36	1	2593	A
36	1	2689	A
36	1	2728	G
36	1	2772	C
36	1	2801	A
36	1	2818	U
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3139	A
36	1	3169	U
36	1	3195	U
36	1	3217	C
36	1	3218	A
36	1	3228	C
36	1	3242	G
36	1	3259	U

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Mol	Chain	Res	Type
36	1	3269	U
36	1	3275	U
36	1	3316	A
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
37	3	13	A
37	3	49	G
38	4	85	G
38	4	111	A
38	4	125	U
1	6	25	C
1	6	66	U
1	6	76	A
1	6	103	A
1	6	114	C
1	6	139	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	249	U
1	6	272	U
1	6	277	U
1	6	352	A
1	6	400	A
1	6	417	A
1	6	434	G
1	6	468	A
1	6	512	A
1	6	542	A
1	6	557	G
1	6	558	U
1	6	717	C
1	6	755	A
1	6	794	U
1	6	829	A
1	6	1051	G
1	6	1058	U

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Mol	Chain	Res	Type
1	6	1097	U
1	6	1098	U
1	6	1137	A
1	6	1207	C
1	6	1238	A
1	6	1244	A
1	6	1255	G
1	6	1344	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	65	A
36	5	151	A
36	5	210	U
36	5	217	U
36	5	221	A
36	5	238	A
36	5	282	G
36	5	397	A
36	5	398	A
36	5	420	G
36	5	438	A
36	5	588	G
36	5	594	U
36	5	715	A
36	5	735	A
36	5	765	C
36	5	786	A
36	5	816	A
36	5	873	C
36	5	894	G
36	5	896	A
36	5	916	G

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Mol	Chain	Res	Type
36	5	978	G
36	5	993	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1160	C
36	5	1181	U
36	5	1192	C
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1317	A
36	5	1329	U
36	5	1352	A
36	5	1355	A
36	5	1434	G
36	5	1481	A
36	5	1560	G
36	5	1580	A
36	5	1716	U
36	5	1750	A
36	5	1793	C
36	5	1816	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	2101	C
36	5	2112	U
36	5	2116	G
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2257	C
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2440	G
36	5	2507	C
36	5	2513	U

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Mol	Chain	Res	Type
36	5	2531	C
36	5	2539	C
36	5	2584	G
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2818	U
36	5	2887	A
36	5	2896	A
36	5	2971	A
36	5	3049	A
36	5	3055	U
36	5	3056	U
36	5	3078	U
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3275	U
36	5	3289	G
36	5	3340	G
36	5	3341	U
36	5	3354	U
36	5	3357	U
38	8	111	A
38	8	126	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
87	OHX	1	4122	-	0,6,6	0.00	-	-		
87	OHX	14	403	-	0,6,6	0.00	-	-		
87	OHX	5	3972	-	0,6,6	0.00	-	-		
87	OHX	6	2149	-	0,6,6	0.00	-	-		
87	OHX	1	4200	-	0,6,6	0.00	-	-		
87	OHX	5	4075	-	0,6,6	0.00	-	-		
87	OHX	1	4191	-	0,6,6	0.00	-	-		
87	OHX	5	3960	-	0,6,6	0.00	-	-		
87	OHX	5	3950	-	0,6,6	0.00	-	-		
87	OHX	2	2028	-	0,6,6	0.00	-	-		
87	OHX	5	4037	-	0,6,6	0.00	-	-		
87	OHX	1	4015	-	0,6,6	0.00	-	-		
87	OHX	1	4119	-	0,6,6	0.00	-	-		
87	OHX	O7	104	-	0,6,6	0.00	-	-		
87	OHX	5	4086	-	0,6,6	0.00	-	-		
87	OHX	1	3909	-	0,6,6	0.00	-	-		
87	OHX	1	3902	-	0,6,6	0.00	-	-		
87	OHX	1	3976	-	0,6,6	0.00	-	-		
87	OHX	6	2175	-	0,6,6	0.00	-	-		
87	OHX	5	4222	-	0,6,6	0.00	-	-		
87	OHX	1	4013	-	0,6,6	0.00	-	-		
87	OHX	1	4008	-	0,6,6	0.00	-	-		
87	OHX	1	4057	-	0,6,6	0.00	-	-		
87	OHX	5	4157	-	0,6,6	0.00	-	-		
87	OHX	1	4068	-	0,6,6	0.00	-	-		
87	OHX	5	3922	-	0,6,6	0.00	-	-		
87	OHX	1	3928	-	0,6,6	0.00	-	-		
87	OHX	2	2056	-	0,6,6	0.00	-	-		
87	OHX	6	2128	-	0,6,6	0.00	-	-		
87	OHX	1	4131	-	0,6,6	0.00	-	-		
87	OHX	1	3915	-	0,6,6	0.00	-	-		
87	OHX	5	4031	-	0,6,6	0.00	-	-		
87	OHX	2	2159	-	0,6,6	0.00	-	-		
87	OHX	6	2129	-	0,6,6	0.00	-	-		
87	OHX	6	2092	-	0,6,6	0.00	-	-		
87	OHX	5	4162	-	0,6,6	0.00	-	-		
87	OHX	1	3904	-	0,6,6	0.00	-	-		
87	OHX	5	4138	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4169	-	0,6,6	0.00	-	-		
87	OHX	3	220	-	0,6,6	0.00	-	-		
87	OHX	6	2194	-	0,6,6	0.00	-	-		
87	OHX	5	4244	-	0,6,6	0.00	-	-		
87	OHX	1	4205	-	0,6,6	0.00	-	-		
87	OHX	6	2174	-	0,6,6	0.00	-	-		
87	OHX	2	2103	-	0,6,6	0.00	-	-		
87	OHX	1	3993	-	0,6,6	0.00	-	-		
87	OHX	5	4074	-	0,6,6	0.00	-	-		
87	OHX	5	4176	-	0,6,6	0.00	-	-		
87	OHX	1	3953	-	0,6,6	0.00	-	-		
87	OHX	5	4181	-	0,6,6	0.00	-	-		
87	OHX	5	3929	-	0,6,6	0.00	-	-		
87	OHX	6	2119	-	0,6,6	0.00	-	-		
87	OHX	19	600	-	0,6,6	0.00	-	-		
87	OHX	5	4093	-	0,6,6	0.00	-	-		
87	OHX	6	2058	-	0,6,6	0.00	-	-		
87	OHX	5	4018	-	0,6,6	0.00	-	-		
87	OHX	1	4202	-	0,6,6	0.00	-	-		
87	OHX	1	3967	-	0,6,6	0.00	-	-		
87	OHX	1	4194	-	0,6,6	0.00	-	-		
87	OHX	5	4058	-	0,6,6	0.00	-	-		
87	OHX	5	4112	-	0,6,6	0.00	-	-		
87	OHX	2	2136	-	0,6,6	0.00	-	-		
87	OHX	5	4227	-	0,6,6	0.00	-	-		
87	OHX	5	4042	-	0,6,6	0.00	-	-		
87	OHX	1	3921	-	0,6,6	0.00	-	-		
87	OHX	5	4101	-	0,6,6	0.00	-	-		
87	OHX	o9	101	-	0,6,6	0.00	-	-		
87	OHX	1	4172	-	0,6,6	0.00	-	-		
87	OHX	1	4106	-	0,6,6	0.00	-	-		
87	OHX	8	215	-	0,6,6	0.00	-	-		
87	OHX	5	3991	-	0,6,6	0.00	-	-		
87	OHX	6	2108	-	0,6,6	0.00	-	-		
87	OHX	6	2107	-	0,6,6	0.00	-	-		
87	OHX	5	4133	-	0,6,6	0.00	-	-		
87	OHX	2	2099	-	0,6,6	0.00	-	-		
87	OHX	1	3988	-	0,6,6	0.00	-	-		
87	OHX	2	2057	-	0,6,6	0.00	-	-		
87	OHX	7	216	-	0,6,6	0.00	-	-		
87	OHX	5	4206	-	0,6,6	0.00	-	-		
87	OHX	6	2155	-	0,6,6	0.00	-	-		
87	OHX	1	4044	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4073	-	0,6,6	0.00	-	-		
87	OHX	6	2085	-	0,6,6	0.00	-	-		
87	OHX	1	4128	-	0,6,6	0.00	-	-		
87	OHX	5	3936	-	0,6,6	0.00	-	-		
87	OHX	5	4102	-	0,6,6	0.00	-	-		
87	OHX	5	4119	-	0,6,6	0.00	-	-		
