



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 07:39 AM BST

PDB ID : 4U6F
Title : Crystal structure of T-2 toxin bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-28
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

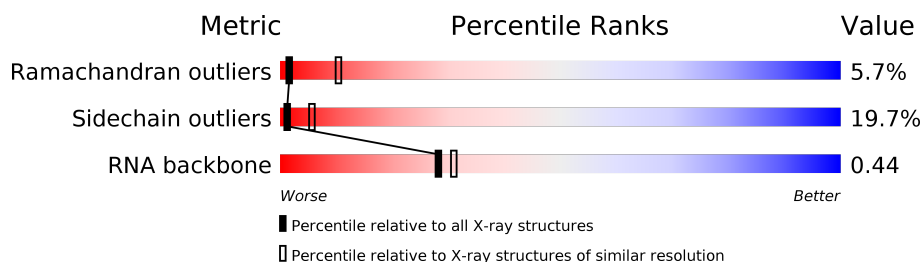
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



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





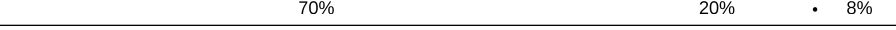
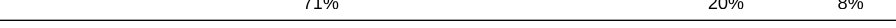

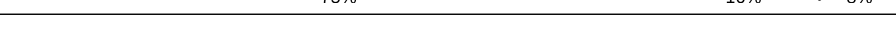
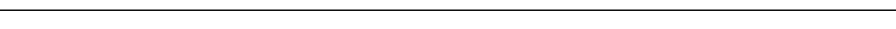
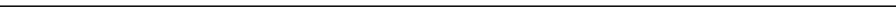















The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	65% 29% 5% .
1	6	1800	65% 31% .
2	S0	251	63% 18% . 18%
2	s0	251	65% 15% . 18%
3	S1	254	57% 24% . 16%
3	s1	254	66% 18% . 15%
4	S2	253	64% 21% . 14%
4	s2	253	67% 17% . 14%


























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















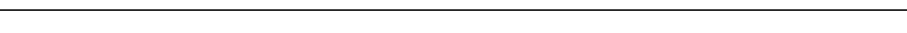




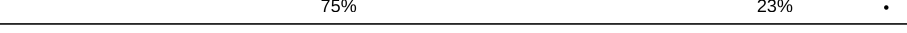





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Mol	Chain	Length	Quality of chain
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107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


























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















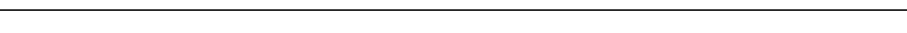




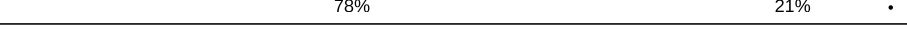





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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6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















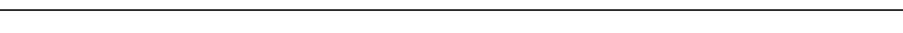




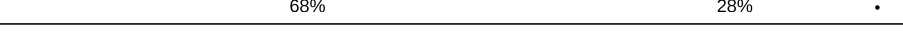





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Mol	Chain	Length	Quality of chain
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9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


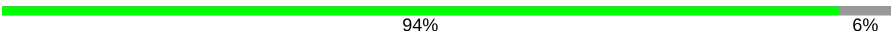


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Mol	Chain	Length	Quality of chain
68	O2	129	 84% 15%
68	o2	129	 75% 23%
69	O3	106	 92% 8%
69	o3	106	 80% 18%
70	O4	120	 78% 14% 7%
70	o4	120	 76% 18% 7%
71	O5	119	 77% 22%
71	o5	119	 79% 21%
72	O6	99	 70% 26%
72	o6	99	 70% 28%
73	O7	87	 79% 21%
73	o7	87	 85% 14%
74	O8	77	 75% 25%
74	o8	77	 70% 30%
75	O9	50	 88% 12%
75	o9	50	 82% 18%
76	Q0	52	 83% 15%
76	q0	52	 83% 15%
77	Q1	25	 68% 28%
77	q1	25	 68% 32%
78	Q2	105	 75% 22%
78	q2	105	 80% 18%
79	Q3	91	 86% 14%
79	q3	91	 80% 20%
80	e0	62	 71% 27%

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Mol	Chain	Length	Quality of chain
81	p0	311	
82	m2	160	
83	p1	47	
84	p2	46	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
88	ZBA	1	4206	X	-	-	-

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411881 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	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			
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 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745
C0	98	SER	THR	conflict	UNP Q08745
c0	89	ALA	GLY	conflict	UNP Q08745
c0	98	SER	THR	conflict	UNP Q08745

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	13	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	14	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	15	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	16	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	17	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	18	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	19	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	4	Total	Mg	0	0
			4	4		
85	n8	3	Total	Mg	0	0
			3	3		
85	o1	1	Total	Mg	0	0
			1	1		
85	N5	1	Total	Mg	0	0
			1	1		
85	6	147	Total	Mg	0	0
			147	147		
85	sM	2	Total	Mg	0	0
			2	2		
85	O4	1	Total	Mg	0	0
			1	1		
85	m5	5	Total	Mg	0	0
			5	5		
85	l3	3	Total	Mg	0	0
			3	3		
85	M1	1	Total	Mg	0	0
			1	1		
85	n0	1	Total	Mg	0	0
			1	1		
85	d6	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	2	126	Total 126	Mg 126	0	0
85	O3	1	Total 1	Mg 1	0	0
85	L4	2	Total 2	Mg 2	0	0
85	l7	1	Total 1	Mg 1	0	0
85	M5	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	o0	1	Total 1	Mg 1	0	0
85	S2	1	Total 1	Mg 1	0	0
85	L8	1	Total 1	Mg 1	0	0
85	o4	1	Total 1	Mg 1	0	0
85	M9	1	Total 1	Mg 1	0	0
85	q0	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	2	Total 2	Mg 2	0	0
85	c1	2	Total 2	Mg 2	0	0
85	5	504	Total 504	Mg 504	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	1	Total 1	Mg 1	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	M4	1	Total 1	Mg 1	0	0

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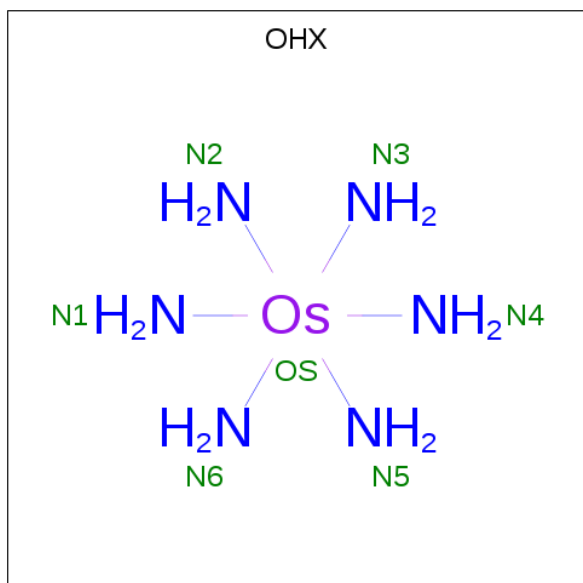
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	n9	1	Total 1	Mg 1	0	0
85	1	465	Total 465	Mg 465	0	0
85	n6	2	Total 2	Mg 2	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	1	Total 1	Mg 1	0	0
85	d3	1	Total 1	Mg 1	0	0
85	q3	2	Total 2	Mg 2	0	0
85	o3	1	Total 1	Mg 1	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	3	Total 3	Mg 3	0	0
85	N8	6	Total 6	Mg 6	0	0
85	4	22	Total 22	Mg 22	0	0
85	L2	2	Total 2	Mg 2	0	0
85	m1	2	Total 2	Mg 2	0	0
85	l5	2	Total 2	Mg 2	0	0
85	m7	4	Total 4	Mg 4	0	0
85	M7	5	Total 5	Mg 5	0	0
85	L6	2	Total 2	Mg 2	0	0
85	s1	1	Total 1	Mg 1	0	0
85	m6	2	Total 2	Mg 2	0	0
85	s8	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	c7	2	Total	Mg	0	0
			2	2		
85	7	17	Total	Mg	0	0
			17	17		
85	n3	2	Total	Mg	0	0
			2	2		
85	L3	3	Total	Mg	0	0
			3	3		
85	d4	1	Total	Mg	0	0
			1	1		
85	N6	1	Total	Mg	0	0
			1	1		
85	8	12	Total	Mg	0	0
			12	12		
85	M6	1	Total	Mg	0	0
			1	1		
85	N0	2	Total	Mg	0	0
			2	2		
85	3	14	Total	Mg	0	0
			14	14		

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



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	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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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
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86	L4	1	Total	N	Os	0	0
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86	M0	1	Total	N	Os	0	0
			7	6	1		
86	M5	1	Total	N	Os	0	0
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86	M6	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	M9	1	Total	N	Os	0	0
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86	N1	1	Total	N	Os	0	0
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86	N9	1	Total	N	Os	0	0
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86	O1	1	Total	N	Os	0	0
			7	6	1		
86	O2	1	Total	N	Os	0	0
			7	6	1		
86	O3	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	Q2	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	7	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l9	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n5	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

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

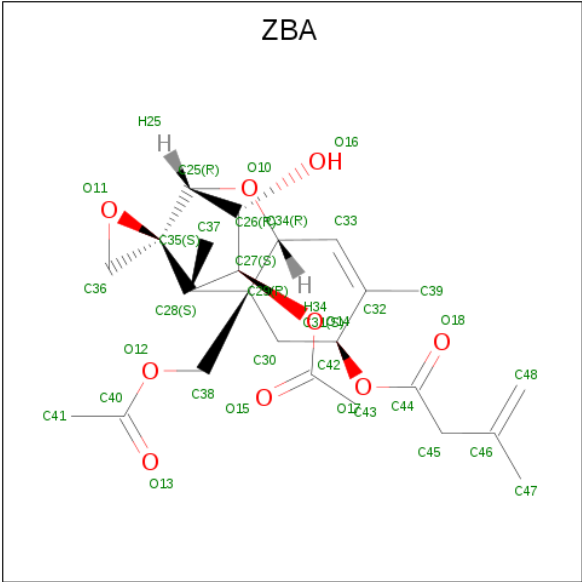
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		

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

- Molecule 88 is 12,13-Epoxytrichothec-9-ene-3,4,8,15-tetrol-4,15-diacetate-8-isovalerate (three-letter code: ZBA) (formula: C₂₄H₃₂O₉).



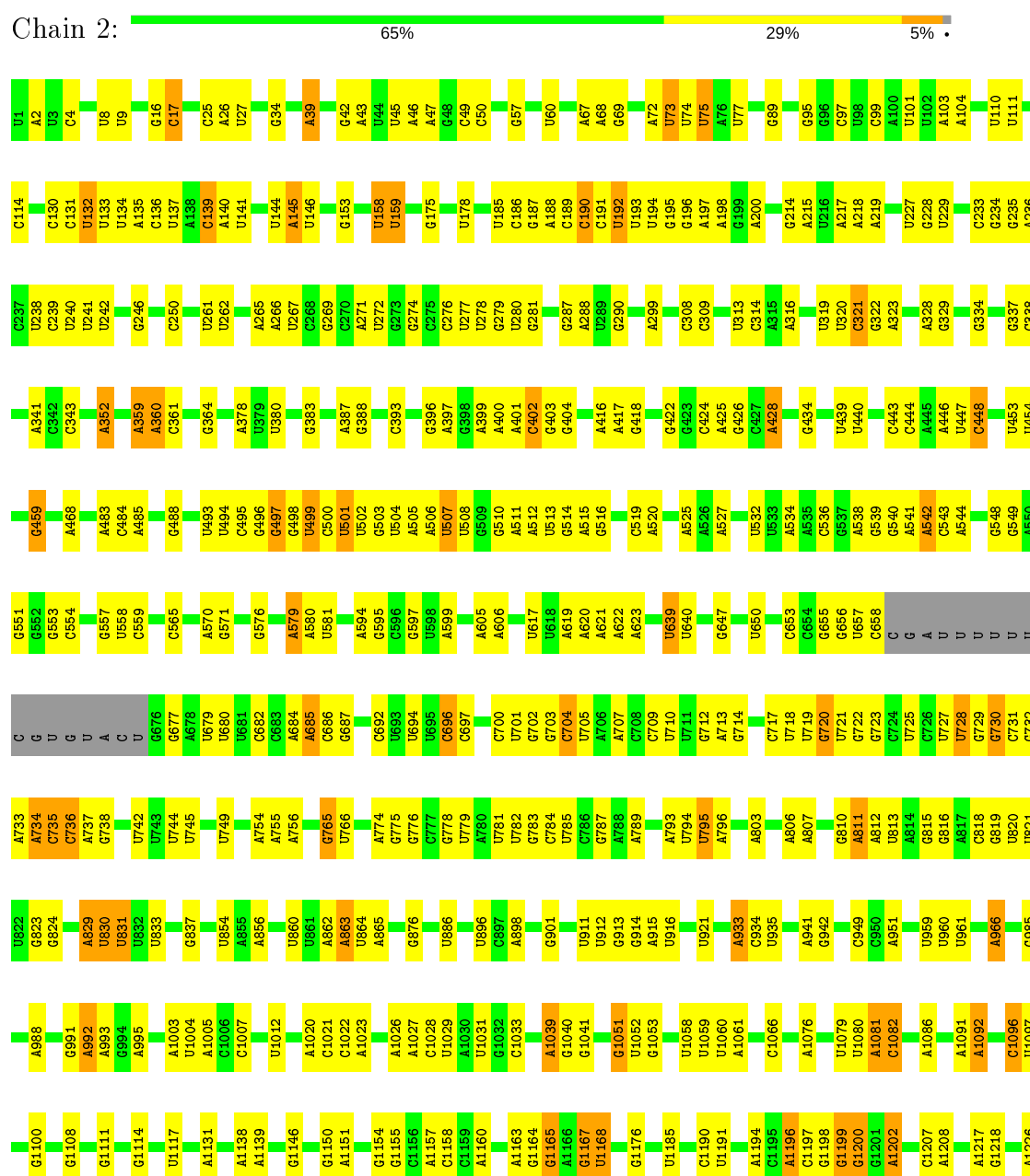
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	C	O	0	0
			33	24	9		
88	5	1	Total	C	O	0	0
			33	24	9		

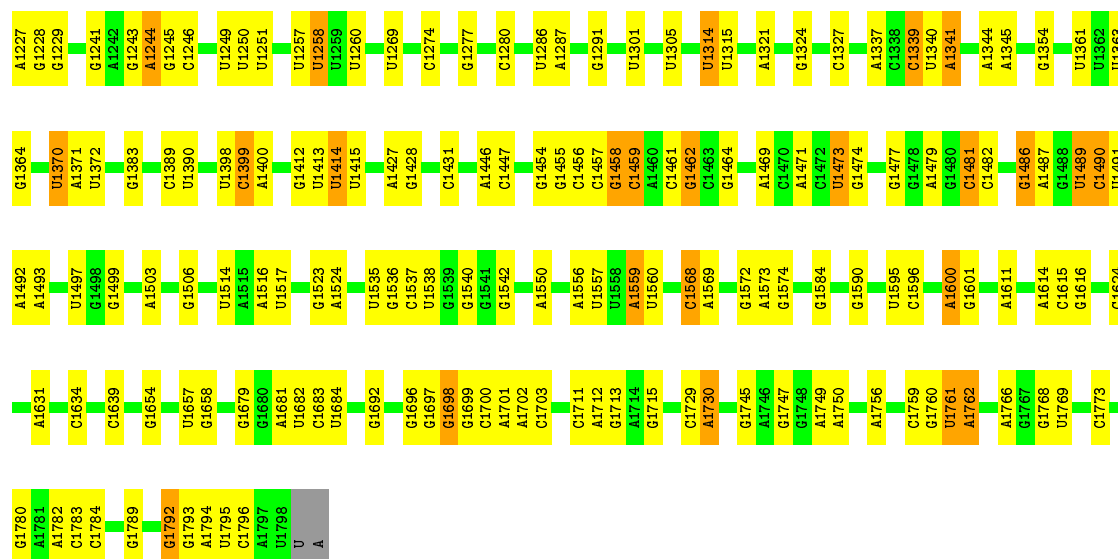
3 Residue-property plots

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

Note EDS failed to run properly.

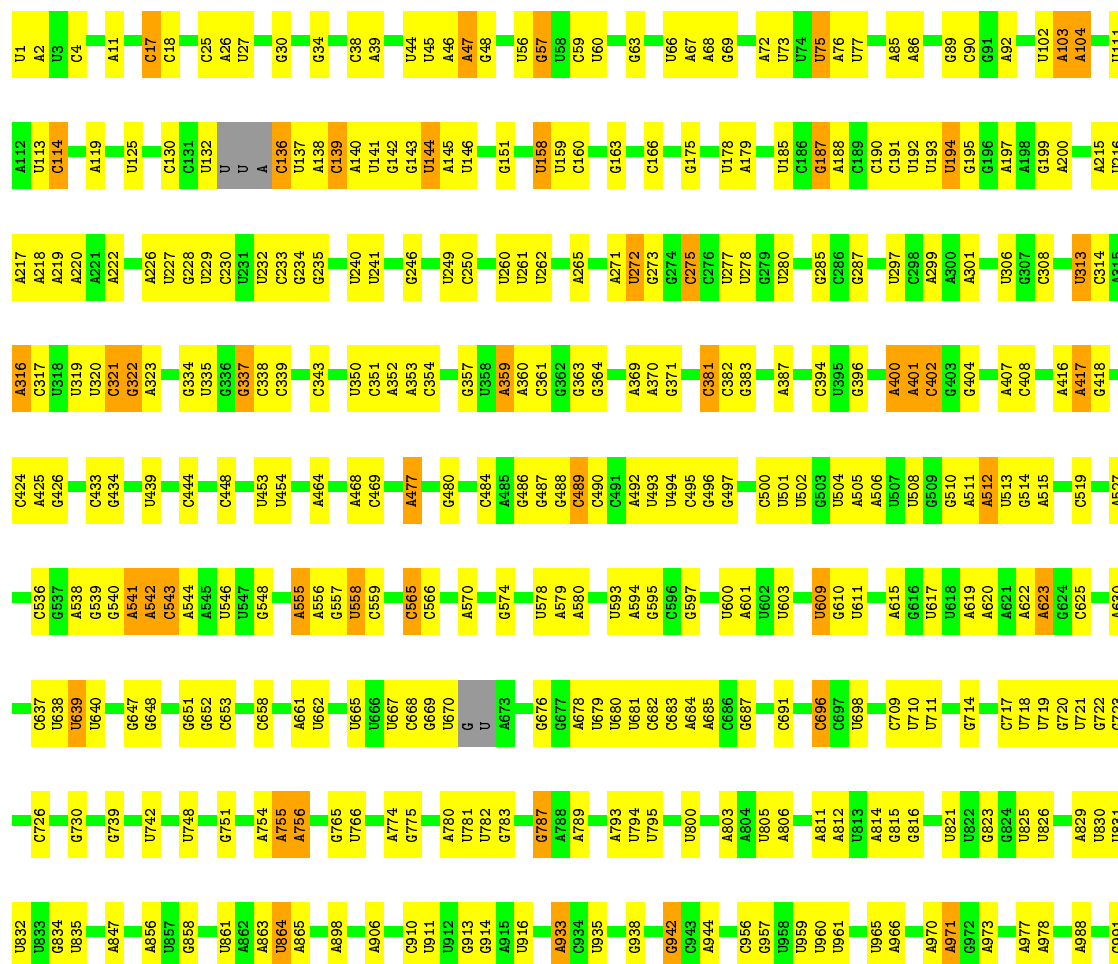
• Molecule 1: 18S ribosomal RNA

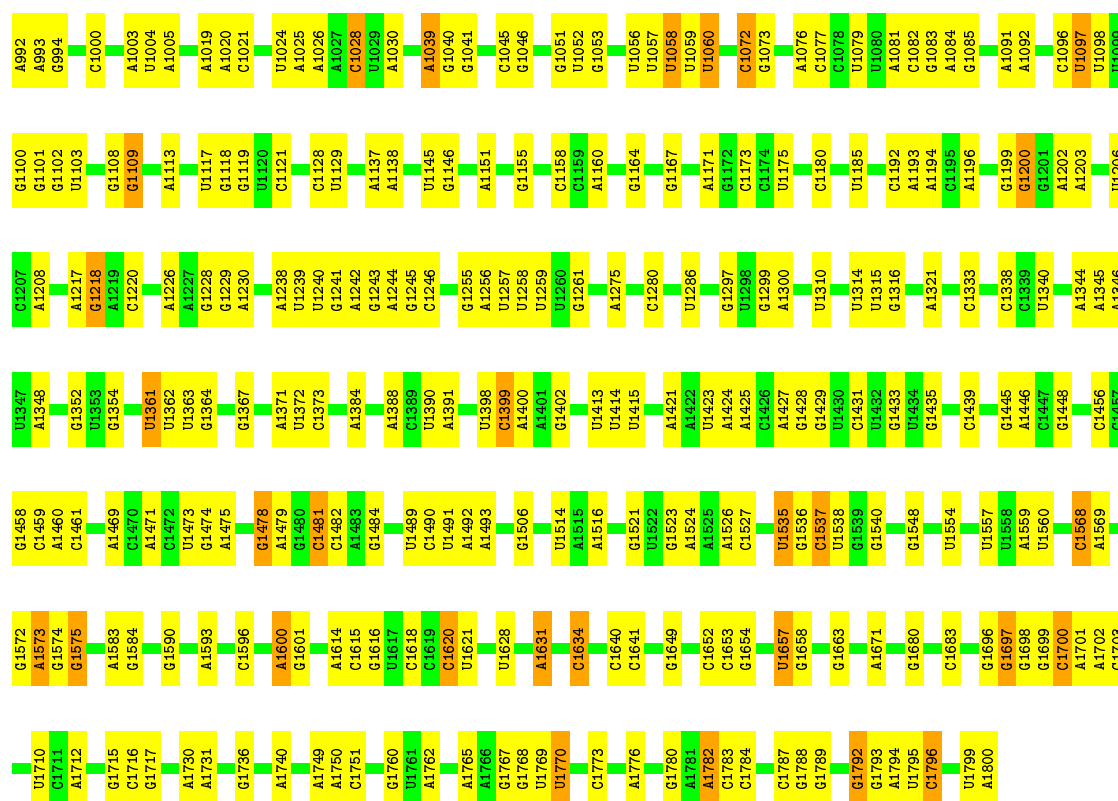




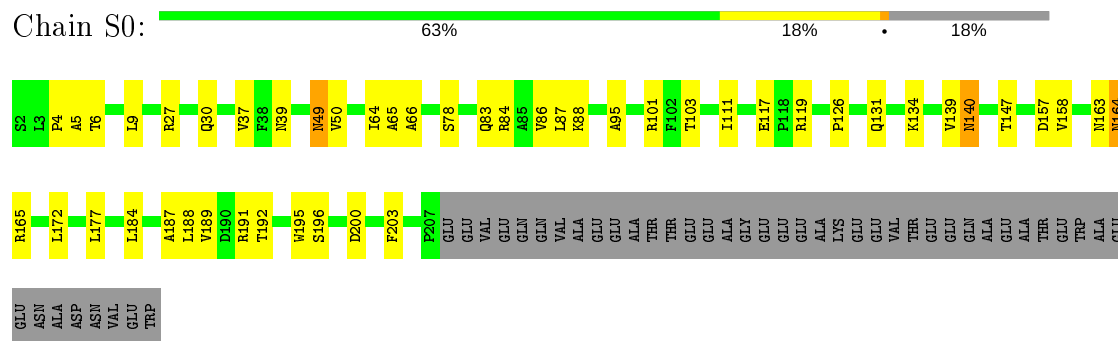
• Molecule 1: 18S ribosomal RNA

Chain 6: 65% 31% .