87	OHX	1	4017	-	0,6,6	0.00	-	-		
87	OHX	5	4214	-	0,6,6	0.00	-	-		
87	OHX	5	4195	-	0,6,6	0.00	-	-		
87	OHX	2	2142	-	0,6,6	0.00	-	-		
87	OHX	6	2127	-	0,6,6	0.00	-	-		
87	OHX	1	4188	-	0,6,6	0.00	-	-		
87	OHX	2	2082	-	0,6,6	0.00	-	-		
87	OHX	2	2104	-	0,6,6	0.00	-	-		
87	OHX	1	4052	-	0,6,6	0.00	-	-		
87	OHX	5	4023	-	0,6,6	0.00	-	-		
87	OHX	8	223	-	0,6,6	0.00	-	-		
87	OHX	5	4124	-	0,6,6	0.00	-	-		
87	OHX	s4	301	-	0,6,6	0.00	-	-		
87	OHX	2	2145	-	0,6,6	0.00	-	-		
87	OHX	5	4054	-	0,6,6	0.00	-	-		
87	OHX	1	4165	-	0,6,6	0.00	-	-		
87	OHX	5	4067	-	0,6,6	0.00	-	-		
87	OHX	1	3944	-	0,6,6	0.00	-	-		
87	OHX	2	2116	-	0,6,6	0.00	-	-		
87	OHX	1	4186	-	0,6,6	0.00	-	-		
87	OHX	1	3985	-	0,6,6	0.00	-	-		
87	OHX	n9	101	-	0,6,6	0.00	-	-		
87	OHX	5	4152	-	0,6,6	0.00	-	-		
87	OHX	5	4038	-	0,6,6	0.00	-	-		
87	OHX	5	4069	-	0,6,6	0.00	-	-		
87	OHX	6	2163	-	0,6,6	0.00	-	-		
87	OHX	5	4015	-	0,6,6	0.00	-	-		
87	OHX	6	2071	-	0,6,6	0.00	-	-		
87	OHX	2	2037	-	0,6,6	0.00	-	-		
87	OHX	6	2074	-	0,6,6	0.00	-	-		
87	OHX	6	2136	-	0,6,6	0.00	-	-		
87	OHX	5	4198	-	0,6,6	0.00	-	-		
87	OHX	1	4022	-	0,6,6	0.00	-	-		
87	OHX	1	4035	-	0,6,6	0.00	-	-		
87	OHX	5	4055	-	0,6,6	0.00	-	-		
87	OHX	2	2071	-	0,6,6	0.00	-	-		
87	OHX	5	4205	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3905	-	0,6,6	0.00	-	-		
87	OHX	2	2179	-	0,6,6	0.00	-	-		
87	OHX	5	3990	-	0,6,6	0.00	-	-		
87	OHX	1	4056	-	0,6,6	0.00	-	-		
87	OHX	1	4170	-	0,6,6	0.00	-	-		
87	OHX	8	228	-	0,6,6	0.00	-	-		
87	OHX	5	4177	-	0,6,6	0.00	-	-		
87	OHX	6	2131	-	0,6,6	0.00	-	-		
87	OHX	5	4172	-	0,6,6	0.00	-	-		
87	OHX	1	3876	-	0,6,6	0.00	-	-		
87	OHX	1	3971	-	0,6,6	0.00	-	-		
87	OHX	6	2116	-	0,6,6	0.00	-	-		
87	OHX	2	2029	-	0,6,6	0.00	-	-		
87	OHX	2	2108	-	0,6,6	0.00	-	-		
87	OHX	6	2105	-	0,6,6	0.00	-	-		
87	OHX	3	221	-	0,6,6	0.00	-	-		
87	OHX	5	4139	-	0,6,6	0.00	-	-		
87	OHX	5	4159	-	0,6,6	0.00	-	-		
87	OHX	5	4156	-	0,6,6	0.00	-	-		
87	OHX	6	2087	-	0,6,6	0.00	-	-		
87	OHX	1	4032	-	0,6,6	0.00	-	-		
87	OHX	5	4026	-	0,6,6	0.00	-	-		
87	OHX	1	3992	-	0,6,6	0.00	-	-		
87	OHX	1	4155	-	0,6,6	0.00	-	-		
87	OHX	5	4220	-	0,6,6	0.00	-	-		
87	OHX	2	2025	-	0,6,6	0.00	-	-		
87	OHX	6	2187	-	0,6,6	0.00	-	-		
87	OHX	2	2100	-	0,6,6	0.00	-	-		
87	OHX	1	4059	-	0,6,6	0.00	-	-		
87	OHX	5	4179	-	0,6,6	0.00	-	-		
87	OHX	6	2089	-	0,6,6	0.00	-	-		
87	OHX	15	304	-	0,6,6	0.00	-	-		
87	OHX	14	404	-	0,6,6	0.00	-	-		
87	OHX	5	4230	-	0,6,6	0.00	-	-		
87	OHX	1	4178	-	0,6,6	0.00	-	-		
87	OHX	N9	101	-	0,6,6	0.00	-	-		
87	OHX	5	4189	-	0,6,6	0.00	-	-		
87	OHX	6	2123	-	0,6,6	0.00	-	-		
87	OHX	8	221	-	0,6,6	0.00	-	-		
87	OHX	6	2073	-	0,6,6	0.00	-	-		
87	OHX	5	4142	-	0,6,6	0.00	-	-		
87	OHX	15	303	-	0,6,6	0.00	-	-		
87	OHX	5	4234	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2081	-	0,6,6	0.00	-	-		
87	OHX	1	3941	-	0,6,6	0.00	-	-		
87	OHX	2	2115	-	0,6,6	0.00	-	-		
87	OHX	1	4055	-	0,6,6	0.00	-	-		
87	OHX	1	3949	-	0,6,6	0.00	-	-		
87	OHX	1	4201	-	0,6,6	0.00	-	-		
87	OHX	1	4204	-	0,6,6	0.00	-	-		
87	OHX	5	4120	-	0,6,6	0.00	-	-		
87	OHX	2	2044	-	0,6,6	0.00	-	-		
87	OHX	Q2	503	-	0,6,6	0.00	-	-		
87	OHX	5	3907	-	0,6,6	0.00	-	-		
87	OHX	5	4241	-	0,6,6	0.00	-	-		
87	OHX	5	3970	-	0,6,6	0.00	-	-		
87	OHX	1	4125	-	0,6,6	0.00	-	-		
87	OHX	1	4198	-	0,6,6	0.00	-	-		
87	OHX	7	219	-	0,6,6	0.00	-	-		
87	OHX	5	3910	-	0,6,6	0.00	-	-		
87	OHX	1	3930	-	0,6,6	0.00	-	-		
87	OHX	N1	201	-	0,6,6	0.00	-	-		
87	OHX	1	4141	-	0,6,6	0.00	-	-		
87	OHX	5	4188	-	0,6,6	0.00	-	-		
87	OHX	5	4182	-	0,6,6	0.00	-	-		
87	OHX	2	2113	-	0,6,6	0.00	-	-		
87	OHX	2	2059	-	0,6,6	0.00	-	-		
87	OHX	1	4053	-	0,6,6	0.00	-	-		
87	OHX	6	2061	-	0,6,6	0.00	-	-		
87	OHX	2	2080	-	0,6,6	0.00	-	-		
87	OHX	6	2142	-	0,6,6	0.00	-	-		
87	OHX	5	4237	-	0,6,6	0.00	-	-		
87	OHX	7	215	-	0,6,6	0.00	-	-		
87	OHX	5	4105	-	0,6,6	0.00	-	-		
87	OHX	5	4184	-	0,6,6	0.00	-	-		
87	OHX	2	2139	-	0,6,6	0.00	-	-		
87	OHX	5	4197	-	0,6,6	0.00	-	-		
87	OHX	1	4173	-	0,6,6	0.00	-	-		
87	OHX	1	4021	-	0,6,6	0.00	-	-		
87	OHX	1	4130	-	0,6,6	0.00	-	-		
87	OHX	5	4081	-	0,6,6	0.00	-	-		
87	OHX	1	3979	-	0,6,6	0.00	-	-		
87	OHX	1	3912	-	0,6,6	0.00	-	-		
87	OHX	6	2047	-	0,6,6	0.00	-	-		
87	OHX	8	218	-	0,6,6	0.00	-	-		
87	OHX	1	3893	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2138	-	0,6,6	0.00	-	-		
87	OHX	1	4007	-	0,6,6	0.00	-	-		
87	OHX	2	2161	-	0,6,6	0.00	-	-		
87	OHX	6	2080	-	0,6,6	0.00	-	-		
87	OHX	7	227	-	0,6,6	0.00	-	-		
87	OHX	5	4160	-	0,6,6	0.00	-	-		
87	OHX	1	4161	-	0,6,6	0.00	-	-		
87	OHX	1	4197	-	0,6,6	0.00	-	-		
87	OHX	5	4144	-	0,6,6	0.00	-	-		
87	OHX	6	2082	-	0,6,6	0.00	-	-		
87	OHX	1	4000	-	0,6,6	0.00	-	-		
87	OHX	2	2149	-	0,6,6	0.00	-	-		
87	OHX	4	232	-	0,6,6	0.00	-	-		
87	OHX	5	4098	-	0,6,6	0.00	-	-		
87	OHX	1	3885	-	0,6,6	0.00	-	-		
87	OHX	1	4081	-	0,6,6	0.00	-	-		
87	OHX	5	4076	-	0,6,6	0.00	-	-		
87	OHX	1	4207	-	0,6,6	0.00	-	-		
87	OHX	5	4072	-	0,6,6	0.00	-	-		
87	OHX	1	3896	-	0,6,6	0.00	-	-		
87	OHX	s1	302	-	0,6,6	0.00	-	-		
87	OHX	2	2109	-	0,6,6	0.00	-	-		
87	OHX	d4	202	-	0,6,6	0.00	-	-		
87	OHX	1	4090	-	0,6,6	0.00	-	-		
87	OHX	1	4126	-	0,6,6	0.00	-	-		
87	OHX	1	3923	-	0,6,6	0.00	-	-		
87	OHX	6	2132	-	0,6,6	0.00	-	-		
87	OHX	1	3908	-	0,6,6	0.00	-	-		
87	OHX	6	2112	-	0,6,6	0.00	-	-		
87	OHX	6	2099	-	0,6,6	0.00	-	-		
87	OHX	5	4146	-	0,6,6	0.00	-	-		