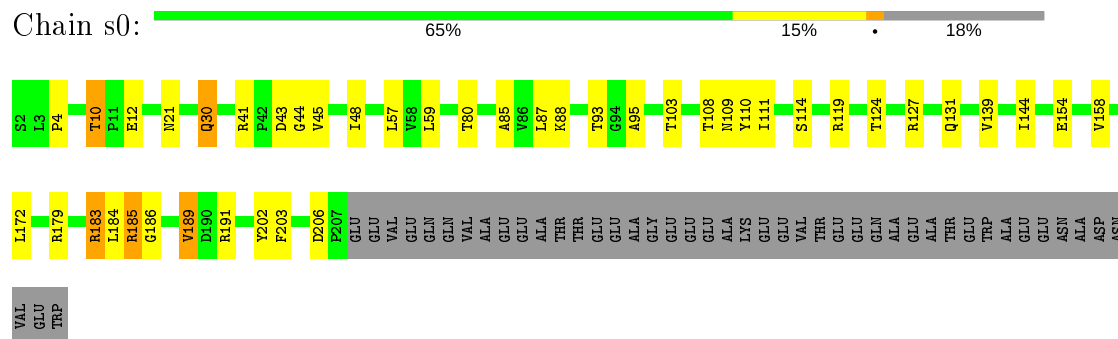




• Molecule 2: 40S ribosomal protein S0-A




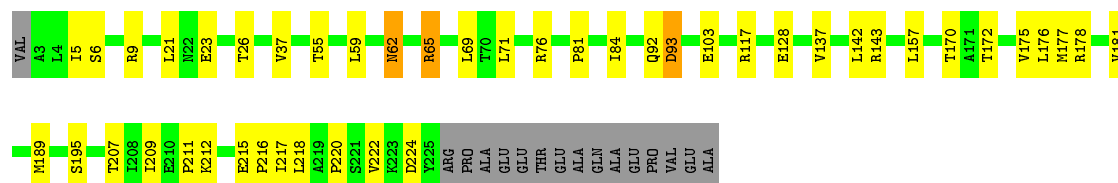
• Molecule 2: 40S ribosomal protein S0-A



• Molecule 3: 40S ribosomal protein S1-A

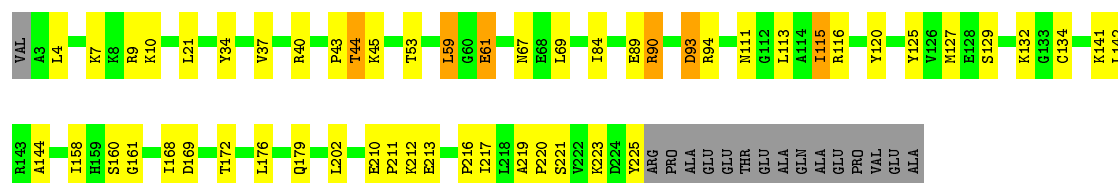
- Molecule 5: 40S ribosomal protein S3

Chain S3: 




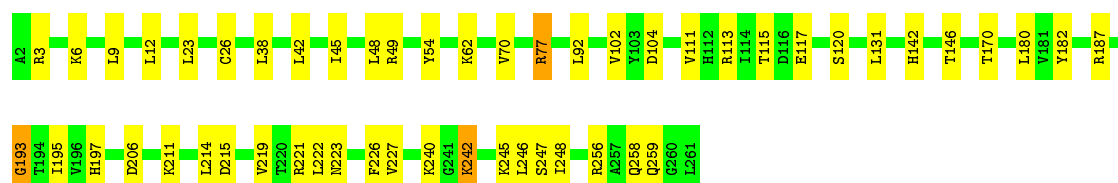
- Molecule 5: 40S ribosomal protein S3

Chain s3: 




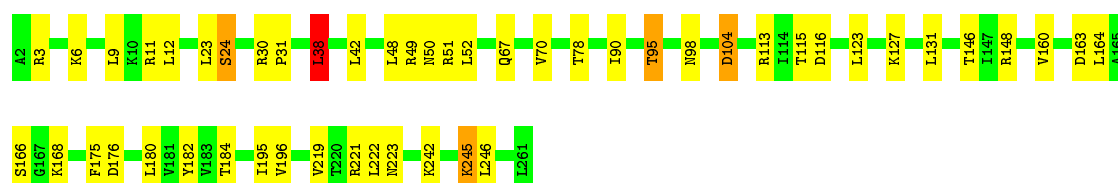
- Molecule 6: 40S ribosomal protein S4-A

Chain S4: 



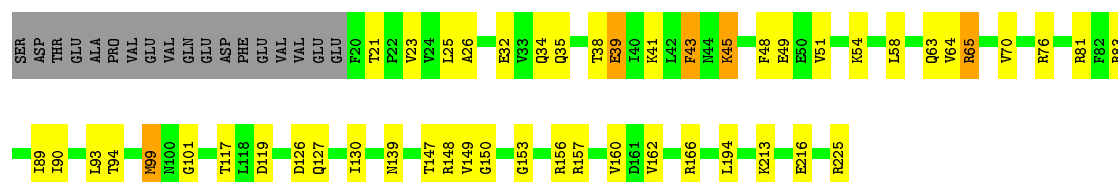
- Molecule 6: 40S ribosomal protein S4-A

Chain s4: 

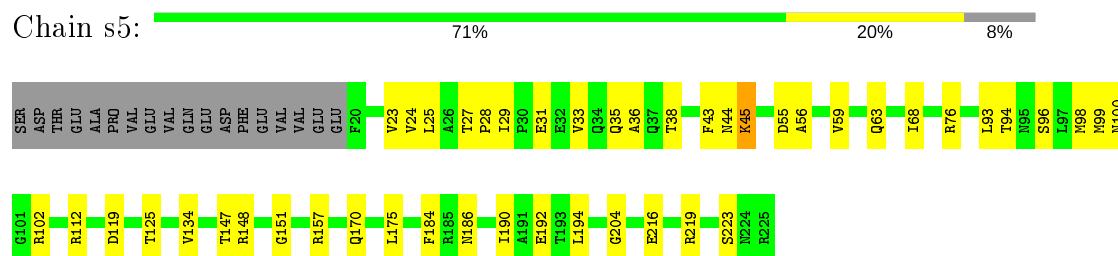


- Molecule 7: 40S ribosomal protein S5

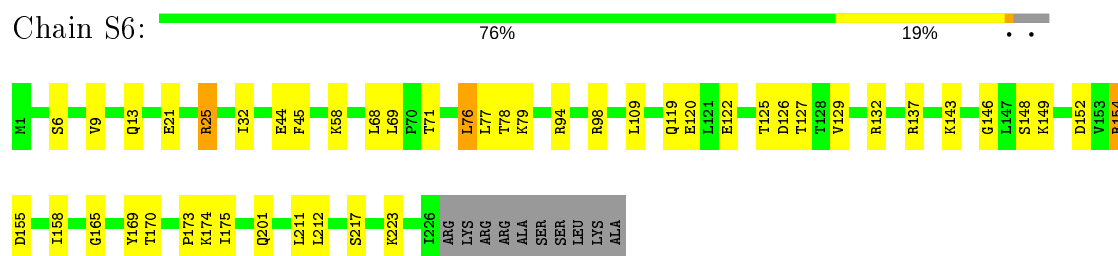
Chain S5: 



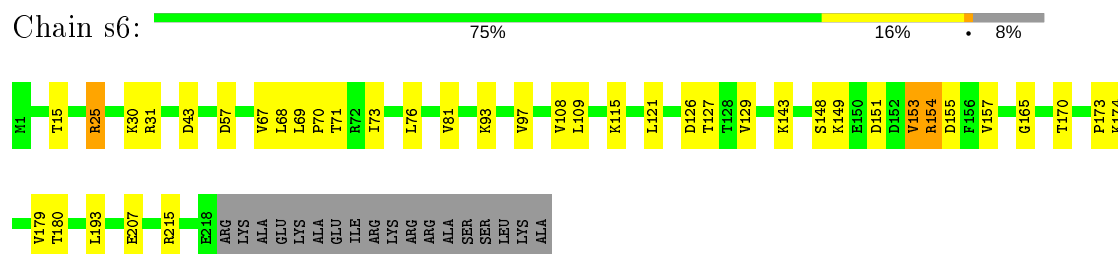
- Molecule 7: 40S ribosomal protein S5



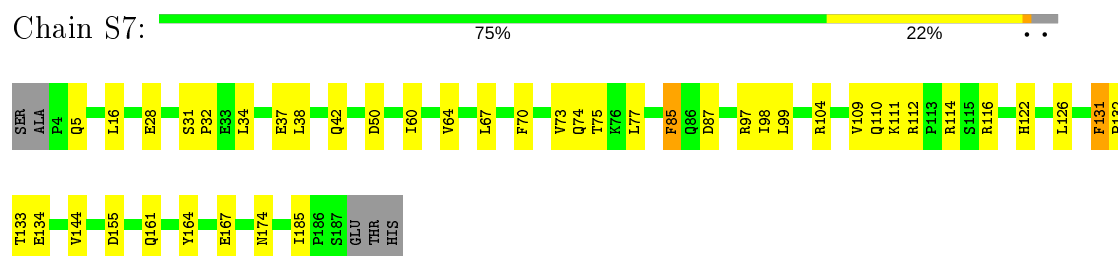
- Molecule 8: 40S ribosomal protein S6-A



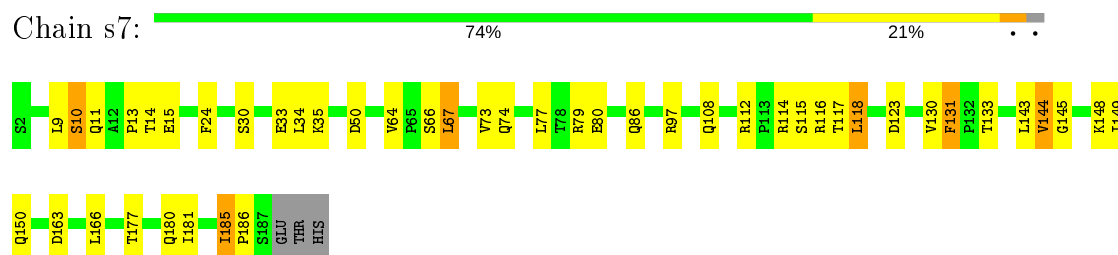
- Molecule 8: 40S ribosomal protein S6-A




- Molecule 9: 40S ribosomal protein S7-A

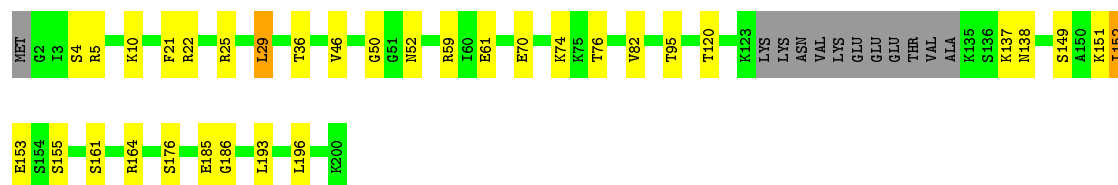


- Molecule 9: 40S ribosomal protein S7-A




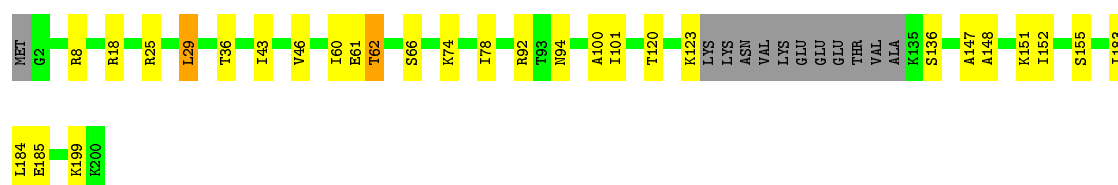
- Molecule 10: 40S ribosomal protein S8-A

Chain S8:  78% 16% • 6%



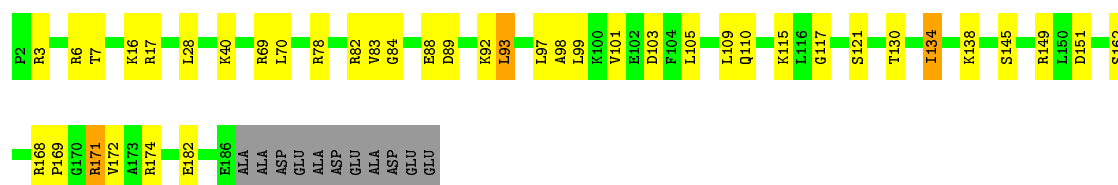
- Molecule 10: 40S ribosomal protein S8-A

Chain s8:  80% 14% • 6%



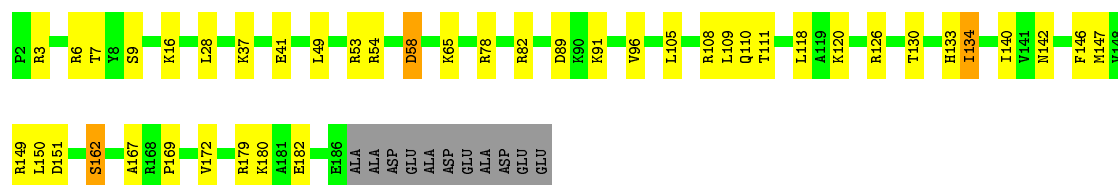
- Molecule 11: 40S ribosomal protein S9-A

Chain S9:  73% 19% • 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9:  72% 20% • 6%

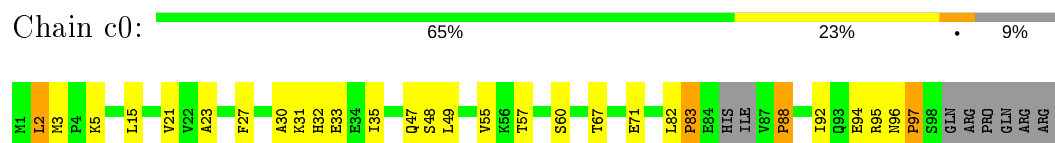


- Molecule 12: 40S ribosomal protein S10-A

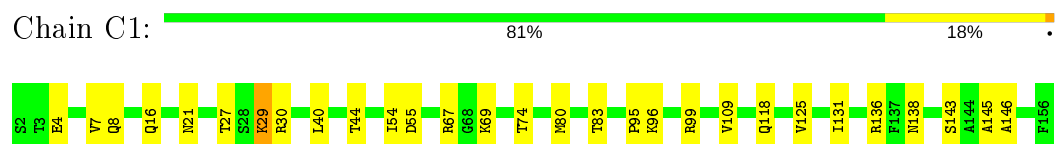
Chain C0:  69% 21% • 9%



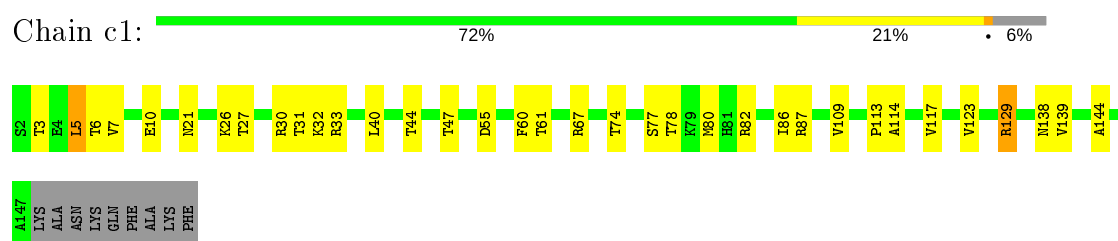
- Molecule 12: 40S ribosomal protein S10-A



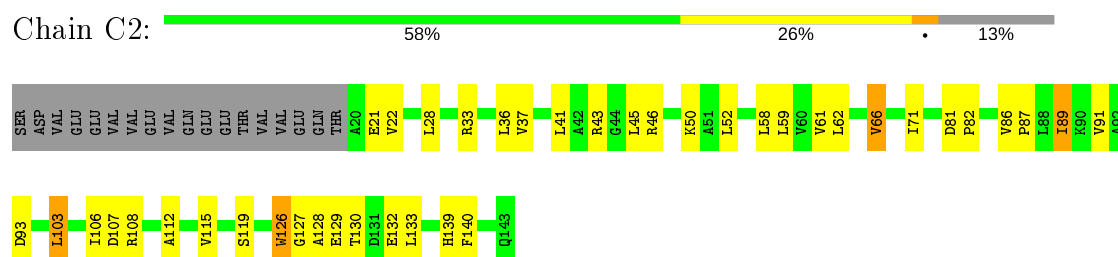
- Molecule 13: 40S ribosomal protein S11-A



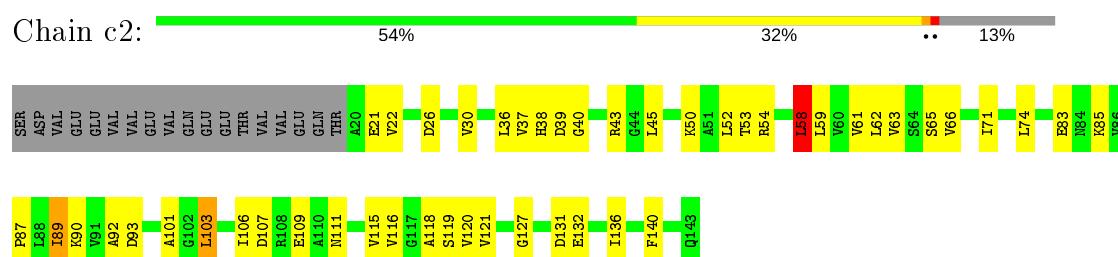
- Molecule 13: 40S ribosomal protein S11-A



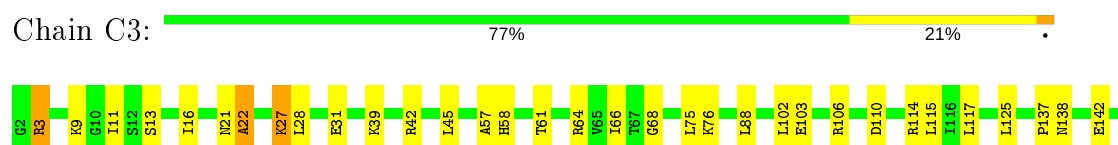
- Molecule 14: 40S ribosomal protein S12



- Molecule 14: 40S ribosomal protein S12



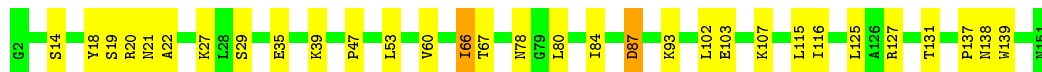
- Molecule 15: 40S ribosomal protein S13





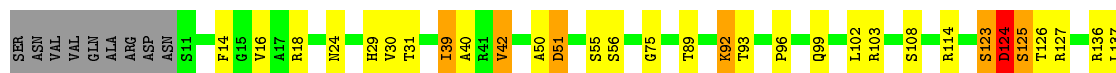
- Molecule 15: 40S ribosomal protein S13

Chain c3: 79% 19%



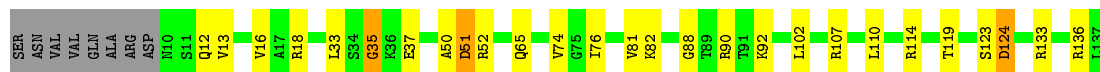
- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 71% 18% 7%



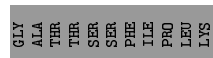
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 74% 18% 6%



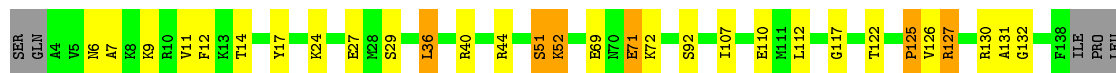
- Molecule 17: 40S ribosomal protein S15

Chain C5: 67% 19% 12%



- Molecule 17: 40S ribosomal protein S15

Chain c5: 74% 17%



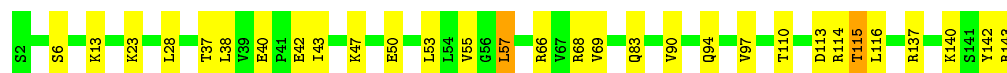
- Molecule 18: 40S ribosomal protein S16-A

Chain C6: 76% 20%



- Molecule 18: 40S ribosomal protein S16-A

Chain c6: 79% 20%



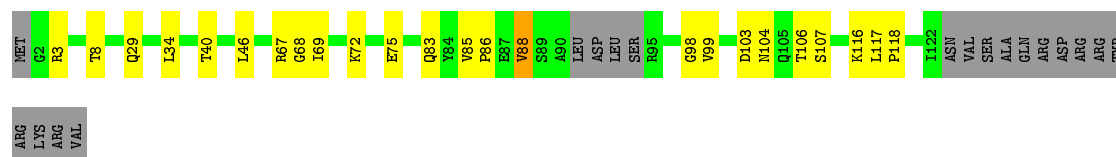
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:  71% 15% • 12%



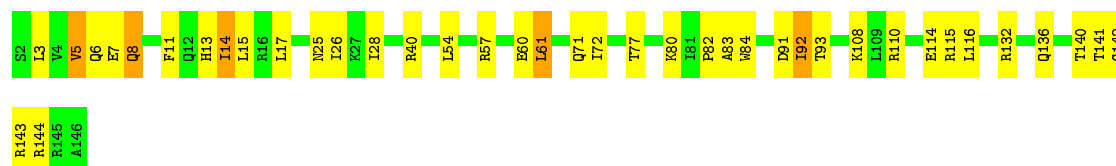
- Molecule 19: 40S ribosomal protein S17-A

Chain c7: 68% 17% • 14%



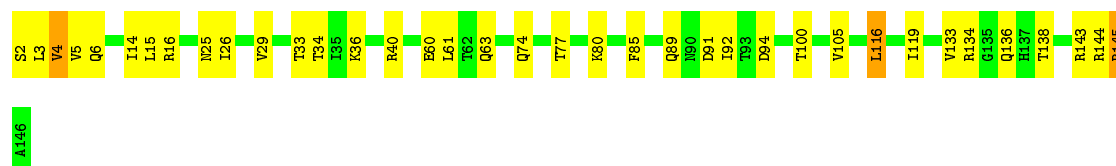
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:  72% 24% .




- Molecule 20: 40S ribosomal protein S18-A

Chain c8: 74% 23% .