87	OHX	6	2100	-	0,6,6	0.00	-	-		
87	OHX	6	2076	-	0,6,6	0.00	-	-		
87	OHX	4	224	-	0,6,6	0.00	-	-		
87	OHX	1	4069	-	0,6,6	0.00	-	-		
87	OHX	M9	202	-	0,6,6	0.00	-	-		
87	OHX	5	4095	-	0,6,6	0.00	-	-		
87	OHX	5	4012	-	0,6,6	0.00	-	-		
87	OHX	1	3911	-	0,6,6	0.00	-	-		
87	OHX	1	3870	-	0,6,6	0.00	-	-		
87	OHX	5	3927	-	0,6,6	0.00	-	-		
87	OHX	2	2047	-	0,6,6	0.00	-	-		
87	OHX	1	4004	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2133	-	0,6,6	0.00	-	-		
87	OHX	1	4124	-	0,6,6	0.00	-	-		
87	OHX	2	2062	-	0,6,6	0.00	-	-		
87	OHX	1	3973	-	0,6,6	0.00	-	-		
87	OHX	o2	201	-	0,6,6	0.00	-	-		
87	OHX	5	4073	-	0,6,6	0.00	-	-		
87	OHX	3	223	-	0,6,6	0.00	-	-		
87	OHX	5	4201	-	0,6,6	0.00	-	-		
87	OHX	5	3909	-	0,6,6	0.00	-	-		
87	OHX	6	2095	-	0,6,6	0.00	-	-		
87	OHX	7	224	-	0,6,6	0.00	-	-		
87	OHX	5	4091	-	0,6,6	0.00	-	-		
87	OHX	1	4199	-	0,6,6	0.00	-	-		
87	OHX	1	3916	-	0,6,6	0.00	-	-		
87	OHX	2	2066	-	0,6,6	0.00	-	-		
87	OHX	5	4175	-	0,6,6	0.00	-	-		
87	OHX	5	4053	-	0,6,6	0.00	-	-		
87	OHX	5	4207	-	0,6,6	0.00	-	-		
87	OHX	1	3900	-	0,6,6	0.00	-	-		
87	OHX	2	2118	-	0,6,6	0.00	-	-		
87	OHX	1	4014	-	0,6,6	0.00	-	-		
87	OHX	1	4050	-	0,6,6	0.00	-	-		
87	OHX	5	3946	-	0,6,6	0.00	-	-		
87	OHX	5	3918	-	0,6,6	0.00	-	-		
87	OHX	5	3947	-	0,6,6	0.00	-	-		
87	OHX	2	2106	-	0,6,6	0.00	-	-		
87	OHX	1	3934	-	0,6,6	0.00	-	-		
87	OHX	5	3902	-	0,6,6	0.00	-	-		
87	OHX	5	4001	-	0,6,6	0.00	-	-		
87	OHX	2	2098	-	0,6,6	0.00	-	-		
87	OHX	1	4181	-	0,6,6	0.00	-	-		
87	OHX	2	2137	-	0,6,6	0.00	-	-		
87	OHX	7	225	-	0,6,6	0.00	-	-		
87	OHX	2	2163	-	0,6,6	0.00	-	-		
87	OHX	5	4211	-	0,6,6	0.00	-	-		
87	OHX	5	4111	-	0,6,6	0.00	-	-		
87	OHX	1	4149	-	0,6,6	0.00	-	-		
87	OHX	1	4110	-	0,6,6	0.00	-	-		
87	OHX	1	3925	-	0,6,6	0.00	-	-		
87	OHX	l3	402	-	0,6,6	0.00	-	-		
87	OHX	6	2162	-	0,6,6	0.00	-	-		
87	OHX	6	2176	-	0,6,6	0.00	-	-		
87	OHX	2	2151	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2048	-	0,6,6	0.00	-	-		
87	OHX	5	3930	-	0,6,6	0.00	-	-		
87	OHX	1	4091	-	0,6,6	0.00	-	-		
87	OHX	1	4140	-	0,6,6	0.00	-	-		
87	OHX	5	3906	-	0,6,6	0.00	-	-		
87	OHX	5	3908	-	0,6,6	0.00	-	-		
87	OHX	6	2078	-	0,6,6	0.00	-	-		
87	OHX	1	3927	-	0,6,6	0.00	-	-		
87	OHX	1	4054	-	0,6,6	0.00	-	-		
87	OHX	5	4003	-	0,6,6	0.00	-	-		
87	OHX	1	4080	-	0,6,6	0.00	-	-		
87	OHX	2	2088	-	0,6,6	0.00	-	-		
87	OHX	5	3998	-	0,6,6	0.00	-	-		
87	OHX	1	4129	-	0,6,6	0.00	-	-		
87	OHX	1	3960	-	0,6,6	0.00	-	-		
87	OHX	6	2048	-	0,6,6	0.00	-	-		
87	OHX	1	4120	-	0,6,6	0.00	-	-		
87	OHX	6	2094	-	0,6,6	0.00	-	-		
87	OHX	O3	202	-	0,6,6	0.00	-	-		
87	OHX	6	2164	-	0,6,6	0.00	-	-		
87	OHX	1	4180	-	0,6,6	0.00	-	-		
87	OHX	2	2164	-	0,6,6	0.00	-	-		
87	OHX	5	4212	-	0,6,6	0.00	-	-		
87	OHX	1	3961	-	0,6,6	0.00	-	-		
87	OHX	1	4196	-	0,6,6	0.00	-	-		
87	OHX	5	4085	-	0,6,6	0.00	-	-		
87	OHX	1	3989	-	0,6,6	0.00	-	-		
87	OHX	M7	208	-	0,6,6	0.00	-	-		
87	OHX	2	2175	-	0,6,6	0.00	-	-		
87	OHX	2	2039	-	0,6,6	0.00	-	-		
87	OHX	1	4142	-	0,6,6	0.00	-	-		
87	OHX	1	3865	-	0,6,6	0.00	-	-		
87	OHX	5	4107	-	0,6,6	0.00	-	-		
87	OHX	5	3917	-	0,6,6	0.00	-	-		
87	OHX	1	3910	-	0,6,6	0.00	-	-		
87	OHX	5	4059	-	0,6,6	0.00	-	-		
87	OHX	2	2132	-	0,6,6	0.00	-	-		
87	OHX	2	2035	-	0,6,6	0.00	-	-		
87	OHX	5	3956	-	0,6,6	0.00	-	-		
87	OHX	2	2141	-	0,6,6	0.00	-	-		
87	OHX	1	3883	-	0,6,6	0.00	-	-		
87	OHX	5	4071	-	0,6,6	0.00	-	-		
87	OHX	1	3879	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2133	-	0,6,6	0.00	-	-		
89	3HE	5	4252	-	21,21,21	0.88	1 (4%)	19,30,30	0.76	0
87	OHX	1	4210	-	0,6,6	0.00	-	-		
87	OHX	o7	103	-	0,6,6	0.00	-	-		
87	OHX	3	222	-	0,6,6	0.00	-	-		
87	OHX	5	4221	-	0,6,6	0.00	-	-		
87	OHX	2	2140	-	0,6,6	0.00	-	-		
87	OHX	2	2052	-	0,6,6	0.00	-	-		
87	OHX	3	215	-	0,6,6	0.00	-	-		
87	OHX	6	2203	-	0,6,6	0.00	-	-		
87	OHX	2	2024	-	0,6,6	0.00	-	-		
87	OHX	1	4026	-	0,6,6	0.00	-	-		
87	OHX	1	3962	-	0,6,6	0.00	-	-		
87	OHX	8	222	-	0,6,6	0.00	-	-		
87	OHX	6	2079	-	0,6,6	0.00	-	-		
87	OHX	6	2098	-	0,6,6	0.00	-	-		
87	OHX	7	217	-	0,6,6	0.00	-	-		
87	OHX	5	4127	-	0,6,6	0.00	-	-		
87	OHX	5	4251	-	0,6,6	0.00	-	-		
87	OHX	6	2189	-	0,6,6	0.00	-	-		
87	OHX	L3	404	-	0,6,6	0.00	-	-		
87	OHX	6	2183	-	0,6,6	0.00	-	-		
87	OHX	5	4238	-	0,6,6	0.00	-	-		
87	OHX	2	2148	-	0,6,6	0.00	-	-		
87	OHX	6	2083	-	0,6,6	0.00	-	-		
87	OHX	6	2126	-	0,6,6	0.00	-	-		
87	OHX	5	4006	-	0,6,6	0.00	-	-		
87	OHX	1	3943	-	0,6,6	0.00	-	-		
87	OHX	5	4224	-	0,6,6	0.00	-	-		
87	OHX	1	3946	-	0,6,6	0.00	-	-		
87	OHX	6	2160	-	0,6,6	0.00	-	-		
87	OHX	1	3958	-	0,6,6	0.00	-	-		
87	OHX	6	2147	-	0,6,6	0.00	-	-		
87	OHX	5	4151	-	0,6,6	0.00	-	-		
87	OHX	5	4185	-	0,6,6	0.00	-	-		
87	OHX	S8	302	-	0,6,6	0.00	-	-		
87	OHX	5	3982	-	0,6,6	0.00	-	-		
87	OHX	1	3901	-	0,6,6	0.00	-	-		
87	OHX	5	4066	-	0,6,6	0.00	-	-		
87	OHX	1	3866	-	0,6,6	0.00	-	-		
87	OHX	1	3913	-	0,6,6	0.00	-	-		
87	OHX	5	4114	-	0,6,6	0.00	-	-		
87	OHX	2	2036	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	M5	303	-	0,6,6	0.00	-	-		
87	OHX	6	2122	-	0,6,6	0.00	-	-		
87	OHX	5	4183	-	0,6,6	0.00	-	-		
87	OHX	5	4046	-	0,6,6	0.00	-	-		
87	OHX	5	4161	-	0,6,6	0.00	-	-		
87	OHX	1	3956	-	0,6,6	0.00	-	-		
87	OHX	1	3935	-	0,6,6	0.00	-	-		
87	OHX	2	2120	-	0,6,6	0.00	-	-		
87	OHX	2	2051	-	0,6,6	0.00	-	-		
87	OHX	6	2193	-	0,6,6	0.00	-	-		
87	OHX	1	3894	-	0,6,6	0.00	-	-		