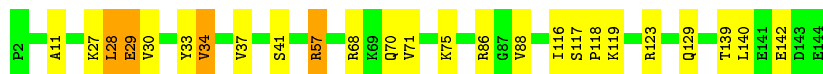
- Molecule 21: 40S ribosomal protein S19-A

Chain C9:  80% 18%



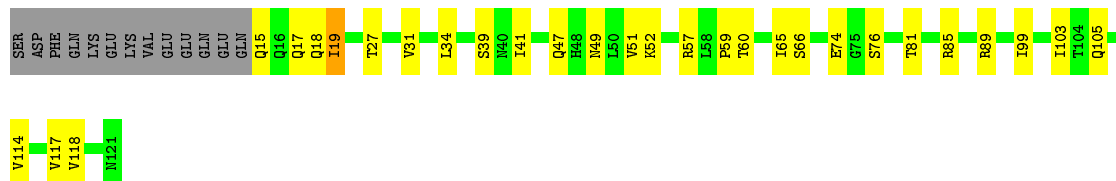
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:  83% 15%



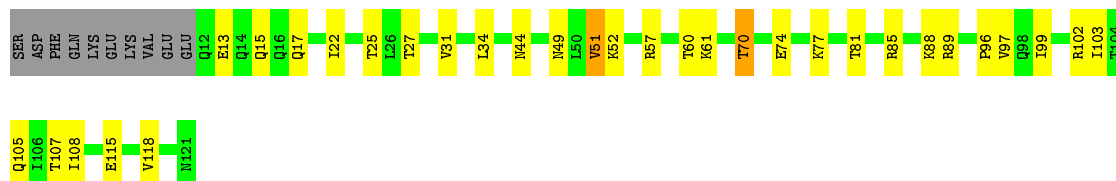
- Molecule 22: 40S ribosomal protein S20

Chain D0:  65% 23% 11%



- Molecule 22: 40S ribosomal protein S20

Chain d0:  65% 25% 8%



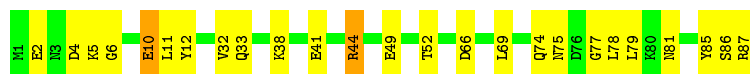
- Molecule 23: 40S ribosomal protein S21-A

Chain D1:  71% 26%




- Molecule 23: 40S ribosomal protein S21-A

Chain d1:  71% 26%




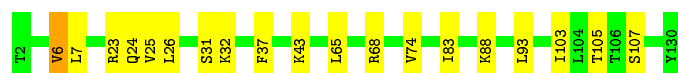
- Molecule 24: 40S ribosomal protein S22-A

Chain D2:  82% 16%




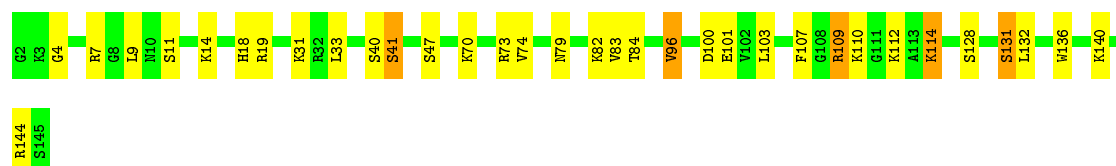
- Molecule 24: 40S ribosomal protein S22-A

Chain d2:  85% 14%




- Molecule 25: 40S ribosomal protein S23-A

Chain D3:  76% 20%




- Molecule 25: 40S ribosomal protein S23-A

Chain d3:  84% 15%




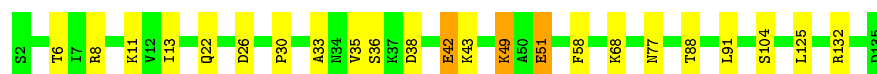
- Molecule 26: 40S ribosomal protein S24-A

Chain D4:  87% 13%



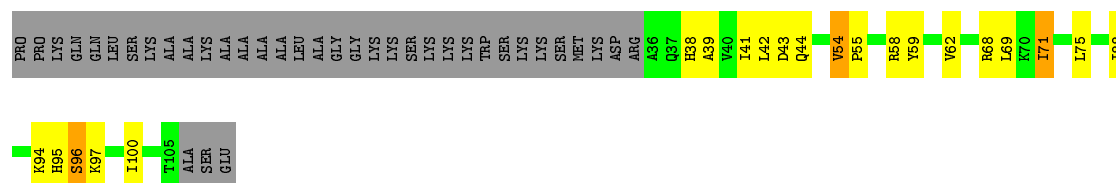
- Molecule 26: 40S ribosomal protein S24-A

Chain d4:  83% 15%



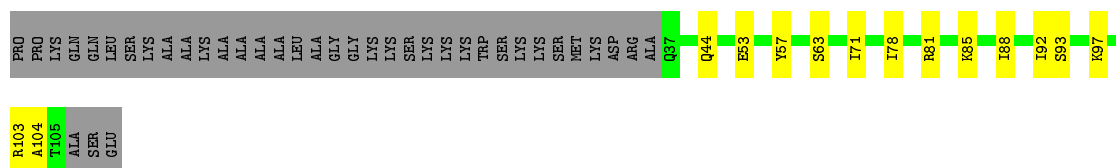
- Molecule 27: 40S ribosomal protein S25-A

Chain D5:  46% 17% 35%



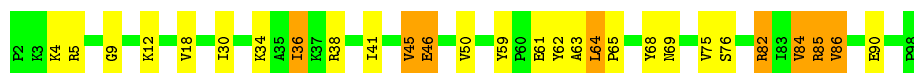
- Molecule 27: 40S ribosomal protein S25-A

Chain d5:  51% 13% 36%



- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 71% 21% 8%



- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 82% 16%



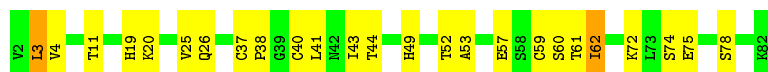
- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 78% 22%



- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 69% 28%



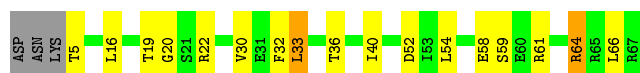
- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 77% 17% 5%




- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 70% 23% 5%



- Molecule 31: 40S ribosomal protein S29-A

Chain D9:  82% 13%




- Molecule 31: 40S ribosomal protein S29-A

Chain d9:  75% 22%



- Molecule 32: 40S ribosomal protein S30-A

Chain E0:  77% 20%



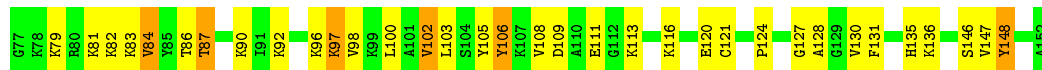
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:  53% 33% 8% 7%




- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:  55% 37% 8%




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

Chain SR:  85% 15%



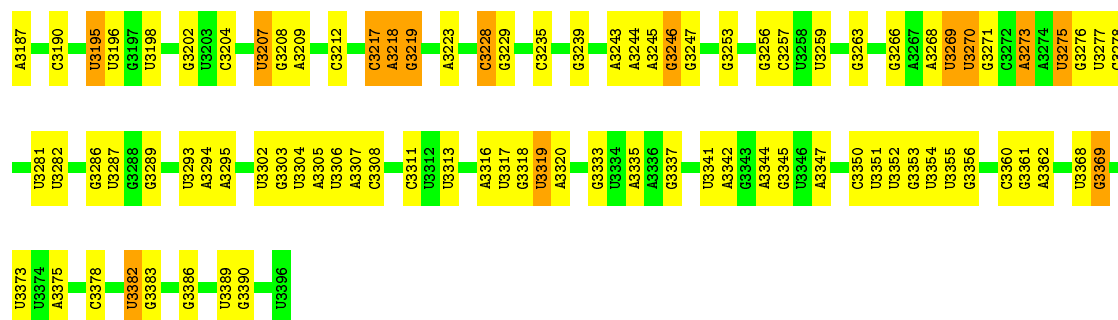
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:  87% 13%



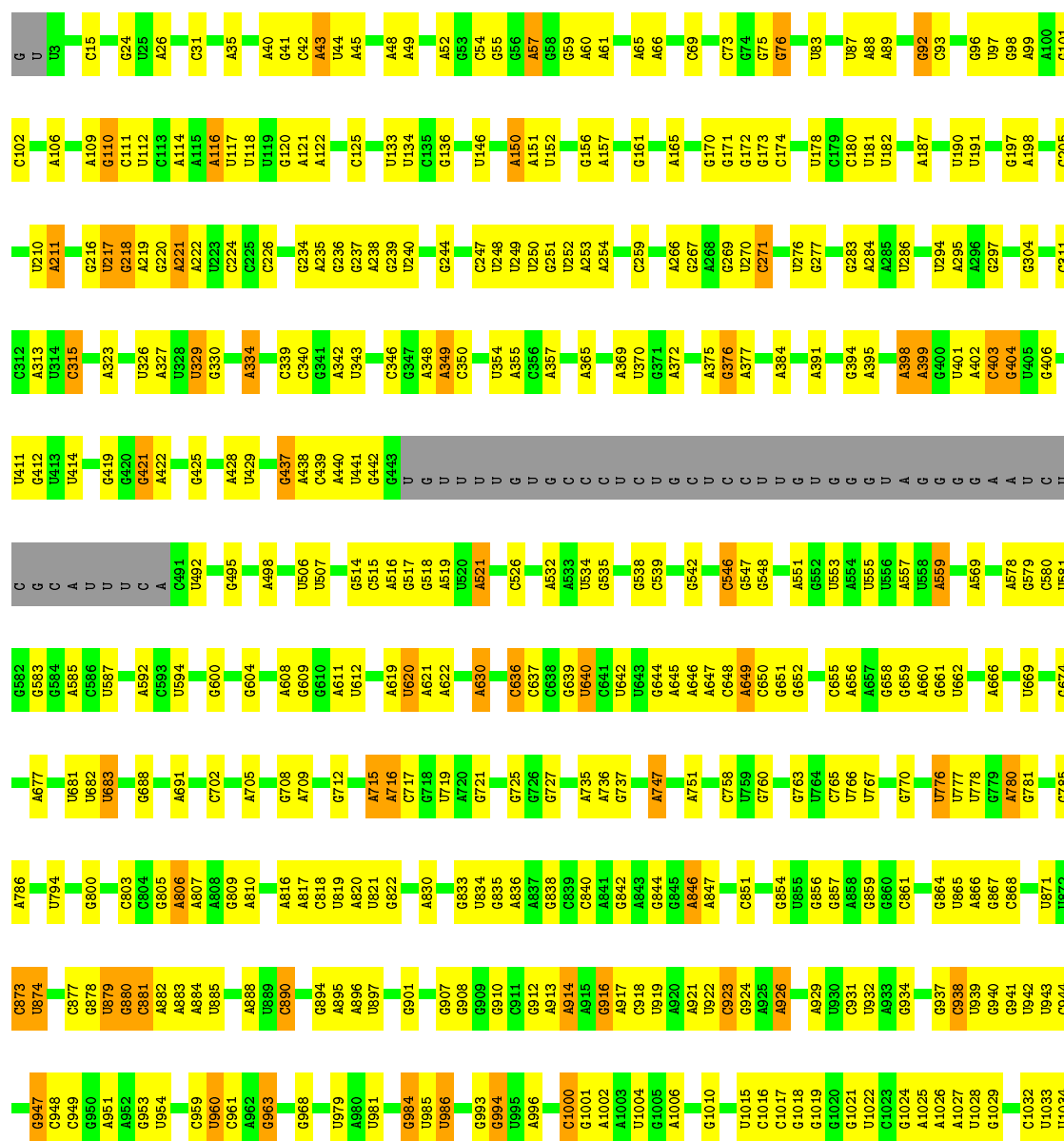
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U1724	U1569	G1476	A1381	C1298	U1211	G1131	U1211	U943	C868	U778	U681	G595	A498	A440
C1726	U1570	A1477	C1385	A1304	G1213	A1133	A1046	C945	G869	A780	U683	U601	C503	U
G1727	A1571	G1480	A1386	U1305	C1216	A1136	A1047	U946	U872	A784	G684	G604	G510	G
G1736	A1481	A1482	U1388	G1306	U1218	C1137	A1048	C947	C873	A785	A691	A608	G517	U
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C1581	U1486	G1486	A1399	G1313	G1226	U1144	C1068	A962	A888	U790	C700	G613	A522	U
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A1583	U1489	A1406	U1405	A1317	G1232	G1146	U1070	A965	C890	U794	G702	U620	G530	U
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A1589	U1495	U1496	U1415	C1327	U1235	G1149	G1077	C969	C894	C804	G708	G628	U541	C
G1592	C1496	U1496	G1416	C1328	G1236	U1151	U1078	A972	A895	A806	A709	A628	U541	U
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A1602	C1508	G1517	G1418	A1330	G1243	A1153	U1079	G974	A896	A808	A711	G633	C543	G
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G1838	G1561	G1561	A1453	U1367	A1271	A1190	G1115	U1009	G924	U850	C753	C655	C577	C
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A1841	U1564	U1564	U1456	G1370	A1274	A1193	G1118	G1017	C927	G853	U759	G661	G582	A
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								G1019	U932	G857	U764	U663	G584	U
								G1020	A933	A858	C765	C663	A585	C
								G1021	A933	A859	C766	C667	C586	A
								G1024	A936	G860	U767	C672	U587	C
								A1025	G937	C861	C768	A672	G588	U
								G1026	C938	G864	G770	G676	A589	G
								G1029	G940	U865		A677	A592	

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C	G	U	C	C	C	A	C	C	A	C	U	G	U	C	A	C	C	C	C	C	C	U	U	A	C	C	G	C	C	U	U	U	U	U	U	U	U	U	U	U	U	U	U	C											
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• Molecule 36: 25S ribosomal RNA

Chain 5: 54% 33% 6% 7%

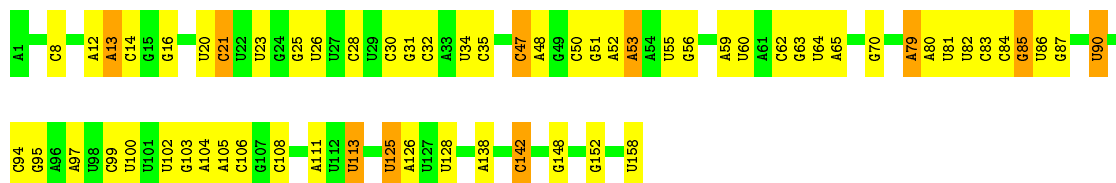


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A2373	A2296	G2206	A2113	A1895	G1796	G1639	G1536	U1442	U1353	A1244	A1154	A1048
G2374	U2297	G2207	G2114	A1896	A1797	G1640	G1537	G1443	G1354	G1245	C1155	C1049
G2375	U2298	A2207	G2115	G1897	U1641	U1641	A1539	U1444	G1355	G1246	G1156	G1050
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G2377	U2301	U2209	A2117	G1899	A1643	C1644	G1552	A1449	G1357	A1253	A1158	
	G2302	G2210	G2118	A1900	U1645	U1645	U1553	G1450	C1359	U1258	A1159	A1064
C2383	G2303	U2211		A1901	A1812	A1813	U1554	G1451	C1360	U1259	A1160	A1065
A2384	C2304	G2212	G2119	G1902	A1814	U1656	U1555	A1452	C1361	G1262	A1161	
G2385	G2305	A2213	A2120	U1903	U1815	A1657	C1556	A1453	G1362	G1263	A1162	G1072
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G2387	A2307	A2215	U2129	G1905	G1817	U1680	G1558	U1455	U1364	U1265	A1164	U1081
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			A2131	C1907		C1682	G1560	U1457	G1366		A1166	A1083
			G2132	U1908	U1821	C1683	G1561	A1458	G1367		A1167	U1084
			U2133	A1910	G1830	U1684	G1562	A1459	G1368		A1168	U1085
			G2134	G1911	U1831	U1685	U1563	A1460	G1369		A1169	U1086
			U2135	C1912	U1832	U1686	U1564	A1461	U1370		A1170	G1087
			G2136	G1913	G1833	U1687	U1565	A1462	G1371		A1171	A1088
			U2137	C1914	U1834	U1688	U1566	A1463	C1372		A1172	A1089
			A2138	U1915	U1835	U1689	U1567	A1464	G1373		A1173	A1090
			A2139	G1916	U1836	U1690	U1568	A1465	G1374		A1174	U1091
				U1917	U1837	U1691	U1569	A1466	G1375		A1175	U1092
				G1918	G1838	U1702	U1570	A1467	A1180		A1176	A1102
				U1919	U1839	U1703	U1571	A1468	U1181		A1177	A1103
				A1920	U1840	A1704	U1572	A1469	A1182		A1178	U1094
				U1921	A1841	U1705	U1573	A1470			A1179	U1095
				G1922	A1842	G1713	U1574	A1471	G1186		A1180	U1096
				U1923	G1843	U1714	U1575	A1472	G1187		A1181	G1097
				A1924	U1844	G1715	U1576	A1473	C1189		A1182	A1098
				G1925	U1845	U1716	U1577	A1474	A1183		A1183	U1099
				U1926	A1846	U1717	U1578	A1475	U1184		A1184	U1100
				G1927	U1847	G1718	U1579	A1476	C1185		A1185	U1101
				U1928	U1848	G1719	U1580	A1477	A1186		A1186	A1102
				A1929	G1849	U1720	U1581	A1478	A1187		A1187	A1103
				U1930	U1850	C1725	U1582	A1479	A1188		A1188	G1104
				U1931	G1851	G1726	U1583	U1480	A1189		A1189	U1105
				G1932	U1852	U1727	U1584	U1481	C1190		A1190	U1106
				U1933	U1853	G1728	U1585	U1482	A1191		A1191	U1107
				G1934	U1854	U1729	U1586	U1483	A1192		A1192	A1108
				U1935	U1855	G1730	U1587	U1484	A1193		A1193	A1109
				G1936	U1856	U1731	U1588	U1485	A1194		A1194	U1110
				U1937	U1857	G1732	U1589	U1486	A1195		A1195	U1111
				G1938	U1858	U1733	U1590	U1487	A1196		A1196	U1112
				U1939	U1859	G1734	U1591	U1488	A1197		A1197	U1113
				G1940	U1860	U1735	U1592	U1489	A1198		A1198	U1114
				U1941	G1861	G1736	U1593	U1490	A1199		A1199	U1115
				G1942	U1862	U1737	U1594	U1491	A1200		A1200	G1116
				U1943	U1863	G1738	U1595	U1492	A1201		A1201	G1117
				G1944	U1864	U1739	U1596	U1493	A1202		A1202	
				U1945	U1865	G1740	U1597	U1494	A1203		A1203	
				G1946	U1866	U1741	U1598	U1495	A1204		A1204	
				U1947	U1867	G1742	U1599	U1496	A1205		A1205	
				G1948	U1868	U1743	U1600	U1497	A1206		A1206	
				U1949	U1869	G1744	U1601	U1498	A1207		A1207	
				G1950	U1870	U1745	U1602	U1499	A1208		A1208	
				U1951	U1871	G1746	U1603	U1500	A1209		A1209	
				G1952	U1872	U1747	U1604	U1501	A1210		A1210	
				U1953	U1873	G1748	U1605	U1502	A1211		A1211	
				G1954	U1874	U1749	U1606	U1503	A1212		A1212	
				U1955	U1875	A1750	U1607	U1504	A1213		A1213	
				G1956	U1876	G1751	U1608	U1505	A1214		A1214	
				U1957	U1877	U1752	U1609	U1506	A1215		A1215	
				G1958	U1878	G1753	U1610	U1507	A1216		A1216	
				U1959	U1879	U1754	U1611	U1508	A1217		A1217	
				G1960	U1880	G1755	U1612	U1509	A1218		A1218	
				U1961	U1881	U1756	U1613	U1510	A1219		A1219	
				G1962	U1882	G1757	U1614	U1511	A1220		A1220	
				U1963	U1883	U1758	U1615	U1512	A1221		A1221	
				G1964	U1884	G1759	U1616	U1513	A1222		A1222	
				U1965	U1885	U1760	U1617	U1514	A1223		A1223	
				G1966	U1886	G1761	U1618	U1515	A1224		A1224	
				U1967	U1887	U1762	U1619	U1516	A1225		A1225	
				G1968	U1888	G1763	U1620	U1517	A1226		A1226	
				U1969	U1889	U1764	U1621	U1518	A1227		A1227	
				G1969	U1890	G1765	U1622	U1519	A1228		A1228	
				U1970	U1891	U1766	U1623	U1520	A1229		A1229	
				G1971	U1892	G1767	U1624	U1521	A1230		A1230	
				U1972	U1893	U1768	U1625	U1522	A1231		A1231	
				G1972	U1894	G1769	U1626	U1523	A1232		A1232	
				U1973	U1895	U1770	U1627	U1524	A1233		A1233	
				G1973	U1896	G1771	U1628	U1525	A1234		A1234	
				U1974	U1897	U1772	U1629	U1526	A1235		A1235	
				G1974	U1898	G1773	U1630	U1527	A1236		A1236	
				U1975	U1899	U1774	U1631	U1528	A1237		A1237	
				G1975	U1900	G1775	U1632	U1529	A1238		A1238	
				U1976	U1901	U1776	U1633	U1530	A1239		A1239	
				G1976	U1902	G1777	U1634	U1531	A1240		A1240	
				U1977	U1903	U1778	U1635	U1532	A1241		A1241	
				G1977	U1904	G1779	U1636	U1533	A1242		A1242	
				U1978	U1905	U1780	U1637	U1534	A1243		A1243	
				G1978	U1906	G1781	U1638	U1535	A1244		A1244	
				U1979	U1907	U1782	U1639	U1536	A1245		A1245	
				G1979	U1908	G1783	U1640	U1537	A1246		A1246	
				U1980	U1909	U1784	U1641	U1538	A1247		A1247	
				G1980	U1910	G1785	U1642	U1539	A1248		A1248	
				U1981	U1911	U1786	U1643	U1540	A1249		A1249	
				G1981	U1912	G1787	U1644	U1541	A1250		A1250	
				U1982	U1913	U1788	U1645	U1542	A1251		A1251	
				G1982	U1914	G1789	U1646	U1543	A1252		A1252	
				U1983	U1915	U1790	U1647	U1544	A1253		A1253	
				G1983	U1916	G1791	U1648	U1545	A1254		A1254	
				U1984	U1917	U1792	U1649	U1546	A1255		A1255	
				G1984	U1918	G1793	U1650	U1547	A1256		A1256	
				U1985	U1919	U1794	U1651	U1548	A1257		A1257	
				G1985	U1920	G1795	U1652	U1549	A1258		A1258	
				U1986	U1921	U1796	U1653	U1550	A1259		A1259	
				G1986	U1922	G1797	U1654	U1551	A1260		A1260	
				U1987	U1923	U1798	U1655	U1552	A1261		A1261	
				G1987	U1924	G1799	U1656	U1553	A1262		A1262	
				U1988	U1925	U1800	U1657	U1554	A1263		A1263	
				G1988	U1926	G1801	U1658	U1555	A1264		A1264	
				U1989	U1927	U1802	U1659	U1556	A1265		A1265	
				G1989	U1928	G1803	U1660	U1557	A1266		A1266	
				U1990	U1929	U1804	U1661	U1558	A1267		A1267	
				G1990	U1930	G1805	U1662	U1559	A1268		A1268	
				U1991	U1931	U1806	U1663	U1560	A1269		A1269	
				G1991	U1932	G1807	U1664	U1561	A1270		A1270	
				U1992	U1933	U1808	U1665	U1562	A1271		A1271	
				G1992	U1934	G1809	U1666	U1563	A1272		A1272	
				U1993	U1935	U1810	U1667	U1564	A1273		A1273	
				G1993	U1936	G1811	U1668	U1565	A1274			