87	OHX	2	2092	-	0,6,6	0.00	-	-		
87	OHX	5	4158	-	0,6,6	0.00	-	-		
87	OHX	1	4108	-	0,6,6	0.00	-	-		
87	OHX	2	2058	-	0,6,6	0.00	-	-		
87	OHX	5	4106	-	0,6,6	0.00	-	-		
87	OHX	1	3881	-	0,6,6	0.00	-	-		
87	OHX	6	2202	-	0,6,6	0.00	-	-		
87	OHX	15	305	-	0,6,6	0.00	-	-		
87	OHX	5	4113	-	0,6,6	0.00	-	-		
87	OHX	1	3937	-	0,6,6	0.00	-	-		
87	OHX	6	2150	-	0,6,6	0.00	-	-		
87	OHX	5	4243	-	0,6,6	0.00	-	-		
87	OHX	1	3920	-	0,6,6	0.00	-	-		
87	OHX	1	3907	-	0,6,6	0.00	-	-		
87	OHX	1	4051	-	0,6,6	0.00	-	-		
87	OHX	6	2186	-	0,6,6	0.00	-	-		
87	OHX	5	4192	-	0,6,6	0.00	-	-		
87	OHX	1	3918	-	0,6,6	0.00	-	-		
87	OHX	1	3917	-	0,6,6	0.00	-	-		
87	OHX	6	2067	-	0,6,6	0.00	-	-		
87	OHX	1	4045	-	0,6,6	0.00	-	-		
87	OHX	5	4208	-	0,6,6	0.00	-	-		
87	OHX	2	2135	-	0,6,6	0.00	-	-		
87	OHX	2	2157	-	0,6,6	0.00	-	-		
87	OHX	1	4029	-	0,6,6	0.00	-	-		
87	OHX	1	4113	-	0,6,6	0.00	-	-		
87	OHX	5	4194	-	0,6,6	0.00	-	-		
87	OHX	5	3987	-	0,6,6	0.00	-	-		
87	OHX	2	2160	-	0,6,6	0.00	-	-		
87	OHX	5	4167	-	0,6,6	0.00	-	-		
87	OHX	5	3925	-	0,6,6	0.00	-	-		
87	OHX	6	2143	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2111	-	0,6,6	0.00	-	-		
87	OHX	5	4209	-	0,6,6	0.00	-	-		
87	OHX	2	2128	-	0,6,6	0.00	-	-		
87	OHX	5	4096	-	0,6,6	0.00	-	-		
87	OHX	1	3889	-	0,6,6	0.00	-	-		
87	OHX	7	226	-	0,6,6	0.00	-	-		
87	OHX	5	4097	-	0,6,6	0.00	-	-		
87	OHX	5	3981	-	0,6,6	0.00	-	-		
87	OHX	2	2083	-	0,6,6	0.00	-	-		
87	OHX	2	2074	-	0,6,6	0.00	-	-		
87	OHX	8	224	-	0,6,6	0.00	-	-		
87	OHX	1	3970	-	0,6,6	0.00	-	-		
87	OHX	6	2177	-	0,6,6	0.00	-	-		
87	OHX	1	3929	-	0,6,6	0.00	-	-		
87	OHX	5	4030	-	0,6,6	0.00	-	-		
87	OHX	5	4082	-	0,6,6	0.00	-	-		
87	OHX	6	2106	-	0,6,6	0.00	-	-		
87	OHX	5	3965	-	0,6,6	0.00	-	-		
87	OHX	2	2061	-	0,6,6	0.00	-	-		
87	OHX	6	2101	-	0,6,6	0.00	-	-		
87	OHX	2	2111	-	0,6,6	0.00	-	-		
87	OHX	6	2118	-	0,6,6	0.00	-	-		
87	OHX	5	4040	-	0,6,6	0.00	-	-		
87	OHX	3	216	-	0,6,6	0.00	-	-		
87	OHX	5	4033	-	0,6,6	0.00	-	-		
87	OHX	D9	102	-	0,6,6	0.00	-	-		
87	OHX	1	4030	-	0,6,6	0.00	-	-		
87	OHX	6	2145	-	0,6,6	0.00	-	-		
87	OHX	1	4003	-	0,6,6	0.00	-	-		
87	OHX	2	2060	-	0,6,6	0.00	-	-		
87	OHX	5	3971	-	0,6,6	0.00	-	-		
87	OHX	5	4131	-	0,6,6	0.00	-	-		
87	OHX	2	2086	-	0,6,6	0.00	-	-		
87	OHX	s8	302	-	0,6,6	0.00	-	-		
87	OHX	4	228	-	0,6,6	0.00	-	-		
87	OHX	5	4223	-	0,6,6	0.00	-	-		
87	OHX	5	4178	-	0,6,6	0.00	-	-		
87	OHX	1	4067	-	0,6,6	0.00	-	-		
87	OHX	2	2176	-	0,6,6	0.00	-	-		
87	OHX	5	4141	-	0,6,6	0.00	-	-		
87	OHX	5	4215	-	0,6,6	0.00	-	-		
87	OHX	1	4212	-	0,6,6	0.00	-	-		
87	OHX	1	4098	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4039	-	0,6,6	0.00	-	-		
87	OHX	4	234	-	0,6,6	0.00	-	-		
87	OHX	1	3895	-	0,6,6	0.00	-	-		
87	OHX	2	2079	-	0,6,6	0.00	-	-		
87	OHX	6	2077	-	0,6,6	0.00	-	-		
87	OHX	6	2096	-	0,6,6	0.00	-	-		
87	OHX	6	2181	-	0,6,6	0.00	-	-		
87	OHX	5	4051	-	0,6,6	0.00	-	-		
87	OHX	C8	201	-	0,6,6	0.00	-	-		
87	OHX	5	4013	-	0,6,6	0.00	-	-		
87	OHX	1	4096	-	0,6,6	0.00	-	-		
87	OHX	5	4170	-	0,6,6	0.00	-	-		
87	OHX	1	4016	-	0,6,6	0.00	-	-		
87	OHX	1	3926	-	0,6,6	0.00	-	-		
87	OHX	5	4024	-	0,6,6	0.00	-	-		
87	OHX	1	3882	-	0,6,6	0.00	-	-		
87	OHX	5	4002	-	0,6,6	0.00	-	-		
87	OHX	7	223	-	0,6,6	0.00	-	-		
87	OHX	7	222	-	0,6,6	0.00	-	-		
87	OHX	5	3926	-	0,6,6	0.00	-	-		
87	OHX	1	4136	-	0,6,6	0.00	-	-		
87	OHX	5	3962	-	0,6,6	0.00	-	-		
87	OHX	5	3924	-	0,6,6	0.00	-	-		
87	OHX	5	4249	-	0,6,6	0.00	-	-		
87	OHX	6	2081	-	0,6,6	0.00	-	-		
87	OHX	5	4204	-	0,6,6	0.00	-	-		
87	OHX	5	4196	-	0,6,6	0.00	-	-		
87	OHX	1	3968	-	0,6,6	0.00	-	-		
87	OHX	c5	201	-	0,6,6	0.00	-	-		
87	OHX	2	2168	-	0,6,6	0.00	-	-		
87	OHX	1	3965	-	0,6,6	0.00	-	-		
87	OHX	5	3985	-	0,6,6	0.00	-	-		
87	OHX	5	4047	-	0,6,6	0.00	-	-		
87	OHX	5	4104	-	0,6,6	0.00	-	-		
87	OHX	5	4020	-	0,6,6	0.00	-	-		
87	OHX	5	4218	-	0,6,6	0.00	-	-		
87	OHX	2	2063	-	0,6,6	0.00	-	-		
87	OHX	2	2166	-	0,6,6	0.00	-	-		
87	OHX	1	4111	-	0,6,6	0.00	-	-		
87	OHX	2	2034	-	0,6,6	0.00	-	-		
87	OHX	2	2076	-	0,6,6	0.00	-	-		
87	OHX	5	4000	-	0,6,6	0.00	-	-		
87	OHX	2	2110	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	4	223	-	0,6,6	0.00	-	-		
87	OHX	1	4211	-	0,6,6	0.00	-	-		
87	OHX	2	2040	-	0,6,6	0.00	-	-		
87	OHX	1	3947	-	0,6,6	0.00	-	-		
87	OHX	2	2045	-	0,6,6	0.00	-	-		
87	OHX	6	2117	-	0,6,6	0.00	-	-		
87	OHX	1	4104	-	0,6,6	0.00	-	-		
87	OHX	2	2032	-	0,6,6	0.00	-	-		
87	OHX	5	3911	-	0,6,6	0.00	-	-		
87	OHX	2	2165	-	0,6,6	0.00	-	-		
87	OHX	6	2157	-	0,6,6	0.00	-	-		
87	OHX	5	4079	-	0,6,6	0.00	-	-		
87	OHX	1	4095	-	0,6,6	0.00	-	-		
87	OHX	1	3987	-	0,6,6	0.00	-	-		
87	OHX	1	3940	-	0,6,6	0.00	-	-		
87	OHX	5	3949	-	0,6,6	0.00	-	-		
87	OHX	1	3991	-	0,6,6	0.00	-	-		
87	OHX	5	4021	-	0,6,6	0.00	-	-		
87	OHX	5	3978	-	0,6,6	0.00	-	-		
87	OHX	5	4005	-	0,6,6	0.00	-	-		
87	OHX	1	4109	-	0,6,6	0.00	-	-		
87	OHX	2	2096	-	0,6,6	0.00	-	-		
87	OHX	1	3873	-	0,6,6	0.00	-	-		
87	OHX	1	3980	-	0,6,6	0.00	-	-		
87	OHX	2	2055	-	0,6,6	0.00	-	-		
87	OHX	6	2196	-	0,6,6	0.00	-	-		
87	OHX	1	3975	-	0,6,6	0.00	-	-		
87	OHX	1	4135	-	0,6,6	0.00	-	-		
87	OHX	5	3915	-	0,6,6	0.00	-	-		
87	OHX	2	2144	-	0,6,6	0.00	-	-		
87	OHX	1	4092	-	0,6,6	0.00	-	-		
87	OHX	6	2205	-	0,6,6	0.00	-	-		
87	OHX	5	3983	-	0,6,6	0.00	-	-		
87	OHX	1	3874	-	0,6,6	0.00	-	-		
87	OHX	6	2114	-	0,6,6	0.00	-	-		
87	OHX	1	4062	-	0,6,6	0.00	-	-		
87	OHX	2	2053	-	0,6,6	0.00	-	-		
87	OHX	5	3961	-	0,6,6	0.00	-	-		
87	OHX	1	4084	-	0,6,6	0.00	-	-		
87	OHX	1	3897	-	0,6,6	0.00	-	-		
87	OHX	1	3977	-	0,6,6	0.00	-	-		
87	OHX	5	4216	-	0,6,6	0.00	-	-		
87	OHX	1	4002	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3919	-	0,6,6	0.00	-	-		
87	OHX	2	2147	-	0,6,6	0.00	-	-		
87	OHX	5	3939	-	0,6,6	0.00	-	-		
87	OHX	5	4099	-	0,6,6	0.00	-	-		
87	OHX	1	4154	-	0,6,6	0.00	-	-		
87	OHX	5	4135	-	0,6,6	0.00	-	-		
87	OHX	5	4129	-	0,6,6	0.00	-	-		
87	OHX	5	4110	-	0,6,6	0.00	-	-		
87	OHX	2	2101	-	0,6,6	0.00	-	-		
87	OHX	1	3995	-	0,6,6	0.00	-	-		
87	OHX	1	4134	-	0,6,6	0.00	-	-		
87	OHX	1	3880	-	0,6,6	0.00	-	-		
87	OHX	2	2129	-	0,6,6	0.00	-	-		
87	OHX	6	2191	-	0,6,6	0.00	-	-		
87	OHX	13	403	-	0,6,6	0.00	-	-		
87	OHX	2	2068	-	0,6,6	0.00	-	-		
87	OHX	6	2115	-	0,6,6	0.00	-	-		
87	OHX	5	4149	-	0,6,6	0.00	-	-		
87	OHX	6	2054	-	0,6,6	0.00	-	-		
87	OHX	1	4182	-	0,6,6	0.00	-	-		
87	OHX	5	4068	-	0,6,6	0.00	-	-		
87	OHX	1	3966	-	0,6,6	0.00	-	-		
87	OHX	2	2085	-	0,6,6	0.00	-	-		
87	OHX	1	4036	-	0,6,6	0.00	-	-		
87	OHX	6	2167	-	0,6,6	0.00	-	-		
87	OHX	1	4185	-	0,6,6	0.00	-	-		
87	OHX	1	4018	-	0,6,6	0.00	-	-		
87	OHX	13	404	-	0,6,6	0.00	-	-		
87	OHX	5	4232	-	0,6,6	0.00	-	-		
87	OHX	5	3999	-	0,6,6	0.00	-	-		
87	OHX	1	4025	-	0,6,6	0.00	-	-		
87	OHX	2	2114	-	0,6,6	0.00	-	-		
87	OHX	2	2119	-	0,6,6	0.00	-	-		
87	OHX	6	2104	-	0,6,6	0.00	-	-		
87	OHX	6	2200	-	0,6,6	0.00	-	-		
87	OHX	1	3869	-	0,6,6	0.00	-	-		
87	OHX	1	3887	-	0,6,6	0.00	-	-		
87	OHX	2	2153	-	0,6,6	0.00	-	-		
87	OHX	2	2131	-	0,6,6	0.00	-	-		
87	OHX	1	3875	-	0,6,6	0.00	-	-		
87	OHX	5	3901	-	0,6,6	0.00	-	-		
87	OHX	5	4118	-	0,6,6	0.00	-	-		
87	OHX	5	3928	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2140	-	0,6,6	0.00	-	-		
87	OHX	5	3923	-	0,6,6	0.00	-	-		
87	OHX	5	4121	-	0,6,6	0.00	-	-		
87	OHX	1	3898	-	0,6,6	0.00	-	-		
87	OHX	1	3972	-	0,6,6	0.00	-	-		
87	OHX	1	4156	-	0,6,6	0.00	-	-		
87	OHX	3	219	-	0,6,6	0.00	-	-		
87	OHX	6	2066	-	0,6,6	0.00	-	-		
87	OHX	1	3986	-	0,6,6	0.00	-	-		
87	OHX	5	4108	-	0,6,6	0.00	-	-		
87	OHX	1	3950	-	0,6,6	0.00	-	-		
87	OHX	2	2138	-	0,6,6	0.00	-	-		
87	OHX	6	2069	-	0,6,6	0.00	-	-		
87	OHX	1	3990	-	0,6,6	0.00	-	-		
87	OHX	5	4228	-	0,6,6	0.00	-	-		
87	OHX	1	4012	-	0,6,6	0.00	-	-		
87	OHX	4	235	-	0,6,6	0.00	-	-		
87	OHX	5	4250	-	0,6,6	0.00	-	-		
87	OHX	2	2107	-	0,6,6	0.00	-	-		
87	OHX	5	3993	-	0,6,6	0.00	-	-		
87	OHX	2	2075	-	0,6,6	0.00	-	-		
87	OHX	5	3969	-	0,6,6	0.00	-	-		
87	OHX	1	3957	-	0,6,6	0.00	-	-		
87	OHX	5	4056	-	0,6,6	0.00	-	-		
87	OHX	5	4011	-	0,6,6	0.00	-	-		
87	OHX	2	2134	-	0,6,6	0.00	-	-		
87	OHX	1	4114	-	0,6,6	0.00	-	-		
87	OHX	2	2069	-	0,6,6	0.00	-	-		
87	OHX	1	4100	-	0,6,6	0.00	-	-		
87	OHX	6	2052	-	0,6,6	0.00	-	-		
87	OHX	5	3967	-	0,6,6	0.00	-	-		
87	OHX	6	2060	-	0,6,6	0.00	-	-		
87	OHX	1	4031	-	0,6,6	0.00	-	-		
87	OHX	1	4203	-	0,6,6	0.00	-	-		
87	OHX	2	2067	-	0,6,6	0.00	-	-		
87	OHX	1	4184	-	0,6,6	0.00	-	-		
87	OHX	4	236	-	0,6,6	0.00	-	-		
87	OHX	5	4048	-	0,6,6	0.00	-	-		
87	OHX	1	4139	-	0,6,6	0.00	-	-		
87	OHX	2	2171	-	0,6,6	0.00	-	-		
87	OHX	2	2124	-	0,6,6	0.00	-	-		
87	OHX	1	4038	-	0,6,6	0.00	-	-		
87	OHX	6	2075	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4036	-	0,6,6	0.00	-	-		
87	OHX	5	4080	-	0,6,6	0.00	-	-		
87	OHX	1	3903	-	0,6,6	0.00	-	-		
87	OHX	m6	202	-	0,6,6	0.00	-	-		
87	OHX	1	4116	-	0,6,6	0.00	-	-		
87	OHX	m4	201	-	0,6,6	0.00	-	-		
87	OHX	6	2197	-	0,6,6	0.00	-	-		
87	OHX	5	4247	-	0,6,6	0.00	-	-		
87	OHX	1	4064	-	0,6,6	0.00	-	-		
87	OHX	2	2078	-	0,6,6	0.00	-	-		
87	OHX	1	4085	-	0,6,6	0.00	-	-		
87	OHX	5	4166	-	0,6,6	0.00	-	-		
87	OHX	1	4061	-	0,6,6	0.00	-	-		
87	OHX	2	2093	-	0,6,6	0.00	-	-		
87	OHX	5	3977	-	0,6,6	0.00	-	-		
87	OHX	1	4097	-	0,6,6	0.00	-	-		
87	OHX	2	2127	-	0,6,6	0.00	-	-		
87	OHX	2	2089	-	0,6,6	0.00	-	-		
87	OHX	n3	203	-	0,6,6	0.00	-	-		
87	OHX	6	2156	-	0,6,6	0.00	-	-		
87	OHX	1	4146	-	0,6,6	0.00	-	-		
87	OHX	1	4189	-	0,6,6	0.00	-	-		
87	OHX	1	4023	-	0,6,6	0.00	-	-		
87	OHX	2	2177	-	0,6,6	0.00	-	-		
87	OHX	1	4086	-	0,6,6	0.00	-	-		
87	OHX	5	4126	-	0,6,6	0.00	-	-		
87	OHX	1	4193	-	0,6,6	0.00	-	-		
87	OHX	5	4134	-	0,6,6	0.00	-	-		
87	OHX	5	4231	-	0,6,6	0.00	-	-		
87	OHX	1	4127	-	0,6,6	0.00	-	-		
87	OHX	m8	201	-	0,6,6	0.00	-	-		
87	OHX	5	4245	-	0,6,6	0.00	-	-		
87	OHX	1	4040	-	0,6,6	0.00	-	-		
87	OHX	6	2064	-	0,6,6	0.00	-	-		
87	OHX	1	3899	-	0,6,6	0.00	-	-		
87	OHX	6	2063	-	0,6,6	0.00	-	-		
87	OHX	6	2053	-	0,6,6	0.00	-	-		
87	OHX	sR	401	-	0,6,6	0.00	-	-		
87	OHX	5	4028	-	0,6,6	0.00	-	-		
87	OHX	5	4136	-	0,6,6	0.00	-	-		
87	OHX	m5	303	-	0,6,6	0.00	-	-		
87	OHX	1	3974	-	0,6,6	0.00	-	-		
87	OHX	8	219	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4001	-	0,6,6	0.00	-	-		
87	OHX	2	2170	-	0,6,6	0.00	-	-		
87	OHX	6	2158	-	0,6,6	0.00	-	-		
87	OHX	5	3935	-	0,6,6	0.00	-	-		
87	OHX	1	4179	-	0,6,6	0.00	-	-		
87	OHX	5	4217	-	0,6,6	0.00	-	-		
87	OHX	6	2059	-	0,6,6	0.00	-	-		
87	OHX	6	2159	-	0,6,6	0.00	-	-		
87	OHX	2	2155	-	0,6,6	0.00	-	-		
87	OHX	1	4171	-	0,6,6	0.00	-	-		
87	OHX	2	2122	-	0,6,6	0.00	-	-		
87	OHX	5	4065	-	0,6,6	0.00	-	-		
87	OHX	1	4093	-	0,6,6	0.00	-	-		
87	OHX	1	4033	-	0,6,6	0.00	-	-		
87	OHX	6	2086	-	0,6,6	0.00	-	-		
87	OHX	5	4044	-	0,6,6	0.00	-	-		