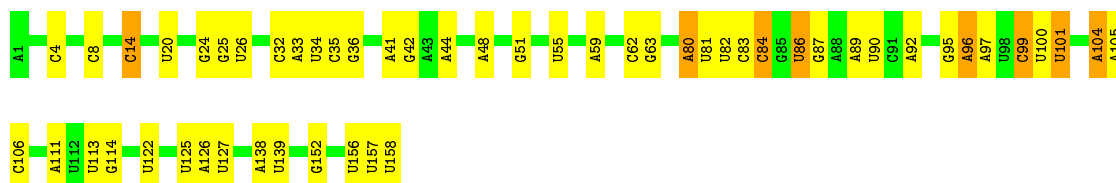
- Molecule 38: 5.8S ribosomal RNA

Chain 4: 61% 33% 6%



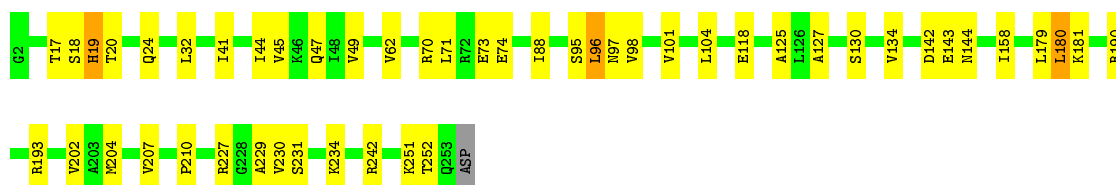
- Molecule 38: 5.8S ribosomal RNA

Chain 8: 66% 28% 5%



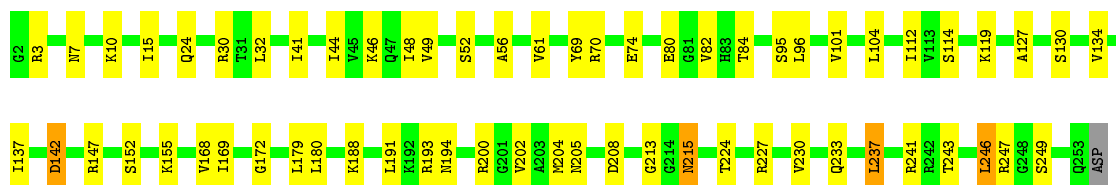
- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 80% 18%



- Molecule 39: 60S ribosomal protein L2-A

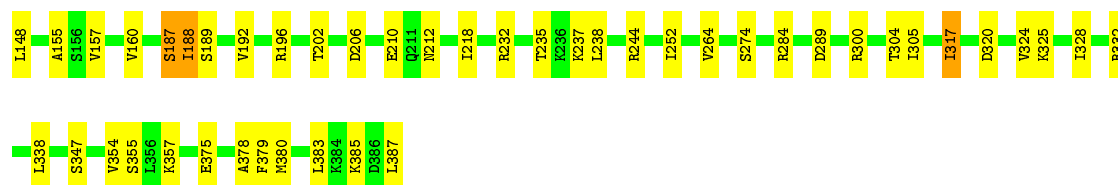
Chain L2: 75% 23%



- Molecule 40: 60S ribosomal protein L3

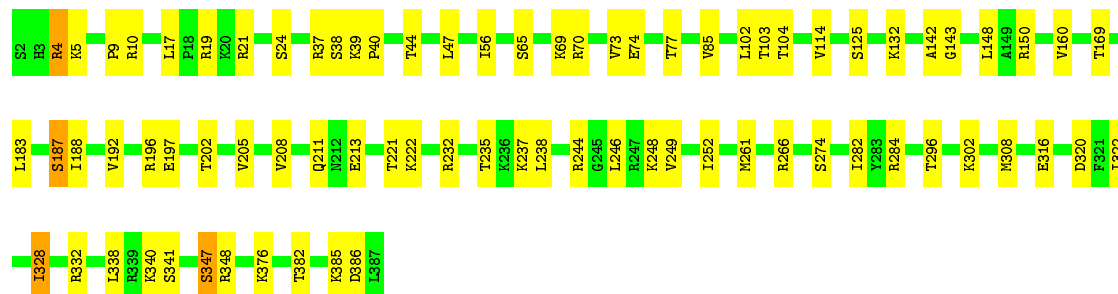
Chain L3: 79% 20%





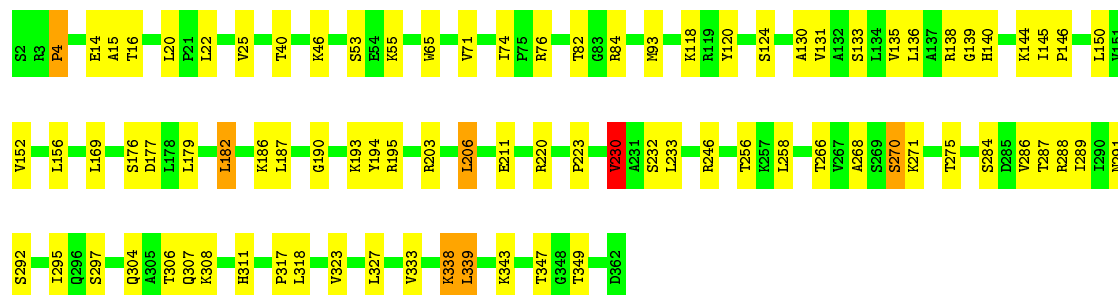
- Molecule 40: 60S ribosomal protein L3

Chain L3: 80% 19%



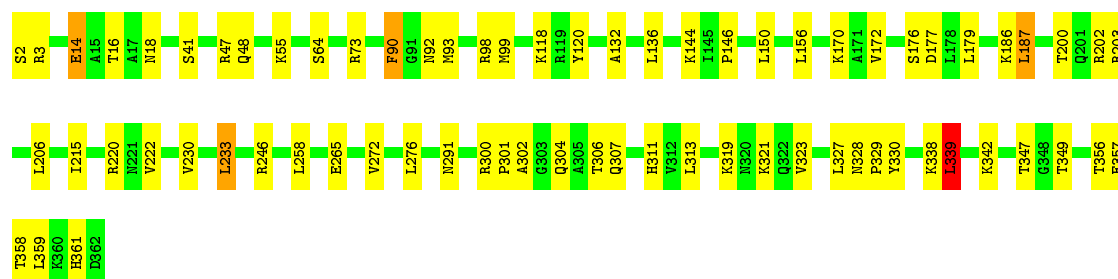
- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 76% 22%



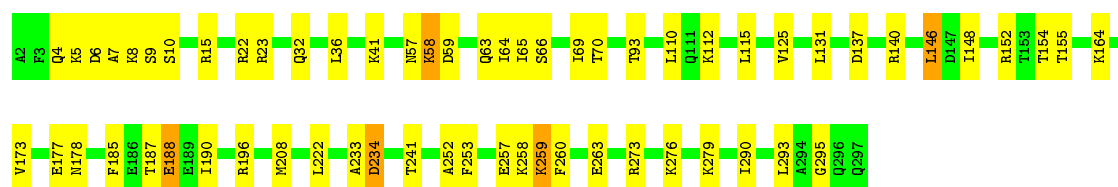
- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 80% 18%

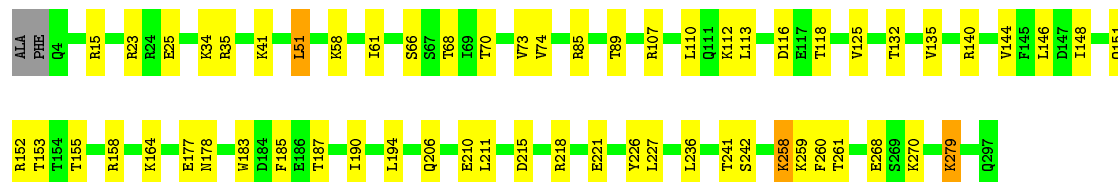
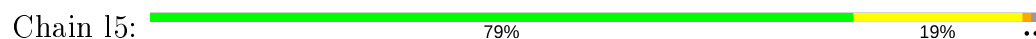


- Molecule 42: 60S ribosomal protein L5

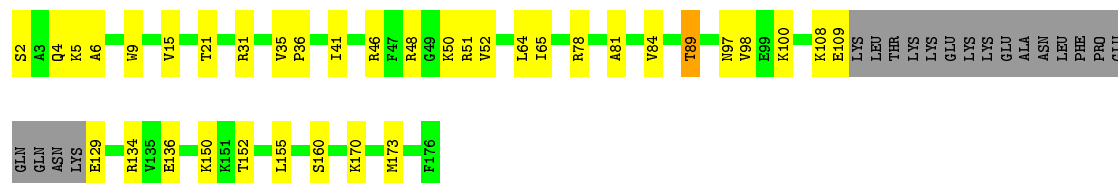
Chain L5: 79% 19%



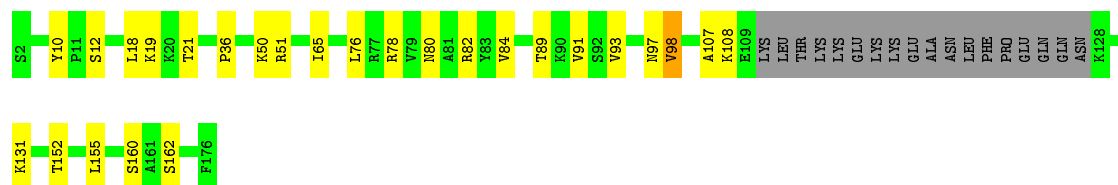
- Molecule 42: 60S ribosomal protein L5



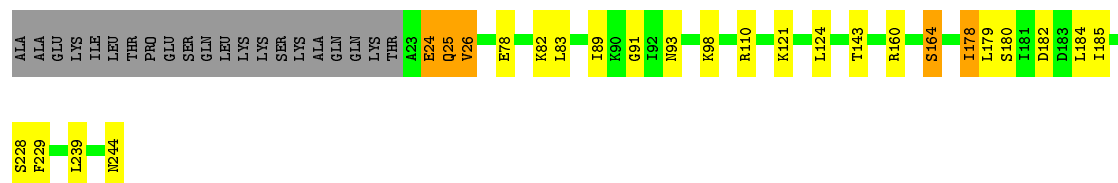
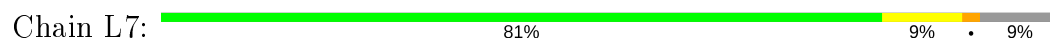
- Molecule 43: 60S ribosomal protein L6-A



- Molecule 43: 60S ribosomal protein L6-A

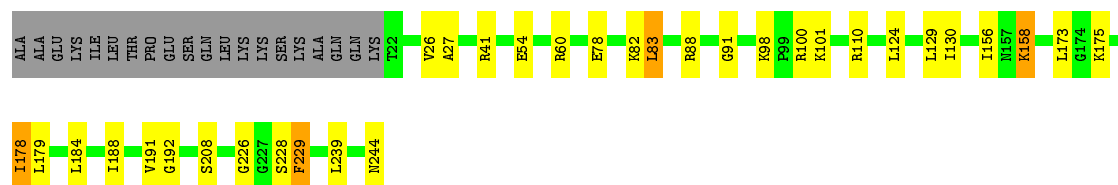


- Molecule 44: 60S ribosomal protein L7-A



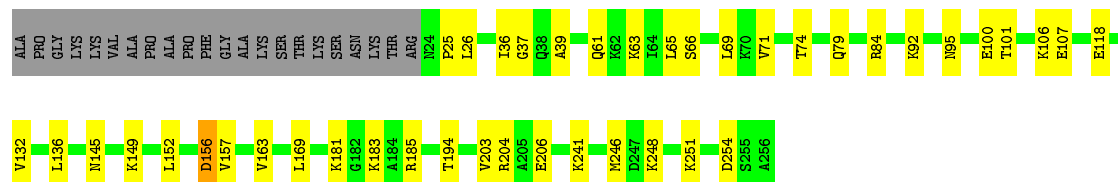
- Molecule 44: 60S ribosomal protein L7-A





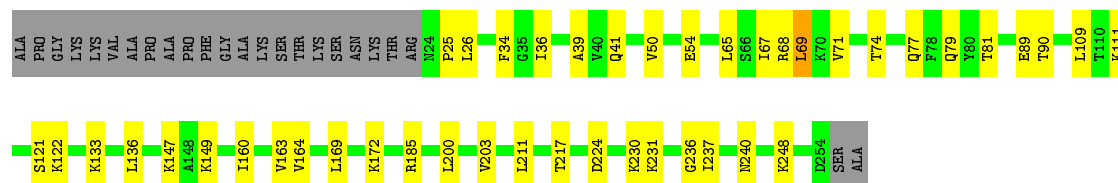
- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 75% 16% 9%



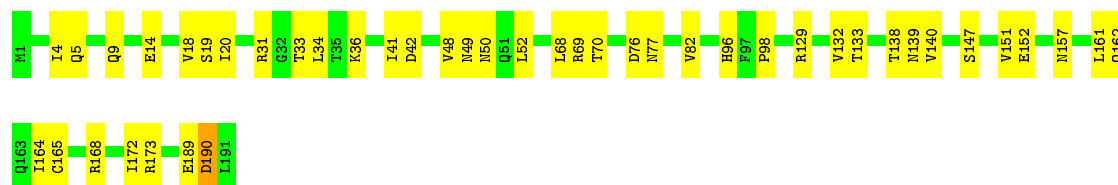
- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 73% 17% 9%



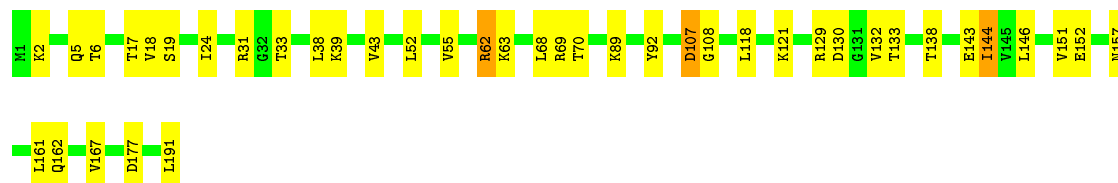
- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 77% 23%



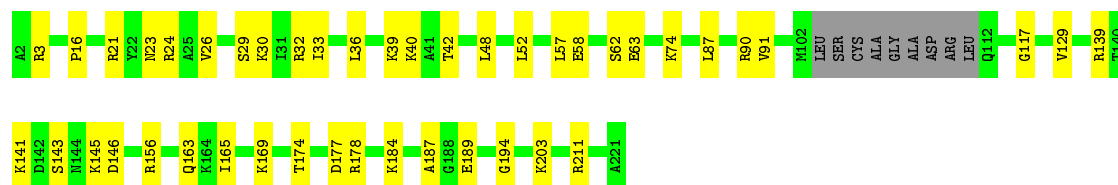
- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 79% 20%



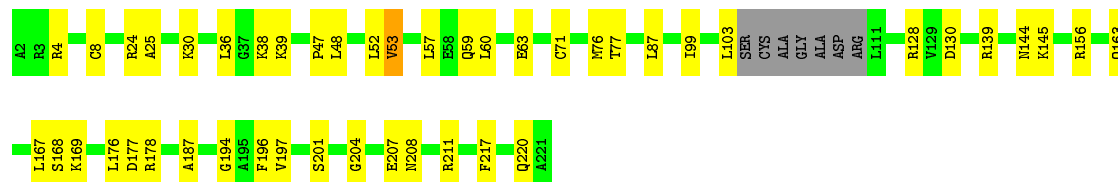
- Molecule 47: 60S ribosomal protein L10

Chain M0: 76% 20%



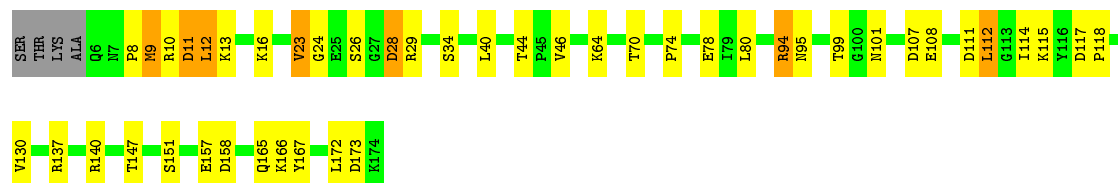
- Molecule 47: 60S ribosomal protein L10

Chain m0: 76% 20% •



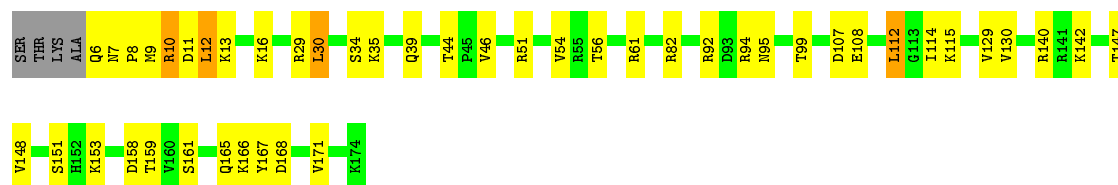
- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 72% 22% • •



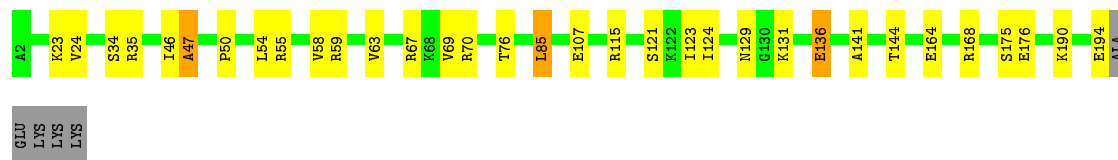
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 71% 24% • •



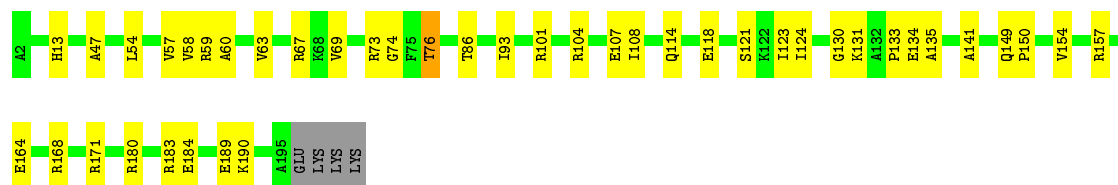
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 81% 15% • •



- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 77% 21% • •



- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 80% 19% .



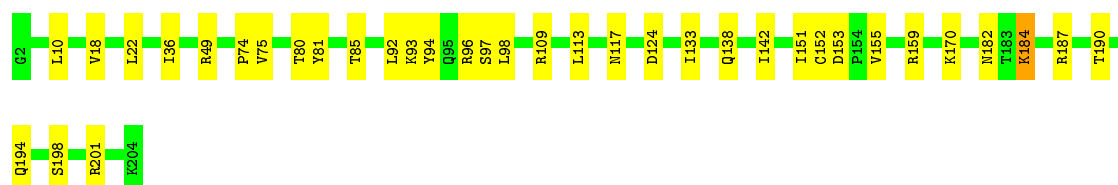
- Molecule 50: 60S ribosomal protein L14-A

Chain m4: 85% 13% .



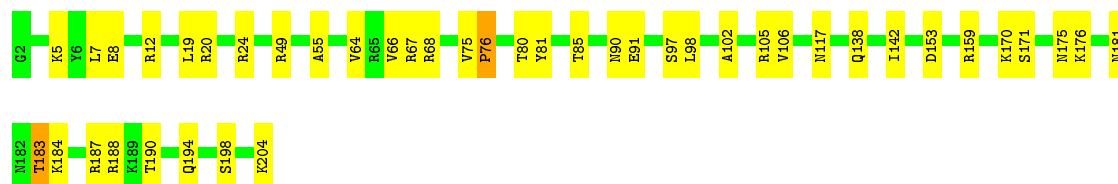
- Molecule 51: 60S ribosomal protein L15-A

Chain M5: 82% 17%



- Molecule 51: 60S ribosomal protein L15-A

Chain m5: 79% 20% .




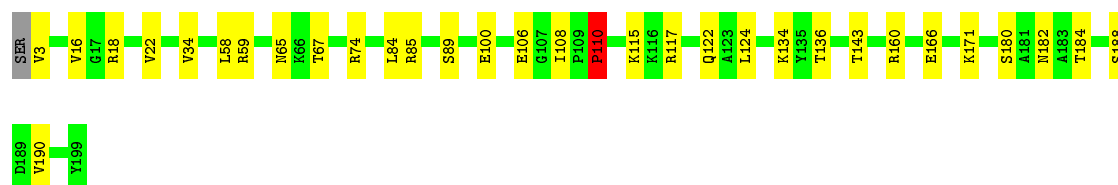
- Molecule 52: 60S ribosomal protein L16-A

Chain M6: 89% 9% ...




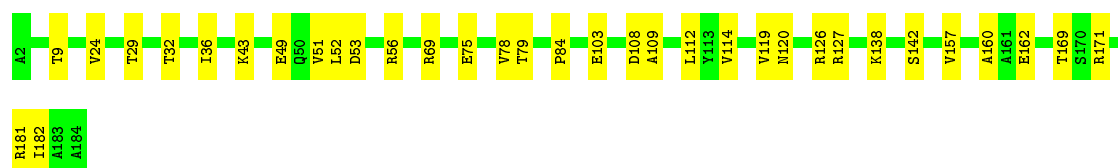
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:  83% 16% ..