87	OHX	5	4225	-	0,6,6	0.00	-	-		
87	OHX	1	4072	-	0,6,6	0.00	-	-		
87	OHX	5	4090	-	0,6,6	0.00	-	-		
87	OHX	1	3997	-	0,6,6	0.00	-	-		
87	OHX	5	4190	-	0,6,6	0.00	-	-		
87	OHX	6	2182	-	0,6,6	0.00	-	-		
87	OHX	5	4088	-	0,6,6	0.00	-	-		
87	OHX	1	3871	-	0,6,6	0.00	-	-		
87	OHX	1	4046	-	0,6,6	0.00	-	-		
87	OHX	5	4122	-	0,6,6	0.00	-	-		
87	OHX	1	4163	-	0,6,6	0.00	-	-		
87	OHX	6	2199	-	0,6,6	0.00	-	-		
87	OHX	5	3912	-	0,6,6	0.00	-	-		
87	OHX	6	2190	-	0,6,6	0.00	-	-		
87	OHX	1	3868	-	0,6,6	0.00	-	-		
87	OHX	5	3931	-	0,6,6	0.00	-	-		
87	OHX	6	2168	-	0,6,6	0.00	-	-		
87	OHX	5	4165	-	0,6,6	0.00	-	-		
87	OHX	1	4137	-	0,6,6	0.00	-	-		
87	OHX	5	3913	-	0,6,6	0.00	-	-		
87	OHX	5	4239	-	0,6,6	0.00	-	-		
87	OHX	6	2152	-	0,6,6	0.00	-	-		
87	OHX	5	4084	-	0,6,6	0.00	-	-		
87	OHX	5	3980	-	0,6,6	0.00	-	-		
87	OHX	5	4128	-	0,6,6	0.00	-	-		
87	OHX	1	4183	-	0,6,6	0.00	-	-		
87	OHX	d9	102	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2180	-	0,6,6	0.00	-	-		
87	OHX	L3	405	-	0,6,6	0.00	-	-		
87	OHX	5	4035	-	0,6,6	0.00	-	-		
87	OHX	1	4074	-	0,6,6	0.00	-	-		
87	OHX	6	2144	-	0,6,6	0.00	-	-		
87	OHX	5	4180	-	0,6,6	0.00	-	-		
87	OHX	5	3944	-	0,6,6	0.00	-	-		
87	OHX	5	4153	-	0,6,6	0.00	-	-		
87	OHX	C3	202	-	0,6,6	0.00	-	-		
87	OHX	5	4145	-	0,6,6	0.00	-	-		
87	OHX	5	4063	-	0,6,6	0.00	-	-		
87	OHX	6	2201	-	0,6,6	0.00	-	-		
87	OHX	c8	203	-	0,6,6	0.00	-	-		
87	OHX	1	4103	-	0,6,6	0.00	-	-		
87	OHX	3	217	-	0,6,6	0.00	-	-		
87	OHX	5	4174	-	0,6,6	0.00	-	-		
87	OHX	1	3981	-	0,6,6	0.00	-	-		
87	OHX	5	4045	-	0,6,6	0.00	-	-		
87	OHX	5	4240	-	0,6,6	0.00	-	-		
87	OHX	8	217	-	0,6,6	0.00	-	-		
87	OHX	6	2102	-	0,6,6	0.00	-	-		
87	OHX	2	2172	-	0,6,6	0.00	-	-		
87	OHX	6	2195	-	0,6,6	0.00	-	-		
87	OHX	1	4070	-	0,6,6	0.00	-	-		
87	OHX	5	3940	-	0,6,6	0.00	-	-		
87	OHX	1	3963	-	0,6,6	0.00	-	-		
87	OHX	5	4029	-	0,6,6	0.00	-	-		
87	OHX	2	2030	-	0,6,6	0.00	-	-		
87	OHX	6	2091	-	0,6,6	0.00	-	-		
87	OHX	5	4200	-	0,6,6	0.00	-	-		
87	OHX	6	2057	-	0,6,6	0.00	-	-		
87	OHX	1	4063	-	0,6,6	0.00	-	-		
87	OHX	6	2188	-	0,6,6	0.00	-	-		
87	OHX	5	3996	-	0,6,6	0.00	-	-		
87	OHX	2	2042	-	0,6,6	0.00	-	-		
87	OHX	6	2103	-	0,6,6	0.00	-	-		
87	OHX	5	4034	-	0,6,6	0.00	-	-		
87	OHX	1	4099	-	0,6,6	0.00	-	-		
87	OHX	L3	406	-	0,6,6	0.00	-	-		
87	OHX	1	3955	-	0,6,6	0.00	-	-		
87	OHX	4	231	-	0,6,6	0.00	-	-		
87	OHX	1	3906	-	0,6,6	0.00	-	-		
87	OHX	2	2022	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4100	-	0,6,6	0.00	-	-		
87	OHX	5	4154	-	0,6,6	0.00	-	-		
87	OHX	2	2094	-	0,6,6	0.00	-	-		
87	OHX	6	2125	-	0,6,6	0.00	-	-		
87	OHX	6	2161	-	0,6,6	0.00	-	-		
87	OHX	1	3877	-	0,6,6	0.00	-	-		
87	OHX	2	2154	-	0,6,6	0.00	-	-		
87	OHX	1	3999	-	0,6,6	0.00	-	-		
87	OHX	c3	201	-	0,6,6	0.00	-	-		
87	OHX	1	4027	-	0,6,6	0.00	-	-		
87	OHX	1	4132	-	0,6,6	0.00	-	-		
87	OHX	1	4133	-	0,6,6	0.00	-	-		
87	OHX	2	2070	-	0,6,6	0.00	-	-		
87	OHX	1	4034	-	0,6,6	0.00	-	-		
87	OHX	5	3937	-	0,6,6	0.00	-	-		
87	OHX	2	2150	-	0,6,6	0.00	-	-		
87	OHX	5	4008	-	0,6,6	0.00	-	-		
87	OHX	1	4177	-	0,6,6	0.00	-	-		
87	OHX	5	4087	-	0,6,6	0.00	-	-		
87	OHX	5	4025	-	0,6,6	0.00	-	-		
87	OHX	2	2167	-	0,6,6	0.00	-	-		
87	OHX	2	2050	-	0,6,6	0.00	-	-		
87	OHX	5	3953	-	0,6,6	0.00	-	-		
87	OHX	5	4092	-	0,6,6	0.00	-	-		
87	OHX	2	2143	-	0,6,6	0.00	-	-		
87	OHX	5	3948	-	0,6,6	0.00	-	-		
87	OHX	5	4062	-	0,6,6	0.00	-	-		
87	OHX	5	3964	-	0,6,6	0.00	-	-		
87	OHX	2	2162	-	0,6,6	0.00	-	-		
87	OHX	5	4125	-	0,6,6	0.00	-	-		
87	OHX	2	2095	-	0,6,6	0.00	-	-		
87	OHX	6	2049	-	0,6,6	0.00	-	-		
87	OHX	4	227	-	0,6,6	0.00	-	-		
87	OHX	2	2090	-	0,6,6	0.00	-	-		
87	OHX	1	3983	-	0,6,6	0.00	-	-		
87	OHX	5	4007	-	0,6,6	0.00	-	-		
87	OHX	6	2185	-	0,6,6	0.00	-	-		
87	OHX	5	4155	-	0,6,6	0.00	-	-		
87	OHX	6	2171	-	0,6,6	0.00	-	-		
87	OHX	5	3920	-	0,6,6	0.00	-	-		
87	OHX	1	4167	-	0,6,6	0.00	-	-		
87	OHX	5	3995	-	0,6,6	0.00	-	-		
87	OHX	6	2146	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3892	-	0,6,6	0.00	-	-		
87	OHX	1	4209	-	0,6,6	0.00	-	-		
87	OHX	5	4057	-	0,6,6	0.00	-	-		
87	OHX	2	2091	-	0,6,6	0.00	-	-		
87	OHX	1	4065	-	0,6,6	0.00	-	-		
87	OHX	5	3989	-	0,6,6	0.00	-	-		
87	OHX	5	4187	-	0,6,6	0.00	-	-		
87	OHX	5	4163	-	0,6,6	0.00	-	-		
87	OHX	1	3936	-	0,6,6	0.00	-	-		
87	OHX	1	4101	-	0,6,6	0.00	-	-		
87	OHX	2	2097	-	0,6,6	0.00	-	-		
87	OHX	1	4019	-	0,6,6	0.00	-	-		
87	OHX	1	3886	-	0,6,6	0.00	-	-		
87	OHX	1	4175	-	0,6,6	0.00	-	-		
87	OHX	4	225	-	0,6,6	0.00	-	-		
87	OHX	1	4048	-	0,6,6	0.00	-	-		
87	OHX	2	2178	-	0,6,6	0.00	-	-		
87	OHX	1	4088	-	0,6,6	0.00	-	-		
87	OHX	5	4004	-	0,6,6	0.00	-	-		
87	OHX	5	4077	-	0,6,6	0.00	-	-		
87	OHX	8	227	-	0,6,6	0.00	-	-		
87	OHX	1	4107	-	0,6,6	0.00	-	-		
87	OHX	1	4066	-	0,6,6	0.00	-	-		
87	OHX	1	3872	-	0,6,6	0.00	-	-		
87	OHX	1	3933	-	0,6,6	0.00	-	-		
87	OHX	1	4006	-	0,6,6	0.00	-	-		
87	OHX	1	4078	-	0,6,6	0.00	-	-		
87	OHX	5	3945	-	0,6,6	0.00	-	-		
87	OHX	6	2093	-	0,6,6	0.00	-	-		
87	OHX	5	4043	-	0,6,6	0.00	-	-		
87	OHX	5	3934	-	0,6,6	0.00	-	-		
87	OHX	2	2065	-	0,6,6	0.00	-	-		
87	OHX	6	2151	-	0,6,6	0.00	-	-		
87	OHX	1	4118	-	0,6,6	0.00	-	-		
87	OHX	1	3954	-	0,6,6	0.00	-	-		
87	OHX	2	2043	-	0,6,6	0.00	-	-		
87	OHX	5	3963	-	0,6,6	0.00	-	-		
87	OHX	5	4009	-	0,6,6	0.00	-	-		
87	OHX	5	3958	-	0,6,6	0.00	-	-		
87	OHX	5	3974	-	0,6,6	0.00	-	-		
87	OHX	2	2146	-	0,6,6	0.00	-	-		