- Molecule 53: 60S ribosomal protein L17-A

Chain M7:  81% 19%




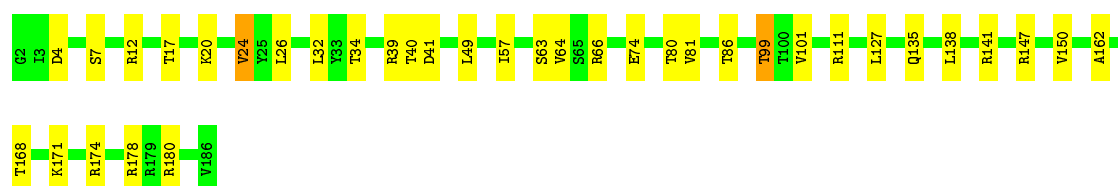
- Molecule 53: 60S ribosomal protein L17-A

Chain m7:  72% 13% 15%




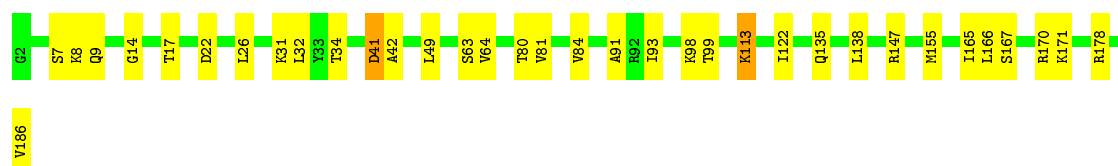
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:  81% 18%




- Molecule 54: 60S ribosomal protein L18-A

Chain m8:  81% 18%




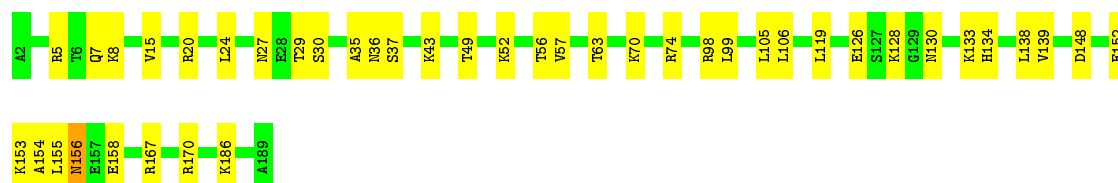
- Molecule 55: 60S ribosomal protein L19-A

Chain M9:  89% 11%




- Molecule 55: 60S ribosomal protein L19-A

Chain m9:  78% 22%




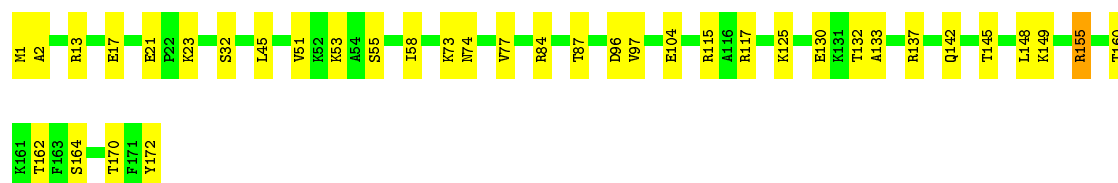
- Molecule 56: 60S ribosomal protein L20-A

Chain N0:  80% 20%




- Molecule 56: 60S ribosomal protein L20-A

Chain n0:  78% 21%




- Molecule 57: 60S ribosomal protein L21-A

Chain N1:  81% 18%



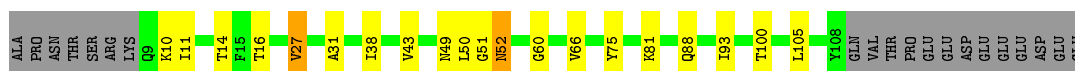
- Molecule 57: 60S ribosomal protein L21-A

Chain n1:  82% 17%

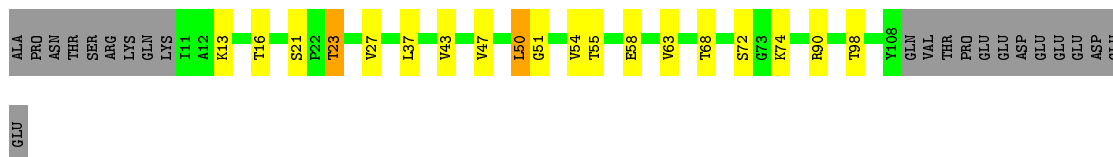


- Molecule 58: 60S ribosomal protein L22-A

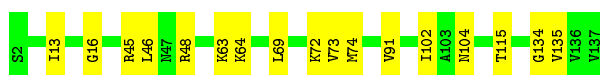
Chain N2:  67% 15% 17%



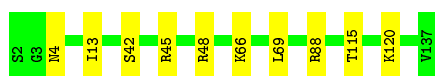
- Molecule 58: 60S ribosomal protein L22-A



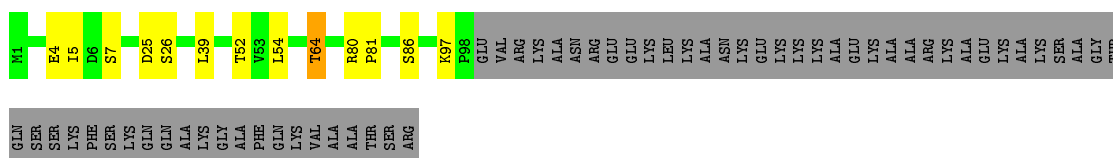
- Molecule 59: 60S ribosomal protein L23-A



- Molecule 59: 60S ribosomal protein L23-A



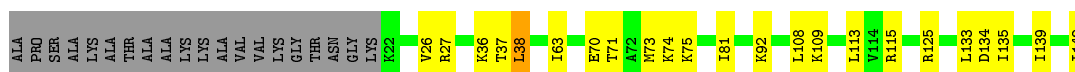
- Molecule 60: 60S ribosomal protein L24-A



- Molecule 60: 60S ribosomal protein L24-A

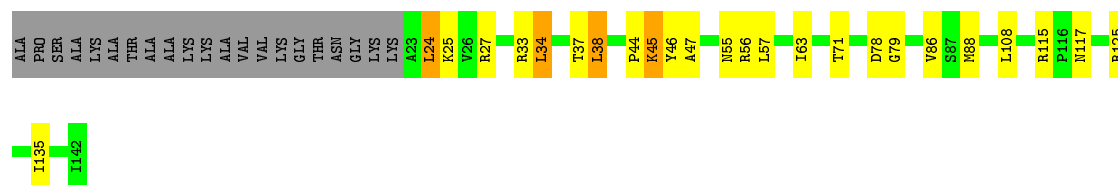


- Molecule 61: 60S ribosomal protein L25




- Molecule 61: 60S ribosomal protein L25

Chain n5:  67% 15% • 15%



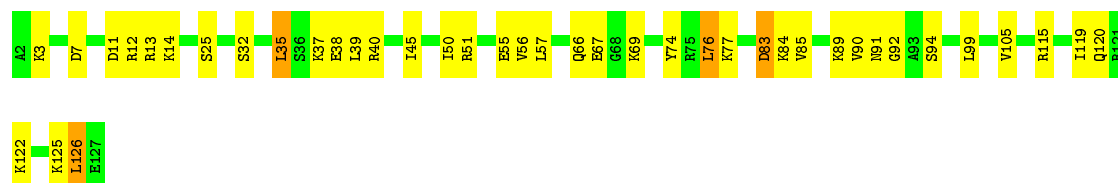
- Molecule 62: 60S ribosomal protein L26-A

Chain N6:  79% 20%




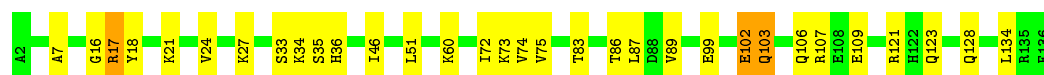
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:  67% 29% .



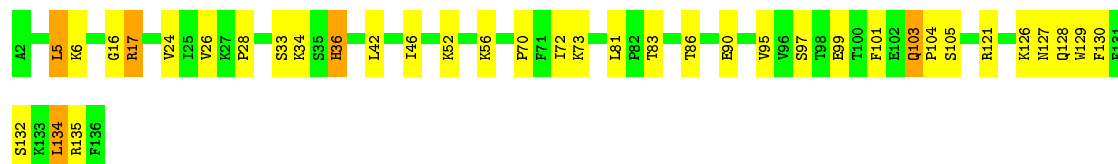
- Molecule 63: 60S ribosomal protein L27-A

Chain N7:  76% 21%




- Molecule 63: 60S ribosomal protein L27-A

Chain n7:  73% 24% .

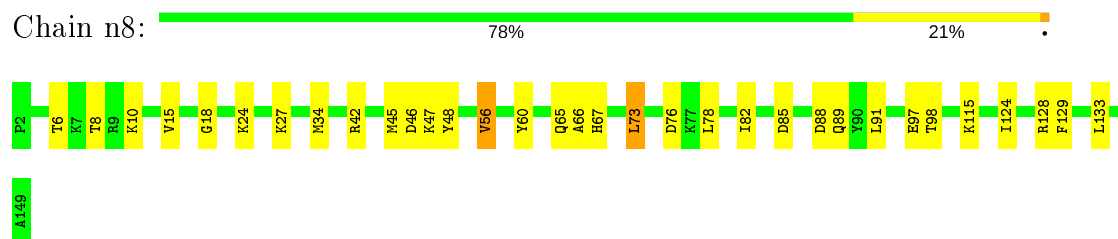


- Molecule 64: 60S ribosomal protein L28

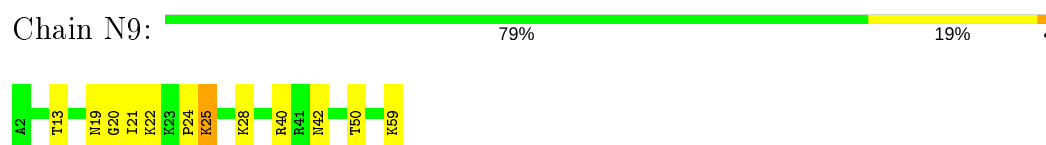
Chain N8:  82% 17%



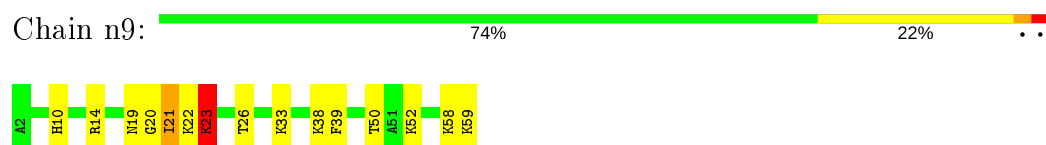
- Molecule 64: 60S ribosomal protein L28



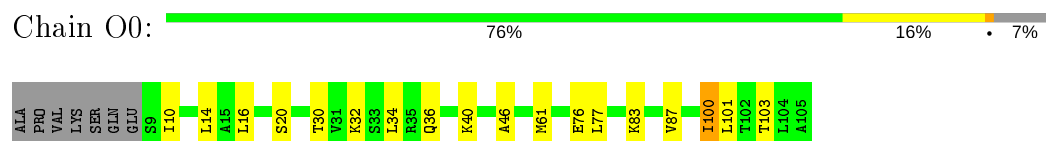
- Molecule 65: 60S ribosomal protein L29



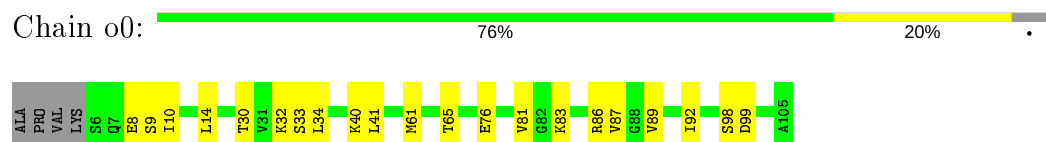
- Molecule 65: 60S ribosomal protein L29



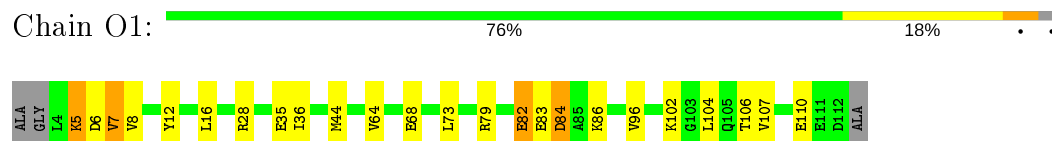
- Molecule 66: 60S ribosomal protein L30



- Molecule 66: 60S ribosomal protein L30

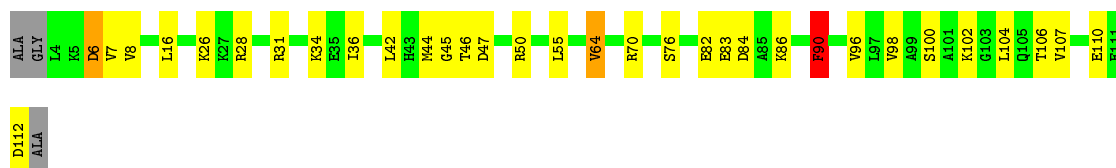


- Molecule 67: 60S ribosomal protein L31-A



- Molecule 67: 60S ribosomal protein L31-A





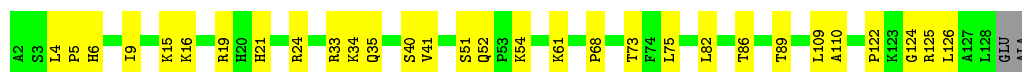
- Molecule 68: 60S ribosomal protein L32

Chain O2: 84% 15%



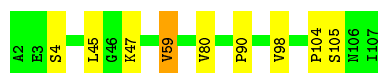
- Molecule 68: 60S ribosomal protein L32

Chain o2: 75% 23%



- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 92% 8%



- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 80% 18%



- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 78% 14% 7%




- Molecule 70: 60S ribosomal protein L34-A

Chain o4: 76% 18% 7%




- Molecule 71: 60S ribosomal protein L35-A

Chain O5:  77% 22%



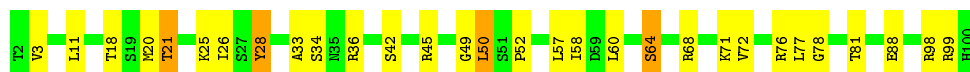
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:  79% 21%



- Molecule 72: 60S ribosomal protein L36-A

Chain O6:  70% 26%




- Molecule 72: 60S ribosomal protein L36-A

Chain o6:  70% 28%




- Molecule 73: 60S ribosomal protein L37-A

Chain O7:  79% 21%



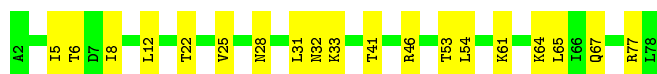
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:  85% 14%



- Molecule 74: 60S ribosomal protein L38

Chain O8:  75% 25%



- Molecule 74: 60S ribosomal protein L38

Chain o8:  70% 30%




- Molecule 75: 60S ribosomal protein L39

Chain O9:  88% 12%




- Molecule 75: 60S ribosomal protein L39

Chain o9:  82% 18%




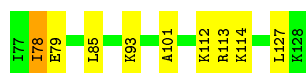
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:  83% 15% .



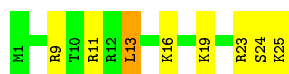
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  83% 15% .



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  68% 28% .




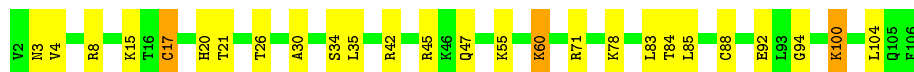
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  68% 32%




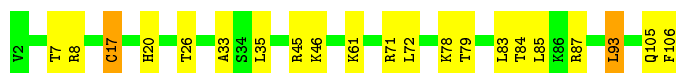
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  75% 22%



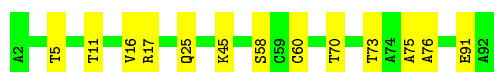
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  80% 18%




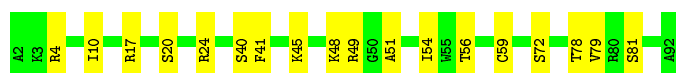
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  86% 14%



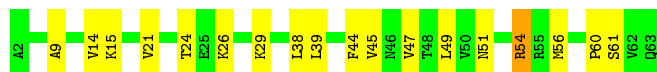
- Molecule 79: 60S ribosomal protein L43-A

Chain q3:  80% 20%




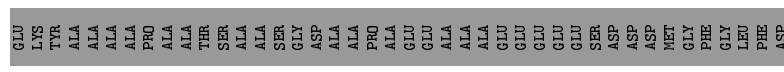
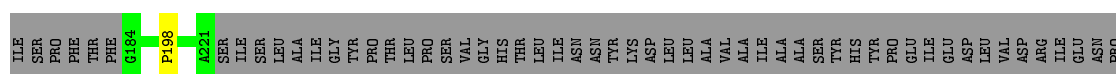
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:  71% 27%



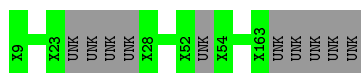
- Molecule 81: 60S acidic ribosomal protein P0

Chain p0:  37% 9% 54%



- Molecule 82: unknown protein chain m2

Chain m2:  94% 6%



- Molecule 83: unknown protein chain p1

Chain p1:  100%

There are no outlier residues recorded for this chain.

- Molecule 84: unknown protein chain p2

Chain p2:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.64Å 287.69Å 304.39Å 90.00° 98.98° 90.00°	Depositor
Resolution (Å)	300.66 – 3.10	Depositor
% Data completeness (in resolution range)	98.7 (300.66-3.10)	Depositor
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.198 , 0.247	Depositor
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.204	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411881	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% 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, ZBA

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	0.68	3/42442 (0.0%)	1.27	308/66130 (0.5%)
1	6	0.78	10/42765 (0.0%)	1.34	367/66634 (0.6%)
2	S0	0.43	0/1617	0.65	0/2215
2	s0	0.49	0/1623	0.71	0/2222
3	S1	0.38	0/1735	0.65	1/2335 (0.0%)
3	s1	0.49	0/1748	0.69	0/2352
4	S2	0.48	0/1665	0.68	0/2263
4	s2	0.51	0/1665	0.73	1/2263 (0.0%)
5	S3	0.45	0/1759	0.64	0/2368
5	s3	0.47	0/1759	0.62	0/2368
6	S4	0.47	0/2109	0.69	1/2839 (0.0%)
6	s4	0.50	0/2109	0.71	1/2839 (0.0%)
7	S5	0.40	0/1629	0.61	0/2202
7	s5	0.45	0/1629	0.65	0/2202
8	S6	0.45	0/1823	0.64	1/2439 (0.0%)
8	s6	0.49	0/1779	0.68	0/2379
9	S7	0.39	0/1506	0.64	0/2028
9	s7	0.45	0/1516	0.71	2/2043 (0.1%)
10	S8	0.52	0/1514	0.70	1/2021 (0.0%)
10	s8	0.56	0/1514	0.76	2/2021 (0.1%)
11	S9	0.44	0/1519	0.64	0/2035
11	s9	0.53	0/1519	0.74	0/2035
12	C0	0.45	0/790	0.73	3/1069 (0.3%)
12	c0	0.39	0/777	0.65	3/1049 (0.3%)
13	C1	0.52	0/1240	0.68	0/1675
13	c1	0.57	0/1194	0.75	2/1610 (0.1%)
14	C2	0.37	0/900	0.66	1/1224 (0.1%)
14	c2	0.30	0/900	0.61	1/1224 (0.1%)
15	C3	0.48	0/1215	0.68	2/1638 (0.1%)
15	c3	0.57	0/1215	0.73	0/1638
16	C4	0.37	0/901	0.66	0/1217
16	c4	0.47	0/960	0.73	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.47	0/998	0.69	0/1341
17	c5	0.45	0/1060	0.68	1/1426 (0.1%)
18	C6	0.46	0/1125	0.72	3/1510 (0.2%)
18	c6	0.49	0/1131	0.70	0/1518
19	C7	0.45	0/935	0.66	0/1254
19	c7	0.47	0/914	0.67	0/1224
20	C8	0.47	0/1211	0.64	0/1628
20	c8	0.51	0/1211	0.69	1/1628 (0.1%)
21	C9	0.45	0/1130	0.62	0/1517
21	c9	0.49	0/1130	0.67	1/1517 (0.1%)
22	D0	0.41	0/865	0.67	0/1169
22	d0	0.44	0/892	0.66	0/1205
23	D1	0.45	0/693	0.65	0/935
23	d1	0.53	0/693	0.73	0/935
24	D2	0.49	0/1038	0.72	2/1395 (0.1%)
24	d2	0.58	0/1038	0.74	0/1395
25	D3	0.61	0/1139	0.77	1/1518 (0.1%)
25	d3	0.63	0/1139	0.77	1/1518 (0.1%)
26	D4	0.43	0/1087	0.61	0/1449
26	d4	0.47	0/1087	0.68	0/1449
27	D5	0.40	0/571	0.72	0/768
27	d5	0.40	0/566	0.65	0/761
28	D6	0.44	0/782	0.66	0/1047
28	d6	0.56	0/782	0.69	0/1047
29	D7	0.43	0/620	0.65	0/838
29	d7	0.49	0/620	0.70	0/838
30	D8	0.37	0/499	0.58	0/670
30	d8	0.42	0/499	0.65	0/670
31	D9	0.55	0/452	0.69	1/600 (0.2%)
31	d9	0.54	0/452	0.75	0/600
32	E0	0.43	0/483	0.61	0/643
33	E1	0.43	0/577	0.78	0/770
33	e1	0.42	0/619	0.75	0/822
34	SR	0.39	0/2494	0.59	0/3393
34	sR	0.39	0/2495	0.58	0/3395
35	SM	0.47	0/1113	0.68	2/1502 (0.1%)
35	sM	0.47	0/683	0.66	1/923 (0.1%)
36	1	1.00	50/75394 (0.1%)	1.56	1409/117545 (1.2%)
36	5	1.02	57/75414 (0.1%)	1.57	1376/117575 (1.2%)
37	3	0.82	0/2883	1.31	19/4491 (0.4%)
37	7	0.99	2/2883 (0.1%)	1.51	45/4491 (1.0%)
38	4	0.94	1/3746 (0.0%)	1.48	50/5832 (0.9%)
38	8	0.90	0/3746	1.44	40/5832 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.64	0/1948	0.85	1/2617 (0.0%)
39	l2	0.70	0/1946	0.88	4/2614 (0.2%)
40	L3	0.69	0/3146	0.81	0/4228
40	l3	0.76	0/3146	0.83	2/4228 (0.0%)
41	L4	0.73	1/2800 (0.0%)	0.88	8/3790 (0.2%)
41	l4	0.68	0/2800	0.81	2/3790 (0.1%)
42	L5	0.53	0/2425	0.66	1/3271 (0.0%)
42	l5	0.67	0/2408	0.75	1/3248 (0.0%)
43	L6	0.68	0/1260	0.79	0/1694
43	l6	0.70	0/1269	0.80	0/1705
44	L7	0.73	0/1821	0.84	0/2451
44	l7	0.77	0/1828	0.84	3/2461 (0.1%)
45	L8	0.51	0/1836	0.65	0/2481
45	l8	0.52	0/1795	0.67	2/2429 (0.1%)
46	L9	0.61	1/1539 (0.1%)	0.75	0/2073
46	l9	0.66	0/1539	0.77	0/2073
47	M0	0.63	0/1741	0.75	0/2335
47	m0	0.67	1/1758 (0.1%)	0.75	0/2358
48	M1	0.51	0/1374	0.72	1/1842 (0.1%)
48	m1	0.62	0/1374	0.80	3/1842 (0.2%)
49	M3	0.71	0/1568	0.81	2/2106 (0.1%)
49	m3	0.60	0/1573	0.82	0/2113
50	M4	0.68	0/1068	0.78	0/1438
50	m4	0.71	0/1074	0.79	2/1446 (0.1%)
51	M5	0.71	1/1757 (0.1%)	0.76	1/2354 (0.0%)
51	m5	0.63	0/1757	0.76	0/2354
52	M6	0.43	0/1585	0.60	1/2128 (0.0%)
52	m6	0.50	0/1585	0.64	0/2128
53	M7	0.72	0/1443	0.82	0/1944
53	m7	0.85	0/1250	0.86	1/1683 (0.1%)
54	M8	0.69	0/1465	0.86	2/1965 (0.1%)
54	m8	0.66	0/1465	0.86	0/1965
55	M9	0.58	0/1538	0.69	0/2050
55	m9	0.60	0/1538	0.71	0/2050
56	N0	0.69	0/1481	0.79	0/1990
56	n0	0.75	0/1481	0.85	1/1990 (0.1%)
57	N1	0.66	0/1300	0.75	0/1743
57	n1	0.78	2/1300 (0.2%)	0.80	0/1743
58	N2	0.43	0/812	0.61	0/1099
58	n2	0.46	0/794	0.65	0/1076
59	N3	0.68	0/1018	0.77	0/1369
59	n3	0.77	0/1018	0.82	0/1369
60	N4	0.51	0/712	0.67	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.61	0/1052	0.73	0/1398
61	N5	0.57	0/979	0.72	1/1321 (0.1%)
61	n5	0.57	0/974	0.74	1/1314 (0.1%)
62	N6	0.64	0/1004	0.83	2/1341 (0.1%)
62	n6	0.60	0/1004	0.80	2/1341 (0.1%)
63	N7	0.49	0/1118	0.68	0/1497
63	n7	0.47	0/1118	0.65	0/1497
64	N8	0.68	0/1204	0.81	1/1612 (0.1%)
64	n8	0.72	0/1204	0.85	1/1612 (0.1%)
65	N9	0.63	0/473	0.75	0/629
65	n9	0.70	0/473	0.90	2/629 (0.3%)
66	O0	0.50	0/751	0.65	0/1008
66	o0	0.52	0/775	0.68	0/1040
67	O1	0.61	0/890	0.75	0/1196
67	o1	0.65	0/897	0.84	2/1205 (0.2%)
68	O2	0.78	0/1041	0.85	0/1394
68	o2	0.75	0/1041	0.84	0/1394
69	O3	0.86	0/868	0.84	0/1168
69	o3	0.85	0/868	0.82	0/1168
70	O4	0.58	1/890 (0.1%)	0.81	3/1189 (0.3%)
70	o4	0.55	0/890	0.74	0/1189
71	O5	0.63	0/978	0.76	0/1301
71	o5	0.52	0/974	0.67	0/1297
72	O6	0.60	0/778	0.75	0/1034
72	o6	0.55	0/777	0.73	0/1033
73	O7	0.70	0/696	0.91	3/923 (0.3%)
73	o7	0.70	0/696	0.85	1/923 (0.1%)
74	O8	0.49	0/618	0.59	0/826
74	o8	0.44	0/614	0.63	0/822
75	O9	0.70	0/443	0.82	0/588
75	o9	0.61	0/443	0.81	0/588
76	Q0	0.61	0/423	0.79	2/562 (0.4%)
76	q0	0.75	0/423	0.83	0/562
77	Q1	0.60	0/234	0.98	1/300 (0.3%)
77	q1	0.63	0/234	0.87	0/300
78	Q2	0.79	1/860 (0.1%)	0.86	2/1136 (0.2%)
78	q2	0.73	1/860 (0.1%)	0.81	2/1136 (0.2%)
79	Q3	0.65	0/701	0.80	1/934 (0.1%)
79	q3	0.68	0/701	0.83	1/934 (0.1%)
80	e0	0.43	0/499	0.72	0/665
81	p0	0.44	0/1091	0.57	0/1472
All	All	0.80	132/430817 (0.0%)	1.24	3717/632520 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	S5	0	1
7	s5	0	2
9	S7	0	1
16	C4	0	2
16	c4	0	1
17	C5	0	1
17	c5	0	1
19	C7	0	1
20	c8	0	1
22	d0	0	1
27	D5	0	3
33	E1	0	2
33	e1	0	1
39	L2	0	1
39	l2	0	1
42	L5	0	1
42	l5	0	1
43	L6	0	2
43	l6	0	1
44	l7	0	2
49	m3	0	1
52	M6	0	1
52	m6	0	1
54	m8	0	1
56	n0	0	2
57	N1	0	1
63	n7	0	1
64	n8	0	2
65	N9	0	2
65	n9	0	2
67	O1	0	1
67	o1	0	2
68	o2	0	1
All	All	0	45