87	OHX	3	218	-	0,6,6	0.00	-	-		
87	OHX	1	4010	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	D3	202	-	0,6,6	0.00	-	-		
87	OHX	3	224	-	0,6,6	0.00	-	-		
87	OHX	5	4248	-	0,6,6	0.00	-	-		
87	OHX	2	2073	-	0,6,6	0.00	-	-		
87	OHX	5	4210	-	0,6,6	0.00	-	-		
87	OHX	2	2046	-	0,6,6	0.00	-	-		
87	OHX	5	4213	-	0,6,6	0.00	-	-		
87	OHX	2	2169	-	0,6,6	0.00	-	-		
87	OHX	1	4169	-	0,6,6	0.00	-	-		
87	OHX	1	3964	-	0,6,6	0.00	-	-		
87	OHX	2	2038	-	0,6,6	0.00	-	-		
87	OHX	1	4005	-	0,6,6	0.00	-	-		
87	OHX	5	4143	-	0,6,6	0.00	-	-		
87	OHX	5	4202	-	0,6,6	0.00	-	-		
87	OHX	1	4187	-	0,6,6	0.00	-	-		
87	OHX	1	3969	-	0,6,6	0.00	-	-		
87	OHX	m7	205	-	0,6,6	0.00	-	-		
87	OHX	7	220	-	0,6,6	0.00	-	-		
87	OHX	6	2065	-	0,6,6	0.00	-	-		
87	OHX	8	214	-	0,6,6	0.00	-	-		
87	OHX	1	3931	-	0,6,6	0.00	-	-		
87	OHX	2	2031	-	0,6,6	0.00	-	-		
87	OHX	6	2110	-	0,6,6	0.00	-	-		
87	OHX	5	4242	-	0,6,6	0.00	-	-		
87	OHX	1	3905	-	0,6,6	0.00	-	-		
87	OHX	6	2124	-	0,6,6	0.00	-	-		
87	OHX	5	4199	-	0,6,6	0.00	-	-		
87	OHX	8	220	-	0,6,6	0.00	-	-		
87	OHX	5	3986	-	0,6,6	0.00	-	-		
87	OHX	1	4024	-	0,6,6	0.00	-	-		
87	OHX	1	3939	-	0,6,6	0.00	-	-		
87	OHX	5	4010	-	0,6,6	0.00	-	-		
87	OHX	1	4121	-	0,6,6	0.00	-	-		
87	OHX	5	3952	-	0,6,6	0.00	-	-		
87	OHX	6	2148	-	0,6,6	0.00	-	-		
87	OHX	6	2051	-	0,6,6	0.00	-	-		
87	OHX	1	3891	-	0,6,6	0.00	-	-		
87	OHX	1	4148	-	0,6,6	0.00	-	-		
87	OHX	2	2117	-	0,6,6	0.00	-	-		
87	OHX	2	2033	-	0,6,6	0.00	-	-		
87	OHX	1	4164	-	0,6,6	0.00	-	-		
87	OHX	1	4166	-	0,6,6	0.00	-	-		
87	OHX	6	2113	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2152	-	0,6,6	0.00	-	-		
87	OHX	6	2056	-	0,6,6	0.00	-	-		
87	OHX	1	3951	-	0,6,6	0.00	-	-		
87	OHX	1	4195	-	0,6,6	0.00	-	-		
87	OHX	2	2041	-	0,6,6	0.00	-	-		
87	OHX	1	4176	-	0,6,6	0.00	-	-		
87	OHX	1	3919	-	0,6,6	0.00	-	-		
87	OHX	5	4022	-	0,6,6	0.00	-	-		
87	OHX	1	4144	-	0,6,6	0.00	-	-		
87	OHX	5	4193	-	0,6,6	0.00	-	-		
87	OHX	M7	207	-	0,6,6	0.00	-	-		
87	OHX	2	2064	-	0,6,6	0.00	-	-		
87	OHX	5	4064	-	0,6,6	0.00	-	-		
87	OHX	5	4078	-	0,6,6	0.00	-	-		
87	OHX	1	4192	-	0,6,6	0.00	-	-		
87	OHX	6	2120	-	0,6,6	0.00	-	-		
87	OHX	1	3932	-	0,6,6	0.00	-	-		
87	OHX	1	3996	-	0,6,6	0.00	-	-		
87	OHX	1	4115	-	0,6,6	0.00	-	-		
87	OHX	6	2070	-	0,6,6	0.00	-	-		
87	OHX	5	4203	-	0,6,6	0.00	-	-		
87	OHX	5	4103	-	0,6,6	0.00	-	-		
87	OHX	6	2192	-	0,6,6	0.00	-	-		
87	OHX	1	4076	-	0,6,6	0.00	-	-		
87	OHX	5	3900	-	0,6,6	0.00	-	-		
87	OHX	5	3954	-	0,6,6	0.00	-	-		
87	OHX	6	2121	-	0,6,6	0.00	-	-		
87	OHX	1	4089	-	0,6,6	0.00	-	-		
87	OHX	6	2141	-	0,6,6	0.00	-	-		
87	OHX	1	4060	-	0,6,6	0.00	-	-		
87	OHX	1	4047	-	0,6,6	0.00	-	-		
87	OHX	6	2135	-	0,6,6	0.00	-	-		
87	OHX	1	4011	-	0,6,6	0.00	-	-		
87	OHX	6	2072	-	0,6,6	0.00	-	-		
87	OHX	4	233	-	0,6,6	0.00	-	-		
87	OHX	5	3938	-	0,6,6	0.00	-	-		
87	OHX	1	4145	-	0,6,6	0.00	-	-		
87	OHX	2	2105	-	0,6,6	0.00	-	-		
87	OHX	5	4235	-	0,6,6	0.00	-	-		
87	OHX	1	4058	-	0,6,6	0.00	-	-		
87	OHX	1	4138	-	0,6,6	0.00	-	-		
87	OHX	5	3904	-	0,6,6	0.00	-	-		
87	OHX	1	4037	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4087	-	0,6,6	0.00	-	-		
87	OHX	1	4039	-	0,6,6	0.00	-	-		
87	OHX	5	4229	-	0,6,6	0.00	-	-		
87	OHX	5	3988	-	0,6,6	0.00	-	-		
87	OHX	5	4117	-	0,6,6	0.00	-	-		
87	OHX	C5	201	-	0,6,6	0.00	-	-		
87	OHX	5	4052	-	0,6,6	0.00	-	-		
87	OHX	1	3948	-	0,6,6	0.00	-	-		
87	OHX	6	2184	-	0,6,6	0.00	-	-		
87	OHX	5	4070	-	0,6,6	0.00	-	-		
87	OHX	5	4050	-	0,6,6	0.00	-	-		
87	OHX	4	226	-	0,6,6	0.00	-	-		
87	OHX	5	4089	-	0,6,6	0.00	-	-		
87	OHX	1	4079	-	0,6,6	0.00	-	-		
87	OHX	1	4009	-	0,6,6	0.00	-	-		
87	OHX	5	4123	-	0,6,6	0.00	-	-		
87	OHX	O2	201	-	0,6,6	0.00	-	-		
87	OHX	6	2172	-	0,6,6	0.00	-	-		
87	OHX	1	4028	-	0,6,6	0.00	-	-		
87	OHX	5	3976	-	0,6,6	0.00	-	-		
87	OHX	1	4020	-	0,6,6	0.00	-	-		
87	OHX	5	4236	-	0,6,6	0.00	-	-		
87	OHX	5	3921	-	0,6,6	0.00	-	-		
87	OHX	5	4233	-	0,6,6	0.00	-	-		
87	OHX	1	4117	-	0,6,6	0.00	-	-		
87	OHX	1	4147	-	0,6,6	0.00	-	-		
87	OHX	5	3994	-	0,6,6	0.00	-	-		
87	OHX	6	2139	-	0,6,6	0.00	-	-		
87	OHX	5	4049	-	0,6,6	0.00	-	-		
87	OHX	2	2102	-	0,6,6	0.00	-	-		
87	OHX	6	2165	-	0,6,6	0.00	-	-		
87	OHX	6	2109	-	0,6,6	0.00	-	-		
87	OHX	1	4213	-	0,6,6	0.00	-	-		
87	OHX	5	4115	-	0,6,6	0.00	-	-		
87	OHX	3	225	-	0,6,6	0.00	-	-		
87	OHX	1	4162	-	0,6,6	0.00	-	-		
87	OHX	1	4168	-	0,6,6	0.00	-	-		
87	OHX	1	4150	-	0,6,6	0.00	-	-		
87	OHX	O7	103	-	0,6,6	0.00	-	-		
87	OHX	6	2068	-	0,6,6	0.00	-	-		
87	OHX	m0	301	-	0,6,6	0.00	-	-		
87	OHX	6	2097	-	0,6,6	0.00	-	-		
87	OHX	o3	202	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	8	226	-	0,6,6	0.00	-	-		
87	OHX	1	4151	-	0,6,6	0.00	-	-		
87	OHX	5	4137	-	0,6,6	0.00	-	-		
87	OHX	1	4157	-	0,6,6	0.00	-	-		
87	OHX	5	3957	-	0,6,6	0.00	-	-		
87	OHX	5	3951	-	0,6,6	0.00	-	-		
87	OHX	1	4071	-	0,6,6	0.00	-	-		
87	OHX	1	3888	-	0,6,6	0.00	-	-		
87	OHX	5	3959	-	0,6,6	0.00	-	-		
87	OHX	2	2027	-	0,6,6	0.00	-	-		
87	OHX	1	4214	-	0,6,6	0.00	-	-		
87	OHX	5	4130	-	0,6,6	0.00	-	-		
87	OHX	1	3938	-	0,6,6	0.00	-	-		
87	OHX	1	3978	-	0,6,6	0.00	-	-		
87	OHX	5	3975	-	0,6,6	0.00	-	-		
87	OHX	2	2130	-	0,6,6	0.00	-	-		
87	OHX	5	3914	-	0,6,6	0.00	-	-		
87	OHX	2	2173	-	0,6,6	0.00	-	-		
87	OHX	5	3955	-	0,6,6	0.00	-	-		
87	OHX	5	4191	-	0,6,6	0.00	-	-		
87	OHX	5	3997	-	0,6,6	0.00	-	-		
87	OHX	m1	203	-	0,6,6	0.00	-	-		