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	11.18	2.01	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C8	9.45	1.44	1.37
36	5	1152	G	N9-C4	-9.34	1.30	1.38
78	q2	17	CYS	CB-SG	9.32	1.98	1.82
36	1	2714	G	N9-C4	-7.82	1.31	1.38
1	2	1749	A	N9-C4	-7.72	1.33	1.37
36	5	2401	A	N9-C4	7.67	1.42	1.37
36	1	2419	A	N9-C4	-7.14	1.33	1.37
36	5	960	U	N1-C2	7.12	1.45	1.38
36	1	2401	A	N7-C5	6.67	1.43	1.39
36	5	3008	A	N3-C4	-6.62	1.30	1.34
36	5	2138	A	N9-C4	-6.47	1.33	1.37
36	1	2401	A	C6-N1	6.44	1.40	1.35
57	n1	104	GLU	CB-CG	6.32	1.64	1.52
36	5	3209	A	C5-C4	6.31	1.43	1.38
36	5	2138	A	N3-C4	-6.26	1.31	1.34
36	1	2640	A	C6-N1	-6.20	1.31	1.35
36	1	39	A	C5-C6	-6.15	1.35	1.41
36	1	943	U	C2-N3	-6.13	1.33	1.37
36	5	3008	A	N9-C4	-6.07	1.34	1.37
36	1	2138	A	N3-C4	-6.02	1.31	1.34
36	5	2358	A	N9-C4	-6.01	1.34	1.37
36	5	1152	G	C8-N7	6.00	1.34	1.30
36	1	2384	A	C5-C6	-5.97	1.35	1.41
36	1	1116	G	N7-C5	-5.96	1.35	1.39
36	5	2375	G	C6-N1	-5.94	1.35	1.39
36	1	2983	C	N3-C4	-5.92	1.29	1.33
36	5	953	G	N7-C5	-5.92	1.35	1.39
37	7	92	A	C5-C6	-5.92	1.35	1.41
36	5	3032	A	N7-C5	-5.91	1.35	1.39
36	5	2954	U	N1-C2	5.86	1.43	1.38
36	1	651	G	N1-C2	-5.85	1.33	1.37
36	5	1199	C	N1-C6	-5.85	1.33	1.37
36	5	2704	A	N9-C4	-5.85	1.34	1.37
36	1	92	G	N1-C2	-5.81	1.33	1.37
36	1	2874	G	N3-C4	-5.80	1.31	1.35
36	5	2243	A	N3-C4	-5.79	1.31	1.34
36	5	2978	U	N1-C2	5.79	1.43	1.38
1	6	337	G	C2-N3	5.78	1.37	1.32
1	6	1537	C	N1-C6	5.78	1.40	1.37
36	5	953	G	C5-C4	-5.77	1.34	1.38
36	1	1304	A	N9-C4	-5.75	1.34	1.37
36	1	2188	A	N9-C4	-5.73	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2811	A	N7-C5	-5.73	1.35	1.39
36	1	639	G	C5-C6	-5.70	1.36	1.42
37	7	92	A	C5-C4	-5.69	1.34	1.38
47	m0	8	CYS	CB-SG	-5.69	1.72	1.81
36	5	2726	C	N3-C4	-5.63	1.30	1.33
36	1	655	C	N1-C6	-5.59	1.33	1.37
36	5	3209	A	N9-C4	5.59	1.41	1.37
36	1	338	A	N7-C5	-5.57	1.35	1.39
36	1	651	G	C6-N1	-5.56	1.35	1.39
36	5	2954	U	C2-N3	5.53	1.41	1.37
1	6	1653	C	N1-C6	-5.53	1.33	1.37
1	6	1030	A	N9-C4	-5.53	1.34	1.37
36	5	2385	G	N9-C4	-5.52	1.33	1.38
36	1	2409	G	N7-C5	-5.51	1.35	1.39
70	O4	47	CYS	CB-SG	-5.51	1.72	1.81
36	1	925	A	N3-C4	-5.50	1.31	1.34
36	5	1847	A	N9-C4	-5.49	1.34	1.37
51	M5	152	CYS	CB-SG	-5.49	1.72	1.81
36	5	45	A	N9-C4	-5.47	1.34	1.37
36	1	1133	A	C5-C4	-5.46	1.34	1.38
1	6	1537	C	C2-N3	5.45	1.40	1.35
36	5	1149	G	N9-C8	-5.43	1.34	1.37
36	1	2355	G	N7-C5	-5.42	1.35	1.39
36	5	2356	A	N3-C4	-5.42	1.31	1.34
41	L4	65	TRP	CB-CG	-5.40	1.40	1.50
36	5	2626	A	N3-C4	-5.39	1.31	1.34
1	6	1765	A	N9-C4	-5.38	1.34	1.37
57	n1	104	GLU	CG-CD	5.38	1.60	1.51
1	6	623	A	N9-C4	-5.35	1.34	1.37
36	5	1152	G	N1-C2	5.35	1.42	1.37
36	1	1158	A	N7-C5	-5.35	1.36	1.39
38	4	28	C	N1-C6	-5.35	1.33	1.37
1	6	1537	C	C5-C6	5.35	1.38	1.34
36	1	29	C	N1-C6	-5.34	1.33	1.37
36	1	1192	C	N1-C2	5.33	1.45	1.40
36	5	2811	A	N9-C4	-5.33	1.34	1.37
36	1	355	A	N9-C4	-5.33	1.34	1.37
36	1	1114	U	C2-N3	-5.31	1.34	1.37
1	2	1469	A	N9-C4	-5.30	1.34	1.37
36	5	1156	C	N3-C4	-5.29	1.30	1.33
36	1	1149	G	N3-C4	-5.28	1.31	1.35
36	5	2364	G	N3-C4	-5.27	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	1299	G	C6-N1	-5.27	1.35	1.39
36	5	2991	A	N3-C4	-5.26	1.31	1.34
36	5	866	A	N9-C4	-5.25	1.34	1.37
36	1	2379	U	N1-C2	-5.25	1.33	1.38
36	5	1115	G	N1-C2	-5.25	1.33	1.37
36	5	3374	U	C2-N3	-5.24	1.34	1.37
36	1	2401	A	N3-C4	5.23	1.38	1.34
36	1	888	A	N7-C5	-5.23	1.36	1.39
36	1	3273	A	N3-C4	-5.22	1.31	1.34
36	5	1902	G	N7-C5	-5.22	1.36	1.39
36	5	3362	A	N7-C5	-5.22	1.36	1.39
36	1	1910	A	N9-C4	-5.21	1.34	1.37
36	5	2922	G	N7-C5	-5.20	1.36	1.39
36	1	2836	C	N3-C4	-5.19	1.30	1.33
36	1	867	G	N3-C4	-5.18	1.31	1.35
36	1	61	A	N3-C4	-5.18	1.31	1.34
36	1	1164	G	C6-N1	-5.16	1.35	1.39
36	5	2320	A	N9-C4	-5.16	1.34	1.37
36	1	912	G	C5-C4	-5.16	1.34	1.38
36	5	1309	U	N1-C2	-5.16	1.33	1.38
36	5	3092	C	N1-C6	-5.15	1.34	1.37
36	5	659	G	N7-C5	-5.15	1.36	1.39
36	5	645	A	C5-C6	5.14	1.45	1.41
36	1	1116	G	C5-C4	-5.14	1.34	1.38
1	2	1131	A	N9-C4	-5.13	1.34	1.37
36	1	913	A	N7-C5	-5.13	1.36	1.39
36	1	2147	A	N9-C4	-5.13	1.34	1.37
36	5	1663	C	N1-C6	-5.11	1.34	1.37
36	1	2877	G	C6-N1	-5.10	1.35	1.39
36	5	2917	G	C8-N7	-5.08	1.27	1.30
36	5	3132	C	N1-C6	-5.08	1.34	1.37
36	1	2398	A	C5-C4	-5.07	1.35	1.38
36	5	2814	G	C5-C4	-5.07	1.34	1.38
46	L9	165	CYS	CB-SG	-5.07	1.73	1.81
36	5	895	A	N9-C4	-5.07	1.34	1.37
36	5	2362	C	N1-C6	-5.07	1.34	1.37
1	6	1119	G	N7-C5	-5.07	1.36	1.39
36	1	1142	G	C5-C4	-5.05	1.34	1.38
36	5	1381	A	N9-C4	-5.05	1.34	1.37
36	5	1449	A	N7-C5	-5.05	1.36	1.39
36	1	1151	U	N1-C2	-5.03	1.34	1.38
36	1	2172	A	N9-C4	-5.03	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1326	A	N9-C4	5.02	1.40	1.37
36	1	1602	A	N3-C4	-5.02	1.31	1.34
36	5	1902	G	C8-N7	-5.02	1.27	1.30
36	5	521	A	N9-C4	-5.01	1.34	1.37
36	1	1313	G	N7-C5	-5.00	1.36	1.39