87	OHX	s9	201	-	0,6,6	0.00	-	-		
87	OHX	1	4112	-	0,6,6	0.00	-	-		
87	OHX	1	4158	-	0,6,6	0.00	-	-		
89	3HE	1	4215	-	21,21,21	0.53	0	19,30,30	0.62	0
87	OHX	1	4094	-	0,6,6	0.00	-	-		
87	OHX	1	4153	-	0,6,6	0.00	-	-		
87	OHX	1	3890	-	0,6,6	0.00	-	-		
87	OHX	2	2121	-	0,6,6	0.00	-	-		
87	OHX	1	4075	-	0,6,6	0.00	-	-		
87	OHX	1	3982	-	0,6,6	0.00	-	-		
87	OHX	1	3867	-	0,6,6	0.00	-	-		
87	OHX	1	4152	-	0,6,6	0.00	-	-		
87	OHX	5	4171	-	0,6,6	0.00	-	-		
87	OHX	6	2173	-	0,6,6	0.00	-	-		
87	OHX	L4	402	-	0,6,6	0.00	-	-		
87	OHX	6	2088	-	0,6,6	0.00	-	-		
87	OHX	2	2084	-	0,6,6	0.00	-	-		
87	OHX	5	4147	-	0,6,6	0.00	-	-		
87	OHX	2	2125	-	0,6,6	0.00	-	-		
87	OHX	5	4168	-	0,6,6	0.00	-	-		
87	OHX	1	3959	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2049	-	0,6,6	0.00	-	-		
87	OHX	2	2174	-	0,6,6	0.00	-	-		
87	OHX	5	4061	-	0,6,6	0.00	-	-		
87	OHX	1	4123	-	0,6,6	0.00	-	-		
87	OHX	6	2055	-	0,6,6	0.00	-	-		
87	OHX	6	2050	-	0,6,6	0.00	-	-		
87	OHX	5	4164	-	0,6,6	0.00	-	-		
87	OHX	1	4102	-	0,6,6	0.00	-	-		
87	OHX	1	4105	-	0,6,6	0.00	-	-		
87	OHX	M0	303	-	0,6,6	0.00	-	-		
87	OHX	2	2087	-	0,6,6	0.00	-	-		
87	OHX	5	4083	-	0,6,6	0.00	-	-		
87	OHX	1	3984	-	0,6,6	0.00	-	-		
87	OHX	6	2084	-	0,6,6	0.00	-	-		
87	OHX	6	2090	-	0,6,6	0.00	-	-		
87	OHX	5	3984	-	0,6,6	0.00	-	-		
87	OHX	5	3942	-	0,6,6	0.00	-	-		
87	OHX	5	4019	-	0,6,6	0.00	-	-		
87	OHX	5	4140	-	0,6,6	0.00	-	-		
87	OHX	5	4094	-	0,6,6	0.00	-	-		
87	OHX	O9	101	-	0,6,6	0.00	-	-		
87	OHX	5	4032	-	0,6,6	0.00	-	-		
87	OHX	5	4017	-	0,6,6	0.00	-	-		
87	OHX	2	2112	-	0,6,6	0.00	-	-		
87	OHX	1	3994	-	0,6,6	0.00	-	-		
87	OHX	2	2054	-	0,6,6	0.00	-	-		
87	OHX	1	4043	-	0,6,6	0.00	-	-		
87	OHX	5	4219	-	0,6,6	0.00	-	-		
87	OHX	1	3864	-	0,6,6	0.00	-	-		
87	OHX	1	4083	-	0,6,6	0.00	-	-		
87	OHX	6	2179	-	0,6,6	0.00	-	-		
87	OHX	6	2134	-	0,6,6	0.00	-	-		
87	OHX	5	3973	-	0,6,6	0.00	-	-		
87	OHX	5	4014	-	0,6,6	0.00	-	-		
87	OHX	2	2126	-	0,6,6	0.00	-	-		
87	OHX	6	2198	-	0,6,6	0.00	-	-		
87	OHX	1	4190	-	0,6,6	0.00	-	-		
87	OHX	1	4082	-	0,6,6	0.00	-	-		
87	OHX	8	229	-	0,6,6	0.00	-	-		
87	OHX	7	221	-	0,6,6	0.00	-	-		
87	OHX	2	2077	-	0,6,6	0.00	-	-		
87	OHX	1	4041	-	0,6,6	0.00	-	-		
87	OHX	6	2062	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	4049	-	0,6,6	0.00	-	-		
87	OHX	1	3878	-	0,6,6	0.00	-	-		
87	OHX	2	2156	-	0,6,6	0.00	-	-		
87	OHX	SR	401	-	0,6,6	0.00	-	-		
87	OHX	5	3943	-	0,6,6	0.00	-	-		
87	OHX	m0	302	-	0,6,6	0.00	-	-		
87	OHX	1	4077	-	0,6,6	0.00	-	-		
87	OHX	7	218	-	0,6,6	0.00	-	-		
87	OHX	5	3933	-	0,6,6	0.00	-	-		
87	OHX	5	3932	-	0,6,6	0.00	-	-		
87	OHX	5	3979	-	0,6,6	0.00	-	-		
87	OHX	1	4042	-	0,6,6	0.00	-	-		
87	OHX	1	3952	-	0,6,6	0.00	-	-		
87	OHX	5	3903	-	0,6,6	0.00	-	-		
87	OHX	1	4206	-	0,6,6	0.00	-	-		
87	OHX	1	4160	-	0,6,6	0.00	-	-		
87	OHX	5	3992	-	0,6,6	0.00	-	-		
87	OHX	1	3998	-	0,6,6	0.00	-	-		
87	OHX	6	2153	-	0,6,6	0.00	-	-		
87	OHX	1	3884	-	0,6,6	0.00	-	-		
87	OHX	4	229	-	0,6,6	0.00	-	-		
87	OHX	2	2023	-	0,6,6	0.00	-	-		
87	OHX	5	3916	-	0,6,6	0.00	-	-		
87	OHX	1	4174	-	0,6,6	0.00	-	-		
87	OHX	5	4041	-	0,6,6	0.00	-	-		
87	OHX	1	3924	-	0,6,6	0.00	-	-		
87	OHX	c1	202	-	0,6,6	0.00	-	-		
87	OHX	5	3968	-	0,6,6	0.00	-	-		
87	OHX	4	230	-	0,6,6	0.00	-	-		
87	OHX	1	3942	-	0,6,6	0.00	-	-		
87	OHX	5	4109	-	0,6,6	0.00	-	-		
87	OHX	6	2204	-	0,6,6	0.00	-	-		
87	OHX	2	2026	-	0,6,6	0.00	-	-		
87	OHX	5	4016	-	0,6,6	0.00	-	-		
87	OHX	1	3914	-	0,6,6	0.00	-	-		
87	OHX	5	4116	-	0,6,6	0.00	-	-		
87	OHX	5	3941	-	0,6,6	0.00	-	-		
87	OHX	q2	502	-	0,6,6	0.00	-	-		
87	OHX	2	2072	-	0,6,6	0.00	-	-		
87	OHX	5	4148	-	0,6,6	0.00	-	-		
87	OHX	6	2178	-	0,6,6	0.00	-	-		
87	OHX	8	225	-	0,6,6	0.00	-	-		
87	OHX	6	2137	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3922	-	0,6,6	0.00	-	-		
87	OHX	1	4208	-	0,6,6	0.00	-	-		
87	OHX	2	2158	-	0,6,6	0.00	-	-		
87	OHX	5	3966	-	0,6,6	0.00	-	-		
87	OHX	6	2170	-	0,6,6	0.00	-	-		
87	OHX	5	4186	-	0,6,6	0.00	-	-		
87	OHX	1	4143	-	0,6,6	0.00	-	-		
87	OHX	5	4060	-	0,6,6	0.00	-	-		
87	OHX	5	4150	-	0,6,6	0.00	-	-		
87	OHX	8	216	-	0,6,6	0.00	-	-		
87	OHX	5	4246	-	0,6,6	0.00	-	-		
87	OHX	5	4226	-	0,6,6	0.00	-	-		
87	OHX	1	3945	-	0,6,6	0.00	-	-		
87	OHX	6	2130	-	0,6,6	0.00	-	-		
87	OHX	5	4027	-	0,6,6	0.00	-	-		
87	OHX	1	4159	-	0,6,6	0.00	-	-		
87	OHX	6	2166	-	0,6,6	0.00	-	-		
87	OHX	5	4173	-	0,6,6	0.00	-	-		
87	OHX	2	2123	-	0,6,6	0.00	-	-		
87	OHX	6	2169	-	0,6,6	0.00	-	-		
87	OHX	6	2154	-	0,6,6	0.00	-	-		
87	OHX	5	4132	-	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
89	3HE	1	4215	-	-	1/8/36/36	0/2/2/2
89	3HE	5	4252	-	-	3/8/36/36	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	5	4252	3HE	C5-C7	3.31	1.58	1.53

There are no bond angle outliers.

There are no chirality outliers.

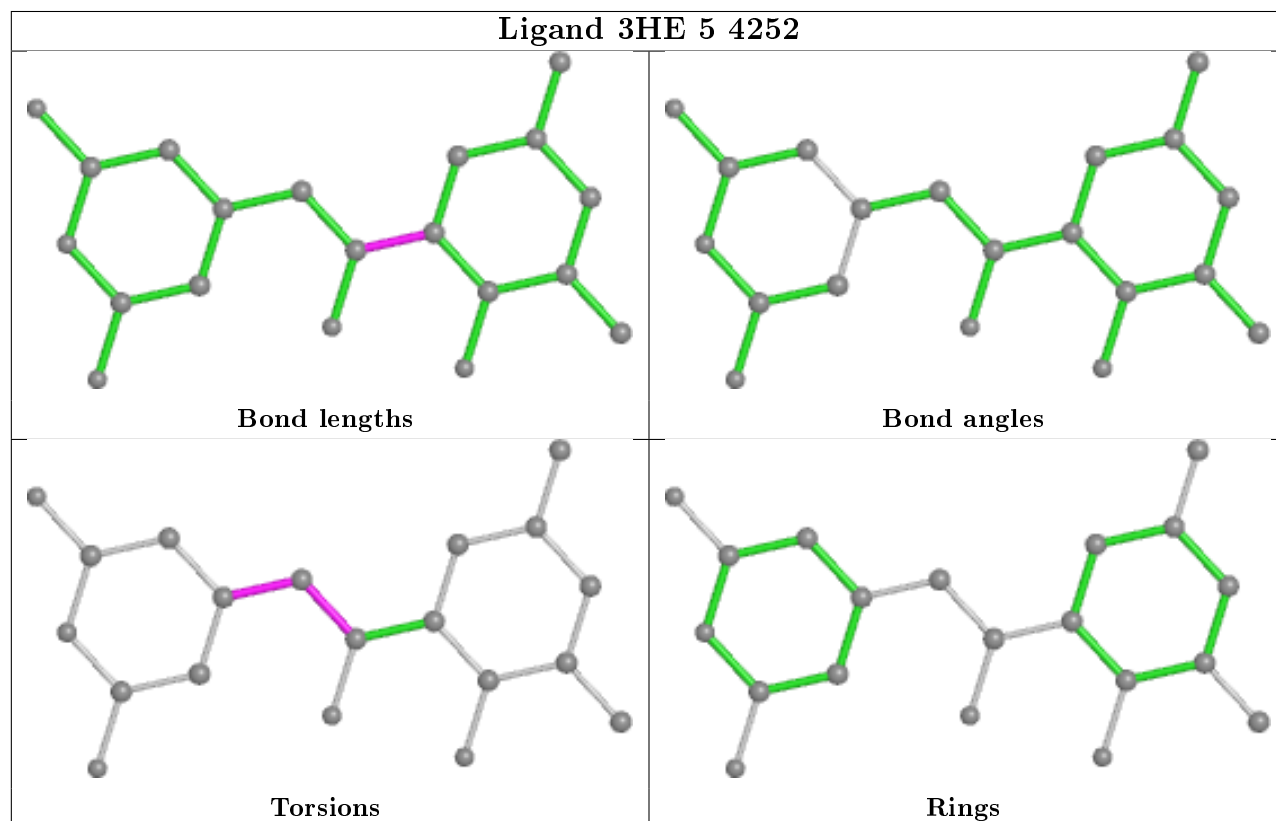
All (4) torsion outliers are listed below:

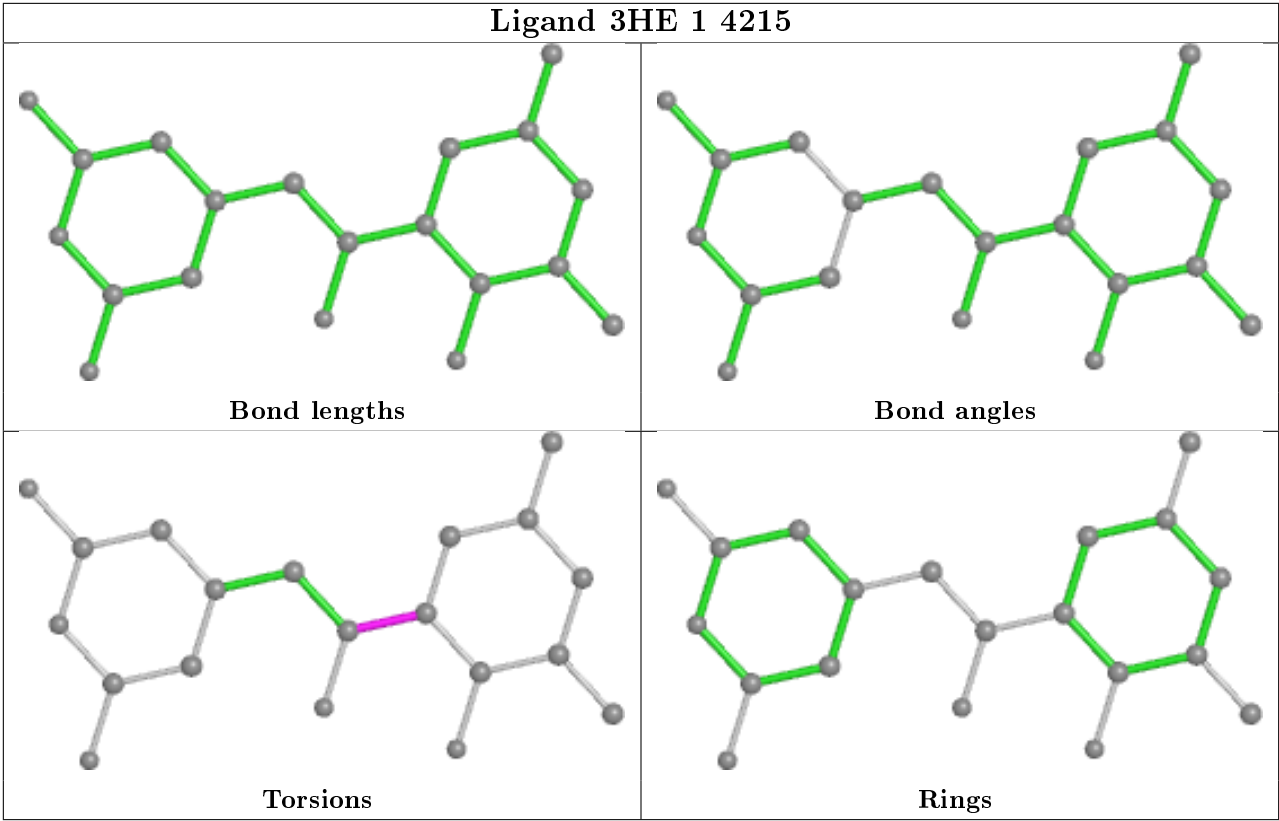
Mol	Chain	Res	Type	Atoms
89	5	4252	3HE	C7-C8-C9-C10
89	5	4252	3HE	C7-C8-C9-C13
89	5	4252	3HE	O3-C7-C8-C9
89	1	4215	3HE	C6-C5-C7-O3

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	SR	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SR	161:LYS	C	162:ALA	N	0.76
1	SR	160:GLU	C	161:LYS	N	0.64

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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