All (3717) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	22.88	140.04	128.60
36	5	1152	G	N3-C4-N9	-22.22	112.67	126.00
36	5	1152	G	C2-N3-C4	-17.60	103.10	111.90
1	6	1537	C	C6-N1-C2	-15.90	113.94	120.30
36	1	2714	G	N3-C4-C5	14.64	135.92	128.60
36	1	2714	G	N3-C4-N9	-13.69	117.79	126.00
36	1	1495	U	C5-C6-N1	-13.64	115.88	122.70
36	5	1152	G	C8-N9-C1'	13.39	144.41	127.00
36	1	2869	U	O5'-P-OP1	-13.22	93.80	105.70
36	1	1368	U	O5'-P-OP1	-13.13	93.88	105.70
36	1	2621	G	C5-C6-O6	-13.06	120.77	128.60
36	5	1152	G	N3-C2-N2	-12.89	110.88	119.90
36	1	2384	A	N1-C6-N6	12.79	126.27	118.60
36	1	960	U	C6-N1-C2	12.73	128.64	121.00
36	1	1308	A	O5'-P-OP2	-12.63	94.33	105.70
36	1	639	G	N1-C6-O6	12.43	127.36	119.90
36	1	960	U	N3-C4-C5	12.13	121.88	114.60
36	5	1152	G	C4-N9-C1'	-12.11	110.76	126.50
1	2	1200	G	N1-C6-O6	12.11	127.16	119.90
36	1	2884	C	N3-C4-C5	12.09	126.74	121.90
36	5	1902	G	N1-C6-O6	11.81	126.98	119.90
36	5	1437	C	C6-N1-C2	-11.64	115.64	120.30
36	1	608	A	N1-C6-N6	11.59	125.55	118.60
36	5	1152	G	C5-N7-C8	-11.57	98.52	104.30
36	1	1308	A	C8-N9-C4	-11.42	101.23	105.80
36	5	1116	G	N3-C4-C5	-11.42	122.89	128.60
36	1	2403	G	O5'-P-OP2	-11.33	95.50	105.70
36	5	2819	A	O5'-P-OP2	-11.30	95.53	105.70
36	5	2704	A	O5'-P-OP1	-11.23	95.59	105.70
36	1	1149	G	N1-C6-O6	11.16	126.59	119.90
36	5	2730	G	N1-C6-O6	11.12	126.57	119.90
1	2	553	G	N1-C6-O6	11.09	126.55	119.90
36	5	1902	G	C6-C5-N7	-11.02	123.79	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1381	A	O5'-P-OP2	11.01	123.91	110.70
36	1	406	G	O4'-C1'-N9	10.95	116.96	108.20
36	1	3278	C	N1-C2-O2	10.94	125.47	118.90
36	5	3245	A	C2-N3-C4	-10.92	105.14	110.60
36	5	2928	C	C6-N1-C2	-10.90	115.94	120.30
36	1	2617	U	C5-C4-O4	10.88	132.43	125.90
1	6	1537	C	N3-C4-C5	-10.88	117.55	121.90
36	5	716	A	O5'-P-OP1	-10.85	95.94	105.70
36	1	2714	G	C2-N3-C4	-10.77	106.51	111.90
36	5	2992	U	O5'-P-OP2	-10.73	96.04	105.70
36	1	2815	G	C8-N9-C4	10.70	110.68	106.40
36	1	3306	U	C5-C4-O4	10.70	132.32	125.90
36	5	2333	C	C6-N1-C2	10.64	124.56	120.30
36	5	2873	U	C2-N3-C4	-10.61	120.64	127.00
36	1	2871	G	O5'-P-OP2	-10.60	96.16	105.70
36	1	1192	C	N1-C2-O2	10.56	125.24	118.90
36	1	639	G	C5-C6-O6	-10.55	122.27	128.60
1	6	144	U	N3-C2-O2	-10.43	114.90	122.20
1	2	453	U	N3-C2-O2	-10.41	114.91	122.20
36	5	2728	G	N9-C4-C5	10.41	109.56	105.40
36	1	2945	G	O5'-P-OP2	-10.40	96.34	105.70
1	2	542	A	O4'-C1'-N9	10.39	116.51	108.20
36	1	1846	C	O5'-P-OP1	-10.21	96.52	105.70
36	1	794	U	O5'-P-OP2	-10.15	96.56	105.70
36	1	3217	C	C2-N1-C1'	10.15	129.97	118.80
36	5	939	U	O5'-P-OP2	-10.12	96.59	105.70
36	5	2873	U	N1-C2-O2	-10.12	115.72	122.80
36	1	3143	C	C6-N1-C2	10.10	124.34	120.30
36	5	1902	G	C5-C6-O6	-10.06	122.56	128.60
36	1	2404	A	C2-N3-C4	-10.05	105.58	110.60
36	5	2858	U	N3-C2-O2	-9.95	115.23	122.20
36	1	776	U	C4-C5-C6	9.94	125.67	119.70
36	5	2913	C	N1-C2-O2	-9.90	112.96	118.90
36	1	517	G	C8-N9-C4	-9.89	102.44	106.40
1	6	163	G	N3-C4-N9	-9.86	120.08	126.00
36	1	2827	U	N3-C4-O4	-9.82	112.53	119.40
36	5	1907	C	N1-C2-O2	-9.80	113.02	118.90
36	1	372	A	O5'-P-OP2	-9.79	96.89	105.70
36	1	1489	A	N1-C6-N6	9.79	124.47	118.60
1	2	1039	A	O4'-C1'-N9	9.78	116.02	108.20
36	1	3362	A	C2-N3-C4	-9.77	105.72	110.60
36	1	2621	G	N1-C6-O6	9.73	125.74	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2846	U	N3-C2-O2	-9.72	115.40	122.20
36	5	2730	G	C5-C6-O6	-9.71	122.77	128.60
36	5	437	G	C8-N9-C4	-9.70	102.52	106.40
36	5	1205	A	O5'-P-OP2	-9.62	97.04	105.70
36	5	2726	C	C5-C4-N4	9.62	126.94	120.20
36	5	2393	G	O5'-P-OP2	-9.61	97.05	105.70
36	5	1897	G	C4-C5-N7	9.60	114.64	110.80
36	1	979	U	C6-N1-C2	-9.54	115.28	121.00
36	5	2698	G	C8-N9-C4	9.53	110.21	106.40
36	1	3306	U	N3-C2-O2	-9.50	115.55	122.20
36	5	398	A	O5'-P-OP2	-9.50	97.15	105.70
36	1	640	U	N3-C4-O4	9.48	126.04	119.40
36	1	2121	G	N1-C6-O6	-9.45	114.23	119.90
36	1	2384	A	C6-C5-N7	-9.43	125.70	132.30
1	6	639	U	N3-C2-O2	-9.43	115.60	122.20
37	7	73	C	C6-N1-C2	-9.41	116.53	120.30
36	1	645	A	N1-C6-N6	-9.39	112.96	118.60
36	5	2150	G	C8-N9-C4	-9.38	102.65	106.40
36	1	435	C	C6-N1-C2	9.38	124.05	120.30
36	1	1158	A	N1-C6-N6	9.35	124.21	118.60
36	1	201	A	O5'-P-OP2	-9.31	97.32	105.70
36	1	2958	A	N1-C6-N6	-9.31	113.02	118.60
36	1	2869	U	O5'-P-OP2	9.29	121.85	110.70
36	5	2572	C	N1-C2-O2	9.29	124.47	118.90
1	2	639	U	N3-C2-O2	-9.24	115.73	122.20
36	5	835	G	C5-C6-O6	-9.24	123.06	128.60
36	5	655	C	N1-C2-O2	-9.21	113.37	118.90
36	1	2393	G	C5-C6-O6	-9.19	123.09	128.60
36	5	3154	C	N1-C2-O2	9.18	124.41	118.90
1	6	1535	U	N3-C2-O2	-9.18	115.78	122.20
36	5	3046	A	O5'-P-OP2	-9.17	97.45	105.70
36	1	86	G	O5'-P-OP2	-9.15	97.46	105.70
36	5	2393	G	N1-C6-O6	9.15	125.39	119.90
36	5	406	G	O4'-C1'-N9	9.13	115.50	108.20
1	6	1473	U	N3-C2-O2	-9.12	115.81	122.20
36	1	3362	A	C5-N7-C8	-9.12	99.34	103.90
36	5	922	U	C5-C6-N1	-9.11	118.14	122.70
36	1	1216	C	C6-N1-C2	-9.09	116.67	120.30
36	5	1876	U	C5-C6-N1	9.09	127.25	122.70
36	1	1443	G	C8-N9-C4	-9.08	102.77	106.40
36	1	1434	G	N7-C8-N9	9.07	117.63	113.10
36	5	1591	G	O5'-P-OP1	-9.07	97.54	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3278	C	N3-C2-O2	-9.03	115.58	121.90
36	1	895	A	C5-N7-C8	-9.02	99.39	103.90
36	5	2283	G	O5'-P-OP2	-9.01	97.59	105.70
36	1	640	U	C5-C4-O4	-9.00	120.50	125.90
36	5	857	G	N1-C6-O6	9.00	125.30	119.90
36	5	2159	U	N3-C2-O2	-8.99	115.91	122.20
36	1	2617	U	N1-C2-N3	8.98	120.29	114.90
36	5	3143	C	C6-N1-C2	8.98	123.89	120.30
1	6	57	G	O5'-P-OP2	-8.97	97.62	105.70
36	1	960	U	C5-C6-N1	-8.97	118.22	122.70
36	1	2797	C	O5'-P-OP1	-8.97	97.63	105.70
1	2	554	C	N1-C2-O2	8.95	124.27	118.90
36	5	3327	G	N1-C6-O6	8.94	125.27	119.90
36	1	2978	U	O4'-C1'-N1	8.93	115.34	108.20
36	5	3209	A	O4'-C1'-N9	8.92	115.33	108.20
36	5	2393	G	C5-C6-O6	-8.91	123.25	128.60
36	1	1495	U	C2-N1-C1'	-8.89	107.03	117.70
36	5	2512	C	C5-C6-N1	8.88	125.44	121.00
36	1	2838	A	O5'-P-OP2	-8.88	97.71	105.70
36	5	2372	A	C8-N9-C4	-8.86	102.25	105.80
36	1	1192	C	C2-N1-C1'	8.85	128.54	118.80
36	1	2351	U	N3-C2-O2	-8.80	116.04	122.20
36	1	2726	C	N3-C2-O2	-8.80	115.74	121.90
1	6	1773	C	N3-C4-C5	-8.78	118.39	121.90
36	1	648	C	C2-N1-C1'	8.77	128.44	118.80
36	5	3245	A	C5-C6-N1	-8.77	113.32	117.70
36	5	2728	G	C8-N9-C4	-8.77	102.89	106.40
36	5	2333	C	N3-C2-O2	8.76	128.03	121.90
36	5	682	U	N3-C4-O4	-8.76	113.27	119.40
36	1	2827	U	C5-C4-O4	8.74	131.14	125.90
1	2	1280	C	N3-C4-C5	-8.73	118.41	121.90
36	5	2646	C	C6-N1-C2	8.73	123.79	120.30
36	1	652	G	O5'-P-OP2	-8.73	97.84	105.70
36	1	2350	C	C5-C6-N1	-8.72	116.64	121.00
36	5	1897	G	N1-C6-O6	8.72	125.13	119.90
36	5	3306	U	C5-C4-O4	-8.71	120.67	125.90
36	1	2314	U	N1-C2-N3	-8.69	109.69	114.90
36	5	1307	G	P-O3'-C3'	8.68	130.12	119.70
1	2	553	G	C5-C6-O6	-8.68	123.39	128.60
36	5	1392	G	C8-N9-C4	8.67	109.87	106.40
36	1	2314	U	C5-C4-O4	-8.66	120.70	125.90
36	5	776	U	C4-C5-C6	8.63	124.88	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1189	C	N1-C2-O2	-8.62	113.73	118.90
1	2	1761	U	C5-C4-O4	8.62	131.07	125.90
36	5	1885	U	C6-N1-C2	8.61	126.17	121.00
36	5	2962	U	O5'-P-OP1	-8.61	97.95	105.70
36	1	1556	C	C6-N1-C2	-8.59	116.86	120.30
36	1	2983	C	C5-C4-N4	8.59	126.21	120.20
36	5	1006	A	O5'-P-OP2	-8.55	98.00	105.70
1	6	1028	C	C6-N1-C2	8.54	123.72	120.30
36	1	2619	G	O5'-P-OP1	-8.53	98.02	105.70
38	4	99	C	C6-N1-C2	8.51	123.70	120.30
36	5	2320	A	C2-N3-C4	-8.51	106.34	110.60
36	1	917	A	O5'-P-OP2	-8.51	98.04	105.70
36	5	2341	A	C8-N9-C4	8.49	109.19	105.80
36	5	2943	G	N9-C4-C5	-8.47	102.01	105.40
36	1	1434	G	C8-N9-C4	-8.47	103.01	106.40
36	1	645	A	C5-C6-N1	8.46	121.93	117.70
36	5	881	C	C5-C6-N1	8.46	125.23	121.00
1	2	75	U	N1-C2-O2	8.45	128.72	122.80
36	1	1365	G	N1-C2-N2	-8.44	108.60	116.20
38	8	33	A	N1-C6-N6	8.44	123.66	118.60
41	14	187	LEU	CA-CB-CG	8.44	134.71	115.30
36	1	1902	G	N9-C4-C5	-8.42	102.03	105.40
36	5	1193	A	N1-C6-N6	8.42	123.65	118.60
36	1	2572	C	N1-C2-O2	8.42	123.95	118.90
36	1	2855	U	C5-C6-N1	-8.41	118.50	122.70
36	1	295	A	C8-N9-C4	-8.40	102.44	105.80
36	1	1158	A	C5-C6-N6	-8.40	116.98	123.70
36	1	2169	G	N1-C6-O6	-8.40	114.86	119.90
36	5	2726	C	N3-C2-O2	-8.39	116.02	121.90
1	6	453	U	N3-C2-O2	-8.39	116.33	122.20
36	5	2866	U	N3-C2-O2	-8.39	116.33	122.20
36	1	718	G	C4-C5-N7	8.37	114.15	110.80
36	1	1854	C	O5'-P-OP2	-8.36	98.17	105.70
36	1	3362	A	N7-C8-N9	8.36	117.98	113.80
36	5	3362	A	N7-C8-N9	8.36	117.98	113.80
36	5	2354	C	N1-C2-O2	-8.36	113.89	118.90
36	1	2572	C	C2-N1-C1'	8.35	127.99	118.80
36	5	2873	U	C5-C6-N1	-8.35	118.53	122.70
36	5	682	U	C2-N1-C1'	-8.34	107.69	117.70
36	5	2873	U	N1-C2-N3	8.34	119.90	114.90
1	6	337	G	C6-C5-N7	-8.34	125.40	130.40
36	5	1897	G	C5-C6-O6	-8.34	123.60	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	25	U	N3-C4-C5	-8.33	109.60	114.60
36	5	2297	U	O5'-P-OP2	-8.33	98.20	105.70
36	5	2215	A	C8-N9-C4	8.33	109.13	105.80
36	1	608	A	C6-C5-N7	-8.32	126.47	132.30
36	5	2375	G	N1-C6-O6	-8.32	114.91	119.90
36	1	1212	A	O5'-P-OP2	-8.31	98.22	105.70
36	5	2726	C	C6-N1-C2	-8.31	116.97	120.30
10	s8	29	LEU	CA-CB-CG	8.31	134.42	115.30
36	5	2699	G	C5-C6-O6	-8.30	123.62	128.60
36	1	1902	G	C4-C5-N7	8.30	114.12	110.80
1	2	323	A	O5'-P-OP2	-8.29	98.24	105.70
36	1	2860	U	N3-C2-O2	8.28	127.99	122.20
36	1	938	C	N1-C2-O2	-8.27	113.94	118.90
36	1	1216	C	C5-C6-N1	8.27	125.13	121.00
38	8	24	G	N1-C6-O6	-8.26	114.94	119.90
36	1	3306	U	N3-C4-O4	-8.26	113.62	119.40
1	6	453	U	C2-N1-C1'	8.26	127.61	117.70
36	5	2385	G	C8-N9-C4	8.26	109.70	106.40
1	6	1731	A	N1-C6-N6	-8.26	113.64	118.60
1	6	1765	A	C8-N9-C4	8.26	109.10	105.80
36	5	518	G	C5-C6-O6	-8.25	123.65	128.60
36	1	3212	C	C6-N1-C2	8.25	123.60	120.30
36	1	2384	A	C5-C6-N6	-8.24	117.11	123.70
36	5	1208	U	N3-C2-O2	-8.24	116.44	122.20
36	1	1495	U	C4-C5-C6	8.23	124.64	119.70
36	1	2846	U	C5-C4-O4	8.23	130.84	125.90
36	1	2200	U	C6-N1-C2	-8.21	116.07	121.00
36	1	939	U	N1-C2-O2	-8.21	117.05	122.80
36	1	3183	A	N1-C6-N6	8.20	123.52	118.60
36	1	3134	A	C8-N9-C4	8.19	109.08	105.80
36	1	979	U	N1-C2-N3	8.18	119.81	114.90
36	5	1902	G	C4-C5-C6	8.18	123.71	118.80
1	6	337	G	N3-C4-N9	8.16	130.90	126.00
36	1	608	A	C5-C6-N6	-8.16	117.17	123.70
36	1	1192	C	N3-C2-O2	-8.16	116.19	121.90
36	1	1433	A	O5'-P-OP1	-8.16	98.36	105.70
36	5	2978	U	N3-C2-O2	-8.16	116.49	122.20
36	5	867	G	O5'-P-OP1	-8.15	98.36	105.70
36	5	894	G	N9-C4-C5	-8.15	102.14	105.40
36	1	2352	A	N1-C6-N6	8.14	123.49	118.60
1	2	1773	C	N3-C4-C5	-8.14	118.64	121.90
36	5	2159	U	N1-C2-O2	8.14	128.50	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3107	U	O5'-P-OP2	-8.13	98.38	105.70
36	1	968	G	N3-C4-C5	-8.13	124.53	128.60
36	1	2377	G	N1-C2-N2	-8.13	108.88	116.20
36	1	1377	G	C4-C5-N7	8.13	114.05	110.80
36	1	2617	U	N3-C2-O2	-8.13	116.51	122.20
36	5	1868	G	N9-C4-C5	-8.12	102.15	105.40
1	2	1749	A	C2-N3-C4	-8.12	106.54	110.60
36	1	2827	U	C5-C6-N1	-8.11	118.65	122.70
36	1	2314	U	C5-C6-N1	8.09	126.75	122.70
36	1	2996	U	N1-C2-O2	8.09	128.47	122.80
1	2	1200	G	C6-C5-N7	-8.09	125.55	130.40
1	2	402	C	C6-N1-C2	8.09	123.54	120.30
36	1	1116	G	O5'-P-OP1	-8.09	98.42	105.70
1	2	1773	C	C6-N1-C2	-8.08	117.07	120.30
36	5	2403	G	C5-C6-O6	-8.07	123.75	128.60
1	6	1641	C	N1-C2-O2	-8.07	114.06	118.90
36	1	2374	C	C6-N1-C2	-8.07	117.07	120.30
1	6	543	C	C6-N1-C2	-8.06	117.08	120.30
36	1	2200	U	N3-C4-C5	-8.06	109.77	114.60
36	5	2572	C	C2-N1-C1'	8.06	127.66	118.80
78	q2	17	CYS	CA-CB-SG	8.06	128.50	114.00
36	5	1592	G	C5-C6-N1	-8.06	107.47	111.50
36	1	1437	C	O5'-P-OP1	-8.05	98.45	105.70
36	5	2943	G	C4-C5-N7	8.05	114.02	110.80
1	6	1537	C	C6-N1-C1'	8.05	130.46	120.80
1	6	1103	U	C5-C4-O4	8.04	130.73	125.90
36	1	3134	A	N9-C4-C5	-8.04	102.58	105.80
36	1	3217	C	N1-C2-O2	8.04	123.72	118.90
36	5	2512	C	C6-N1-C2	-8.04	117.09	120.30
36	1	2899	C	N3-C2-O2	-8.03	116.28	121.90
36	5	1193	A	C6-C5-N7	-8.02	126.69	132.30
1	2	73	U	O4'-C1'-N1	8.02	114.61	108.20
36	1	2944	U	O5'-P-OP1	-8.02	98.48	105.70
36	5	1452	A	N1-C6-N6	8.02	123.41	118.60
1	2	1762	A	C8-N9-C4	8.01	109.00	105.80
36	1	1495	U	N1-C2-O2	-8.01	117.19	122.80
1	6	337	G	C4-N9-C1'	8.01	136.91	126.50
36	1	908	G	O4'-C1'-N9	-8.00	101.80	108.20
36	1	2401	A	C8-N9-C4	8.00	109.00	105.80
36	5	2644	C	C6-N1-C2	8.00	123.50	120.30
36	5	1902	G	N3-C4-N9	8.00	130.80	126.00
36	5	2683	U	C5-C6-N1	8.00	126.70	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2819	A	N1-C6-N6	-8.00	113.80	118.60
36	1	960	U	C2-N3-C4	-8.00	122.20	127.00
36	1	1838	G	N1-C6-O6	7.99	124.70	119.90
36	5	877	C	N3-C4-C5	7.96	125.08	121.90
36	5	1152	G	N1-C6-O6	7.95	124.67	119.90
36	1	960	U	C2-N1-C1'	-7.94	108.17	117.70
1	6	194	U	C2-N1-C1'	7.93	127.21	117.70
36	5	340	C	C6-N1-C2	7.92	123.47	120.30
36	5	3050	U	C5-C4-O4	7.92	130.65	125.90
36	5	2899	C	C6-N1-C2	-7.91	117.14	120.30
38	8	80	A	C8-N9-C4	-7.91	102.64	105.80
36	5	2912	G	O5'-P-OP1	-7.90	98.59	105.70
36	1	1495	U	C2-N3-C4	-7.89	122.26	127.00
36	5	2199	G	C4-C5-N7	7.89	113.96	110.80
36	1	884	A	N1-C6-N6	7.89	123.33	118.60
36	1	2621	G	N3-C2-N2	-7.89	114.38	119.90
1	2	966	A	C8-N9-C4	7.89	108.95	105.80
1	2	145	A	C8-N9-C4	-7.88	102.65	105.80
36	1	864	G	N9-C4-C5	7.87	108.55	105.40
36	1	2956	A	O5'-P-OP1	-7.86	98.63	105.70
37	7	92	A	N9-C4-C5	-7.86	102.66	105.80
36	5	942	U	N3-C4-O4	7.85	124.89	119.40
36	1	2899	C	C2-N1-C1'	7.84	127.43	118.80
48	m1	112	LEU	CA-CB-CG	7.83	133.32	115.30
1	6	163	G	C8-N9-C4	-7.82	103.27	106.40
36	5	1435	A	P-O3'-C3'	7.82	129.09	119.70
36	5	669	U	C5-C6-N1	-7.81	118.79	122.70
36	5	2283	G	N1-C6-O6	7.81	124.59	119.90
36	1	2984	C	C5-C4-N4	7.81	125.67	120.20
36	5	3123	A	C8-N9-C4	7.81	108.92	105.80
36	1	895	A	N7-C8-N9	7.80	117.70	113.80
12	C0	88	PRO	N-CA-CB	7.80	112.66	103.30
36	1	893	C	N1-C2-O2	7.80	123.58	118.90
36	1	1336	U	O5'-P-OP2	-7.80	98.68	105.70
36	5	429	U	O5'-P-OP2	-7.80	98.68	105.70
36	1	1662	G	C6-C5-N7	-7.79	125.72	130.40
36	5	2375	G	C5-C6-O6	7.78	133.27	128.60
1	2	1560	U	N3-C2-O2	-7.78	116.76	122.20
1	2	639	U	N1-C2-O2	7.77	128.24	122.80
36	5	2943	G	C6-C5-N7	-7.76	125.74	130.40
38	4	94	C	C6-N1-C2	7.76	123.40	120.30
36	1	1148	G	C8-N9-C4	7.75	109.50	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	13	A	N1-C6-N6	7.75	123.25	118.60
36	1	2953	U	N1-C2-O2	-7.75	117.37	122.80
36	1	646	A	O5'-P-OP2	-7.74	98.73	105.70
36	1	2983	C	C5-C6-N1	-7.74	117.13	121.00
36	5	2572	C	N3-C2-O2	-7.73	116.49	121.90
36	5	1796	G	N1-C6-O6	-7.73	115.26	119.90
36	1	584	G	N1-C6-O6	-7.73	115.26	119.90
1	6	1700	C	C2-N1-C1'	7.73	127.30	118.80
36	1	1489	A	N9-C4-C5	-7.72	102.71	105.80
36	1	3024	A	O5'-P-OP1	-7.72	98.75	105.70
38	4	32	C	O5'-P-OP2	-7.70	98.77	105.70
1	2	810	G	C6-C5-N7	-7.70	125.78	130.40
36	1	2384	A	N9-C4-C5	-7.70	102.72	105.80
36	1	789	A	N1-C6-N6	-7.69	113.98	118.60
1	6	1596	C	N3-C2-O2	-7.69	116.52	121.90
36	1	776	U	N1-C2-N3	7.69	119.51	114.90
36	5	211	A	O5'-P-OP1	-7.68	98.79	105.70
36	1	2550	U	C6-N1-C2	-7.68	116.39	121.00
1	6	647	G	N3-C4-N9	-7.68	121.39	126.00
36	5	3362	A	C8-N9-C4	-7.68	102.73	105.80
1	2	1761	U	N3-C2-O2	-7.67	116.83	122.20
36	1	645	A	C6-N1-C2	-7.66	114.00	118.60
36	5	1152	G	C4-C5-N7	7.66	113.86	110.80
1	2	554	C	C2-N1-C1'	7.65	127.22	118.80
1	2	553	G	C6-C5-N7	-7.65	125.81	130.40
36	1	59	G	N1-C6-O6	7.64	124.49	119.90
36	1	933	A	C4-C5-C6	7.64	120.82	117.00
36	1	3057	U	C5-C4-O4	7.64	130.49	125.90
36	5	776	U	C5-C6-N1	-7.64	118.88	122.70
36	5	2294	U	O5'-P-OP1	-7.64	98.82	105.70
36	5	3154	C	C2-N1-C1'	7.64	127.21	118.80
36	5	2637	A	C8-N9-C4	7.64	108.86	105.80
1	2	453	U	C2-N1-C1'	7.64	126.87	117.70
1	2	448	C	C6-N1-C2	-7.64	117.25	120.30
36	1	2366	C	O5'-P-OP2	-7.63	98.83	105.70
36	5	2231	C	C2-N1-C1'	7.63	127.20	118.80
36	1	1308	A	N7-C8-N9	7.63	117.61	113.80
36	5	1129	A	O5'-P-OP2	-7.63	98.83	105.70
36	1	2887	A	N1-C6-N6	7.63	123.18	118.60
36	1	2983	C	N3-C4-N4	-7.62	112.66	118.00
36	1	3217	C	N3-C2-O2	-7.62	116.56	121.90
36	5	838	G	C5-C6-O6	7.62	133.17	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2899	C	N3-C2-O2	-7.61	116.58	121.90
36	1	682	U	C2-N1-C1'	-7.60	108.58	117.70
1	6	102	U	O5'-P-OP1	-7.60	98.86	105.70
36	1	843	A	C2-N3-C4	-7.59	106.80	110.60
36	5	2392	C	N3-C4-C5	7.59	124.94	121.90
38	4	125	U	C2-N1-C1'	7.59	126.81	117.70
1	6	337	G	N3-C2-N2	7.59	125.21	119.90
36	5	3362	A	C5-N7-C8	-7.59	100.11	103.90
36	1	3344	A	N7-C8-N9	7.59	117.59	113.80
36	5	2880	U	N3-C2-O2	-7.58	116.89	122.20
36	1	3022	G	O4'-C1'-N9	7.58	114.26	108.20
36	5	3092	C	N3-C2-O2	-7.58	116.59	121.90
36	1	2194	G	C6-C5-N7	-7.57	125.86	130.40
36	5	1420	C	C5-C6-N1	-7.57	117.21	121.00
36	1	42	C	C6-N1-C2	-7.57	117.27	120.30
36	1	2869	U	C2-N1-C1'	7.57	126.78	117.70
36	1	969	C	N1-C2-O2	-7.56	114.36	118.90
36	5	2231	C	O4'-C1'-N1	7.56	114.25	108.20
36	1	517	G	N7-C8-N9	7.56	116.88	113.10
1	6	337	G	C8-N9-C1'	-7.56	117.17	127.00
36	1	3217	C	C6-N1-C1'	-7.56	111.73	120.80
36	5	1193	A	C4-C5-C6	7.55	120.78	117.00
36	5	2880	U	N1-C2-O2	7.55	128.09	122.80
36	1	2237	C	C6-N1-C2	7.55	123.32	120.30
36	1	1495	U	N1-C2-N3	7.55	119.43	114.90
44	17	229	PHE	CB-CG-CD1	7.55	126.08	120.80
36	5	1152	G	C4-C5-C6	-7.54	114.28	118.80
10	S8	29	LEU	CA-CB-CG	7.54	132.63	115.30
36	5	2145	A	C6-N1-C2	-7.53	114.08	118.60
38	8	33	A	C8-N9-C4	7.53	108.81	105.80
36	1	39	A	N1-C6-N6	7.52	123.11	118.60
36	1	1409	G	N1-C6-O6	-7.52	115.39	119.90
36	1	1437	C	C2-N1-C1'	7.52	127.07	118.80
36	1	946	U	O5'-P-OP2	-7.52	98.94	105.70
37	7	53	U	O5'-P-OP2	-7.51	98.94	105.70
36	5	1380	G	C8-N9-C4	7.51	109.40	106.40
36	1	417	A	N1-C6-N6	7.51	123.11	118.60
38	8	44	A	C8-N9-C4	7.51	108.80	105.80
36	5	2699	G	N1-C6-O6	7.50	124.40	119.90
36	1	895	A	C4-C5-N7	7.50	114.45	110.70
36	1	2403	G	N3-C4-N9	7.49	130.50	126.00
36	5	922	U	C5-C4-O4	7.49	130.40	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2384	A	C4-C5-N7	7.49	114.45	110.70
36	1	1484	U	P-O3'-C3'	7.49	128.69	119.70
36	5	1841	A	N1-C6-N6	7.49	123.09	118.60
36	1	672	A	N1-C6-N6	7.49	123.09	118.60
36	5	3245	A	C6-C5-N7	-7.48	127.06	132.30
36	1	2796	G	C2-N3-C4	-7.48	108.16	111.90
1	2	1280	C	N1-C2-O2	-7.47	114.42	118.90
36	1	2550	U	C5-C4-O4	7.46	130.38	125.90
36	1	2628	A	N1-C2-N3	7.46	133.03	129.30
1	6	1019	A	C8-N9-C4	7.46	108.78	105.80
36	5	2953	U	N1-C2-O2	-7.45	117.58	122.80
36	5	2608	G	C8-N9-C4	7.45	109.38	106.40
36	1	296	A	O5'-P-OP1	-7.45	98.99	105.70
36	5	981	U	C5-C6-N1	7.45	126.43	122.70
36	5	2634	U	C2-N3-C4	-7.45	122.53	127.00
36	1	908	G	C5-C6-O6	-7.45	124.13	128.60
1	6	1596	C	C5-C4-N4	7.44	125.41	120.20
1	6	163	G	C2-N3-C4	-7.44	108.18	111.90
36	5	1856	C	O5'-P-OP1	-7.43	99.01	105.70
36	5	2870	C	N3-C4-N4	-7.43	112.80	118.00
1	2	728	U	C2-N1-C1'	7.42	126.61	117.70
36	5	2816	G	N9-C4-C5	-7.41	102.44	105.40
36	5	2354	C	N3-C2-O2	7.41	127.08	121.90
36	5	2866	U	N1-C2-O2	7.40	127.98	122.80
38	4	125	U	N1-C2-O2	7.40	127.98	122.80
1	2	359	A	C8-N9-C4	7.39	108.76	105.80
36	1	2404	A	N1-C6-N6	7.39	123.04	118.60
36	1	2831	G	N1-C6-O6	7.39	124.34	119.90
36	5	1160	C	N1-C2-O2	-7.39	114.46	118.90
36	5	2278	C	C5-C6-N1	7.39	124.70	121.00
36	1	2355	G	C5-C6-O6	-7.39	124.17	128.60
36	1	2816	G	C5-C6-O6	-7.39	124.17	128.60
36	5	939	U	O5'-P-OP1	7.39	119.56	110.70
36	1	702	C	C6-N1-C2	-7.38	117.35	120.30
37	3	82	G	C8-N9-C4	-7.38	103.45	106.40
36	5	3245	A	N1-C6-N6	7.37	123.02	118.60
36	1	1662	G	C5-C6-O6	-7.37	124.18	128.60
37	3	82	G	N9-C4-C5	7.37	108.35	105.40
36	5	2317	A	O5'-P-OP1	-7.37	99.06	105.70
36	1	2879	C	N1-C2-O2	-7.37	114.48	118.90
36	5	1513	G	C8-N9-C4	-7.37	103.45	106.40
1	2	364	G	N3-C4-N9	7.37	130.42	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	992	A	C2-N3-C4	-7.36	106.92	110.60
36	1	917	A	O5'-P-OP1	7.36	119.54	110.70
36	1	2360	C	C5-C6-N1	-7.36	117.32	121.00
36	5	1897	G	C5-N7-C8	-7.36	100.62	104.30
36	1	65	A	P-O3'-C3'	7.34	128.51	119.70
37	3	5	G	N3-C4-N9	-7.34	121.60	126.00
36	1	1450	G	O5'-P-OP1	-7.33	99.10	105.70
36	5	2144	A	O4'-C1'-N9	7.33	114.06	108.20
36	5	514	G	C5-C6-O6	-7.33	124.20	128.60
36	1	2634	U	C2-N3-C4	-7.32	122.61	127.00
36	5	3245	A	N7-C8-N9	7.32	117.46	113.80
1	2	554	C	C2-N3-C4	7.32	123.56	119.90
1	6	1634	C	C2-N1-C1'	7.31	126.84	118.80
20	c8	116	LEU	CA-CB-CG	7.31	132.12	115.30
36	5	3327	G	C5-C6-O6	-7.31	124.21	128.60
36	5	1868	G	C6-C5-N7	-7.31	126.02	130.40
36	1	1308	A	O5'-P-OP1	7.31	119.47	110.70
36	1	1113	G	N1-C6-O6	7.30	124.28	119.90
36	5	1441	G	C5-C6-N1	7.30	115.15	111.50
1	2	75	U	N3-C2-O2	-7.30	117.09	122.20
36	5	1704	A	C8-N9-C4	7.30	108.72	105.80
36	5	2639	G	C4-N9-C1'	7.30	135.99	126.50
48	M1	112	LEU	CA-CB-CG	7.29	132.08	115.30
36	5	776	U	N1-C2-N3	7.29	119.28	114.90
36	1	2355	G	N1-C6-O6	7.29	124.27	119.90
36	5	922	U	N3-C2-O2	-7.29	117.10	122.20
36	1	1365	G	N7-C8-N9	7.28	116.74	113.10
36	5	1116	G	N9-C4-C5	7.28	108.31	105.40
36	5	2621	G	N3-C2-N2	-7.28	114.80	119.90
1	2	1200	G	C5-C6-O6	-7.28	124.23	128.60
36	5	514	G	N1-C6-O6	7.28	124.27	119.90
36	5	2830	G	N1-C2-N3	7.28	128.27	123.90
36	1	1646	G	N1-C6-O6	7.28	124.27	119.90
36	5	894	G	C4-C5-N7	7.27	113.71	110.80
36	1	285	A	C8-N9-C4	7.27	108.71	105.80
38	8	33	A	C5-C6-N6	-7.27	117.88	123.70
15	C3	22	ALA	C-N-CD	-7.27	104.61	120.60
36	1	2617	U	N3-C4-O4	-7.27	114.31	119.40
1	6	1596	C	C6-N1-C2	-7.27	117.39	120.30
1	2	1611	A	N1-C2-N3	7.26	132.93	129.30
36	5	932	U	C6-N1-C2	7.25	125.35	121.00
1	6	1787	C	O5'-P-OP1	-7.25	99.17	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1222	G	P-O3'-C3'	7.25	128.40	119.70
36	1	645	A	N3-C4-C5	-7.25	121.73	126.80
36	1	2836	C	C4-C5-C6	7.24	121.02	117.40
36	5	437	G	N9-C4-C5	7.24	108.30	105.40
36	1	3207	U	C2-N1-C1'	-7.24	109.01	117.70
1	2	75	U	C2-N1-C1'	7.24	126.38	117.70
36	1	3057	U	N3-C4-O4	-7.24	114.33	119.40
36	1	1306	G	C5-C6-O6	-7.24	124.26	128.60
1	6	1025	A	N9-C4-C5	-7.24	102.91	105.80
36	5	838	G	N1-C6-O6	-7.23	115.56	119.90
36	5	2385	G	N3-C4-C5	7.23	132.22	128.60
36	5	2816	G	C5-C6-O6	-7.23	124.26	128.60
36	5	857	G	C6-C5-N7	-7.23	126.06	130.40
36	1	1433	A	C5-C6-N6	-7.22	117.92	123.70
36	1	3362	A	O4'-C1'-N9	7.22	113.98	108.20
36	5	2762	A	O5'-P-OP2	-7.22	99.20	105.70
36	1	1306	G	N1-C6-O6	7.22	124.23	119.90
37	7	49	G	N1-C6-O6	7.22	124.23	119.90
36	5	1116	G	C4-C5-N7	-7.22	107.91	110.80
36	1	1897	G	N1-C6-O6	7.21	124.22	119.90
1	6	1280	C	C6-N1-C2	-7.20	117.42	120.30
1	2	810	G	N1-C6-O6	7.20	124.22	119.90
36	1	2819	A	O5'-P-OP2	-7.20	99.22	105.70
36	1	2404	A	C5-C6-N1	-7.20	114.10	117.70
36	1	1377	G	C5-C6-O6	-7.19	124.28	128.60
36	5	1412	G	C8-N9-C4	-7.19	103.52	106.40
36	1	639	G	C6-C5-N7	-7.19	126.09	130.40
36	1	404	G	O5'-P-OP2	-7.18	99.23	105.70
36	1	650	C	N1-C2-O2	-7.18	114.59	118.90
36	5	1452	A	N9-C4-C5	-7.18	102.93	105.80
36	5	2994	A	N1-C6-N6	7.18	122.91	118.60
36	1	1437	C	C6-N1-C2	-7.18	117.43	120.30
36	1	651	G	N3-C4-N9	7.17	130.30	126.00
36	1	1891	A	C2-N3-C4	-7.17	107.01	110.60
36	1	2101	C	P-O3'-C3'	7.17	128.30	119.70
36	5	2879	C	C6-N1-C2	7.17	123.17	120.30
36	5	650	C	C2-N3-C4	-7.16	116.32	119.90
1	6	1596	C	N3-C4-N4	-7.16	112.99	118.00
36	1	1680	G	O5'-P-OP1	-7.14	99.27	105.70
36	5	3245	A	N1-C2-N3	7.14	132.87	129.30
1	2	1600	A	C5-C6-N1	-7.14	114.13	117.70
36	5	1116	G	C6-N1-C2	-7.14	120.82	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2698	G	N7-C8-N9	-7.13	109.53	113.10
36	1	1151	U	N1-C2-O2	-7.13	117.81	122.80
36	1	1151	U	N3-C4-O4	7.13	124.39	119.40
36	1	895	A	C6-C5-N7	-7.12	127.31	132.30
36	1	2945	G	O5'-P-OP1	7.12	119.25	110.70
36	5	3362	A	C6-C5-N7	-7.12	127.31	132.30
36	5	2858	U	N1-C2-N3	7.12	119.17	114.90
36	1	835	G	O4'-C1'-N9	7.12	113.89	108.20
36	5	2939	G	O5'-P-OP1	-7.12	99.30	105.70
36	5	2360	C	C4-C5-C6	7.11	120.96	117.40
1	2	1280	C	N3-C4-N4	7.11	122.98	118.00
36	1	1279	C	C6-N1-C2	-7.11	117.46	120.30
36	1	2814	G	C5-C6-O6	-7.11	124.33	128.60
36	5	2327	U	C5-C6-N1	-7.11	119.15	122.70
36	5	73	C	C5-C4-N4	-7.10	115.23	120.20
36	1	857	G	N1-C6-O6	7.10	124.16	119.90
36	5	2726	C	N1-C2-N3	7.10	124.17	119.20
36	1	1164	G	C5-C6-O6	7.10	132.86	128.60
36	1	39	A	C4-C5-N7	7.09	114.25	110.70
36	5	283	G	C6-C5-N7	-7.09	126.14	130.40
36	5	2709	C	N3-C4-C5	7.09	124.74	121.90
36	5	2805	G	N3-C4-N9	7.09	130.26	126.00
36	1	1119	C	C5-C6-N1	-7.09	117.46	121.00
36	1	2833	A	C8-N9-C4	7.08	108.63	105.80
36	1	2996	U	C2-N1-C1'	7.08	126.20	117.70
1	2	287	G	O4'-C1'-N9	7.08	113.87	108.20
36	1	2360	C	C4-C5-C6	7.08	120.94	117.40
1	6	1121	C	C6-N1-C2	7.07	123.13	120.30
36	5	346	C	N1-C2-O2	7.07	123.14	118.90
1	6	1117	U	N1-C2-O2	-7.06	117.86	122.80
36	5	2331	C	N3-C4-C5	-7.06	119.08	121.90
1	6	1640	C	C5-C6-N1	7.05	124.53	121.00
36	5	2929	C	C2-N3-C4	-7.05	116.37	119.90
36	1	1151	U	N3-C4-C5	-7.05	110.37	114.60
36	1	2899	C	C6-N1-C1'	-7.05	112.34	120.80
36	1	3344	A	O4'-C1'-N9	7.05	113.84	108.20
36	5	1605	A	O4'-C1'-N9	7.05	113.84	108.20
36	5	2804	A	O5'-P-OP1	-7.05	99.35	105.70
36	5	780	A	N1-C6-N6	7.05	122.83	118.60
36	5	890	C	O5'-P-OP2	-7.05	99.36	105.70
36	5	894	G	N3-C2-N2	7.05	124.83	119.90
1	2	831	U	C5-C6-N1	7.04	126.22	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3119	U	N3-C2-O2	-7.04	117.27	122.20
1	6	163	G	N9-C4-C5	7.04	108.22	105.40
1	2	453	U	N1-C2-O2	7.04	127.73	122.80
36	1	2418	G	OP1-P-O3'	7.04	120.68	105.20
36	5	1938	U	C6-N1-C2	7.04	125.22	121.00
36	1	1396	C	C6-N1-C2	7.03	123.11	120.30
36	1	776	U	C5-C6-N1	-7.03	119.19	122.70
1	2	1455	G	C5-C6-N1	-7.03	107.99	111.50
1	6	1700	C	N1-C2-O2	7.03	123.11	118.90
36	5	1004	U	N3-C2-O2	-7.03	117.28	122.20
36	5	1513	G	N3-C4-C5	-7.01	125.09	128.60
38	8	20	U	O5'-P-OP2	-7.01	99.39	105.70
1	2	1473	U	N3-C2-O2	-7.01	117.30	122.20
36	1	2892	A	N1-C6-N6	-7.01	114.40	118.60
36	5	1200	A	N1-C6-N6	7.00	122.80	118.60
36	1	1481	A	O5'-P-OP1	7.00	119.10	110.70
36	1	3244	A	N1-C6-N6	7.00	122.80	118.60
36	1	1793	C	C5-C6-N1	-7.00	117.50	121.00
36	5	283	G	C4-C5-N7	7.00	113.60	110.80
36	5	949	C	C4-C5-C6	7.00	120.90	117.40
1	2	1241	G	O4'-C1'-N9	6.99	113.80	108.20
36	1	517	G	C4-N9-C1'	6.99	135.59	126.50
36	1	1157	G	N9-C4-C5	6.99	108.20	105.40
1	6	387	A	N1-C6-N6	-6.99	114.41	118.60
36	5	1858	A	O4'-C1'-N9	6.99	113.79	108.20
36	1	2347	U	O5'-P-OP2	-6.99	99.41	105.70
1	6	755	A	O4'-C1'-N9	6.99	113.79	108.20
36	5	3245	A	C5-N7-C8	-6.99	100.41	103.90
36	5	2273	G	C5-C6-N1	6.98	114.99	111.50
36	5	2980	U	O5'-P-OP1	6.98	119.08	110.70
36	5	1484	U	C6-N1-C2	6.98	125.19	121.00
36	1	576	C	C6-N1-C2	6.98	123.09	120.30
1	6	617	U	C2-N1-C1'	6.98	126.07	117.70
36	5	940	G	C5-C6-O6	-6.98	124.41	128.60
36	1	942	U	N3-C4-O4	6.98	124.28	119.40
36	1	339	C	N1-C2-N3	6.97	124.08	119.20
36	1	789	A	C5-C6-N6	6.97	129.28	123.70
36	5	1507	G	O5'-P-OP1	-6.97	99.42	105.70
1	6	144	U	O4'-C1'-N1	6.97	113.78	108.20
1	6	1535	U	N1-C2-O2	6.97	127.68	122.80
36	1	1048	A	N1-C6-N6	-6.97	114.42	118.60
36	1	1683	A	N1-C6-N6	6.97	122.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2140	U	C5-C4-O4	6.97	130.08	125.90
1	6	558	U	N1-C2-O2	6.97	127.68	122.80
1	6	1634	C	N1-C2-O2	6.96	123.08	118.90
36	5	2913	C	N3-C4-C5	-6.96	119.11	121.90
36	1	2400	G	C5-C6-O6	-6.96	124.42	128.60
1	6	794	U	C2-N1-C1'	6.96	126.05	117.70
36	1	1332	A	O5'-P-OP1	-6.95	99.44	105.70
36	5	2353	G	N1-C6-O6	6.95	124.07	119.90
36	1	713	U	C5-C6-N1	-6.95	119.23	122.70
40	l3	4	ARG	NE-CZ-NH1	6.95	123.77	120.30
36	5	1305	U	O5'-P-OP1	-6.95	99.45	105.70
36	1	116	A	O4'-C1'-N9	6.94	113.75	108.20
36	1	1306	G	C8-N9-C4	6.94	109.18	106.40
36	1	3181	C	N3-C4-N4	-6.94	113.14	118.00
1	6	337	G	C4-C5-N7	6.94	113.58	110.80
36	5	1472	U	C5-C4-O4	-6.93	121.74	125.90
36	1	2621	G	N1-C2-N2	6.93	122.44	116.20
36	1	1820	U	P-O3'-C3'	6.93	128.01	119.70
36	1	1158	A	C6-C5-N7	-6.92	127.45	132.30
36	1	2393	G	N1-C6-O6	6.92	124.06	119.90
36	1	351	A	N1-C6-N6	-6.92	114.45	118.60
36	1	1082	U	C6-N1-C2	-6.92	116.85	121.00
36	5	859	G	O5'-P-OP1	-6.92	99.47	105.70
36	5	2295	A	O5'-P-OP2	-6.92	99.48	105.70
1	2	1314	U	N3-C2-O2	-6.91	117.36	122.20
36	5	821	U	N1-C2-O2	-6.91	117.96	122.80
36	5	2639	G	C8-N9-C1'	-6.91	118.02	127.00
36	5	3364	C	C6-N1-C2	-6.91	117.54	120.30
1	2	1092	A	N1-C6-N6	6.91	122.74	118.60
1	6	1641	C	N3-C2-O2	6.91	126.73	121.90
36	5	2339	C	O4'-C1'-N1	-6.91	102.68	108.20
1	6	136	C	C2-N1-C1'	6.90	126.39	118.80
1	6	543	C	C5-C6-N1	6.90	124.45	121.00
36	5	662	U	O5'-P-OP1	-6.90	99.49	105.70
36	1	2403	G	N9-C4-C5	-6.90	102.64	105.40
36	5	1928	G	C5-C6-O6	-6.90	124.46	128.60
36	1	2772	C	C2-N1-C1'	6.90	126.39	118.80
37	7	27	A	N1-C6-N6	-6.90	114.46	118.60
36	5	2199	G	C5-N7-C8	-6.90	100.85	104.30
36	1	2816	G	N1-C6-O6	6.90	124.04	119.90
1	6	1478	G	C4-N9-C1'	6.90	135.47	126.50
36	1	339	C	C6-N1-C2	-6.89	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1307	G	P-O3'-C3'	6.89	127.97	119.70
36	1	2408	U	O5'-P-OP1	-6.89	99.50	105.70
36	5	2385	G	C2-N3-C4	-6.89	108.45	111.90
36	1	2279	A	N1-C6-N6	6.89	122.73	118.60
36	5	926	A	C2-N3-C4	-6.89	107.16	110.60
36	1	613	G	C5-C6-O6	-6.89	124.47	128.60
1	2	1131	A	O5'-P-OP1	-6.88	99.51	105.70
36	5	1902	G	N9-C4-C5	-6.88	102.65	105.40
36	5	1833	G	N1-C6-O6	-6.88	115.77	119.90
36	5	1500	G	C8-N9-C4	6.88	109.15	106.40
36	1	587	U	N3-C4-C5	6.88	118.73	114.60
36	5	1117	G	O5'-P-OP1	-6.88	99.51	105.70
1	6	1300	A	O5'-P-OP1	-6.88	99.51	105.70
36	1	2846	U	N3-C4-O4	-6.87	114.59	119.40
36	5	1309	U	N1-C2-O2	-6.87	117.99	122.80
36	1	285	A	N1-C6-N6	6.87	122.72	118.60
36	1	895	A	N1-C6-N6	6.87	122.72	118.60
1	2	380	U	N3-C2-O2	-6.87	117.39	122.20
1	2	1274	C	N3-C4-N4	-6.87	113.19	118.00
36	1	2606	G	C6-C5-N7	-6.87	126.28	130.40
36	5	587	U	C6-N1-C2	6.87	125.12	121.00
1	2	1486	G	C5-N7-C8	-6.86	100.87	104.30
36	5	2406	C	N1-C2-O2	-6.86	114.78	118.90
37	7	27	A	N9-C4-C5	6.85	108.54	105.80
36	1	1313	G	C5-C6-O6	-6.85	124.49	128.60
1	6	1299	G	N3-C4-C5	-6.85	125.17	128.60
36	1	1113	G	C5-C6-N1	-6.85	108.08	111.50
36	1	1476	G	N1-C6-O6	-6.85	115.79	119.90
36	5	1788	C	C6-N1-C2	-6.84	117.56	120.30
36	5	1391	C	N1-C2-O2	-6.84	114.80	118.90
36	5	1803	C	C6-N1-C2	6.84	123.04	120.30
36	1	1334	U	N1-C2-N3	6.84	119.00	114.90
36	5	2808	A	C8-N9-C4	6.84	108.53	105.80
1	6	805	U	O5'-P-OP1	-6.84	99.55	105.70
1	6	1560	U	N3-C2-O2	-6.84	117.42	122.20
1	6	400	A	O5'-P-OP2	-6.83	99.55	105.70
36	5	1494	U	C2-N1-C1'	-6.83	109.50	117.70
36	5	914	A	N1-C6-N6	6.83	122.70	118.60
1	2	352	A	C8-N9-C4	6.83	108.53	105.80
36	1	142	C	C6-N1-C2	-6.83	117.57	120.30
36	5	636	C	C6-N1-C2	6.83	123.03	120.30
36	5	1124	U	N3-C4-C5	6.83	118.70	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2836	C	N3-C2-O2	-6.83	117.12	121.90
1	2	1399	C	C5-C6-N1	6.82	124.41	121.00
36	5	2993	G	C4-C5-N7	6.82	113.53	110.80
36	5	3137	C	O5'-P-OP2	-6.82	99.56	105.70
36	1	339	C	N3-C2-O2	-6.82	117.13	121.90
36	1	2784	G	N3-C4-N9	6.82	130.09	126.00
1	2	190	C	O4'-C1'-N1	6.81	113.65	108.20
36	1	810	A	N1-C6-N6	-6.81	114.51	118.60
36	1	1846	C	N3-C4-C5	-6.81	119.17	121.90
1	6	1751	C	C6-N1-C2	6.81	123.03	120.30
37	7	92	A	C8-N9-C4	6.81	108.52	105.80
36	5	648	C	O5'-P-OP1	-6.81	99.57	105.70
36	1	1836	C	N1-C2-O2	6.80	122.98	118.90
1	6	1479	A	N1-C6-N6	6.80	122.68	118.60
36	5	1850	A	C5-C6-N1	-6.80	114.30	117.70
1	6	17	C	C6-N1-C2	-6.80	117.58	120.30
36	5	2403	G	O5'-P-OP2	-6.80	99.58	105.70
37	7	92	A	C5-C6-N6	-6.80	118.26	123.70
36	1	651	G	N3-C4-C5	-6.80	125.20	128.60
36	5	947	G	N3-C4-C5	-6.80	125.20	128.60
35	SM	167	PRO	N-CA-CB	6.80	111.45	103.30
36	5	1000	C	C6-N1-C2	6.80	123.02	120.30
36	5	3121	U	C5-C4-O4	6.80	129.98	125.90
36	5	2943	G	N1-C6-O6	6.79	123.98	119.90
36	1	2692	A	N1-C6-N6	6.79	122.67	118.60
38	8	100	U	C5-C4-O4	-6.79	121.83	125.90
36	1	49	A	N1-C6-N6	6.78	122.67	118.60
36	5	890	C	N3-C2-O2	-6.78	117.15	121.90
38	4	53	A	C5-C6-N1	6.78	121.09	117.70
31	D9	36	LEU	CA-CB-CG	6.78	130.89	115.30
36	1	1835	A	O5'-P-OP1	-6.78	99.60	105.70
36	5	661	G	O5'-P-OP1	-6.78	99.60	105.70
36	1	2144	A	C5-C6-N6	-6.78	118.28	123.70
36	5	655	C	C6-N1-C2	-6.78	117.59	120.30
36	1	225	C	C5-C4-N4	-6.77	115.46	120.20
36	1	843	A	N1-C6-N6	6.77	122.66	118.60
36	1	2808	A	N1-C6-N6	6.77	122.66	118.60
36	1	585	A	C8-N9-C4	6.77	108.51	105.80
1	6	1473	U	C2-N1-C1'	6.77	125.82	117.70
36	5	2116	G	N1-C6-O6	6.77	123.96	119.90
1	2	132	U	P-O3'-C3'	6.77	127.82	119.70
36	1	2923	U	O5'-P-OP1	-6.76	99.61	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1452	A	C2-N3-C4	-6.76	107.22	110.60
36	1	3278	C	C2-N1-C1'	6.76	126.24	118.80
36	5	343	U	N1-C2-O2	-6.76	118.07	122.80
1	6	1481	C	C6-N1-C2	-6.76	117.60	120.30
36	5	2550	U	C5-C4-O4	6.76	129.96	125.90
1	2	736	C	C2-N1-C1'	6.76	126.23	118.80
1	2	1082	C	C6-N1-C2	-6.76	117.60	120.30
36	5	1384	U	N3-C4-C5	-6.76	110.55	114.60
36	5	2954	U	C2-N1-C1'	6.75	125.81	117.70
36	1	1906	G	C5-C6-O6	-6.75	124.55	128.60
1	6	30	G	N3-C2-N2	-6.75	115.17	119.90
1	2	830	U	N3-C2-O2	-6.75	117.48	122.20
37	7	87	G	C5-C6-O6	-6.75	124.55	128.60
36	5	365	A	N1-C6-N6	6.75	122.65	118.60
36	5	3154	C	N3-C2-O2	-6.75	117.18	121.90
1	6	1481	C	N3-C2-O2	-6.74	117.18	121.90
36	5	894	G	N1-C2-N2	-6.74	110.13	116.20
36	5	2870	C	C2-N1-C1'	-6.74	111.39	118.80
36	5	217	U	OP1-P-O3'	6.73	120.02	105.20
36	1	103	G	N1-C6-O6	-6.73	115.86	119.90
36	5	1876	U	C6-N1-C2	-6.73	116.96	121.00
36	1	218	G	O5'-P-OP2	-6.73	99.64	105.70
36	1	2878	G	N9-C4-C5	-6.73	102.71	105.40
36	1	2169	G	C6-C5-N7	6.72	134.44	130.40
36	1	3275	U	C5-C6-N1	6.72	126.06	122.70
36	1	913	A	C4-C5-C6	6.72	120.36	117.00
36	1	1606	U	N1-C2-O2	-6.72	118.09	122.80
36	1	39	A	C2-N3-C4	-6.72	107.24	110.60
36	5	1902	G	C8-N9-C1'	-6.72	118.26	127.00
1	2	1568	C	P-O3'-C3'	6.72	127.76	119.70
36	5	1796	G	C5-C6-O6	6.72	132.63	128.60
36	1	343	U	N1-C2-N3	6.71	118.93	114.90
36	1	1842	A	N1-C6-N6	-6.71	114.57	118.60
36	1	2242	A	N1-C2-N3	6.71	132.66	129.30
52	M6	78	ARG	NE-CZ-NH1	6.71	123.66	120.30
37	7	73	C	C5-C6-N1	6.71	124.36	121.00
36	1	2714	G	C8-N9-C1'	6.71	135.72	127.00
25	d3	16	ARG	NE-CZ-NH2	-6.71	116.94	120.30
36	5	1161	G	N1-C6-O6	-6.71	115.87	119.90
36	1	885	U	N3-C2-O2	-6.71	117.50	122.20
36	1	868	C	C6-N1-C2	6.71	122.98	120.30
38	8	104	A	C8-N9-C4	6.71	108.48	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2836	C	C5-C4-N4	6.71	124.89	120.20
38	4	113	U	C5-C4-O4	6.71	129.92	125.90
36	5	2728	G	C4-C5-N7	-6.71	108.12	110.80
36	1	2307	G	C4-C5-N7	-6.70	108.12	110.80
36	5	3133	C	N1-C2-O2	-6.70	114.88	118.90
36	1	805	G	C5-C6-O6	-6.70	124.58	128.60
36	5	776	U	N3-C2-O2	-6.70	117.51	122.20
41	14	339	LEU	CA-CB-CG	6.70	130.71	115.30
36	5	922	U	C4-C5-C6	6.70	123.72	119.70
36	1	1367	G	C6-C5-N7	-6.70	126.38	130.40
36	1	2195	C	O5'-P-OP2	-6.70	99.67	105.70
36	5	835	G	C4-C5-N7	6.70	113.48	110.80
36	1	1202	A	O5'-P-OP2	-6.69	99.68	105.70
36	1	1607	U	O5'-P-OP2	-6.69	99.68	105.70
36	1	1675	G	N1-C6-O6	-6.69	115.89	119.90
36	1	1049	C	O5'-P-OP2	-6.69	99.68	105.70
36	1	1157	G	C4-C5-N7	-6.69	108.12	110.80
36	1	2513	U	O4'-C1'-N1	6.69	113.55	108.20
36	5	1834	U	C6-N1-C2	-6.69	116.99	121.00
36	1	922	U	N1-C2-O2	6.68	127.48	122.80
36	1	1662	G	N1-C6-O6	6.68	123.91	119.90
36	1	1891	A	C8-N9-C4	6.68	108.47	105.80
1	6	1028	C	C5-C6-N1	-6.68	117.66	121.00
36	1	746	A	N1-C6-N6	6.68	122.61	118.60
36	1	1848	G	C5-C6-O6	-6.68	124.59	128.60
36	1	2409	G	C6-C5-N7	-6.68	126.39	130.40
36	1	718	G	C5-N7-C8	-6.68	100.96	104.30
36	1	2714	G	C4-N9-C1'	-6.67	117.83	126.50
36	1	1316	C	C4-C5-C6	6.66	120.73	117.40
36	5	43	A	C8-N9-C4	6.66	108.47	105.80
36	5	2957	G	O5'-P-OP1	-6.66	99.70	105.70
37	3	95	A	N1-C6-N6	6.66	122.60	118.60
36	1	895	A	C2-N3-C4	-6.66	107.27	110.60
37	3	92	A	N1-C6-N6	6.66	122.60	118.60
36	1	1396	C	N1-C2-N3	-6.66	114.54	119.20
36	1	2176	U	N3-C2-O2	-6.66	117.54	122.20
36	5	2282	U	O5'-P-OP1	-6.66	99.71	105.70
36	1	1365	G	C8-N9-C4	-6.65	103.74	106.40
36	5	645	A	C6-N1-C2	-6.65	114.61	118.60
1	6	1121	C	O5'-P-OP2	-6.65	99.71	105.70
36	5	76	G	C8-N9-C4	6.65	109.06	106.40
36	5	873	C	P-O3'-C3'	6.65	127.68	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	651	G	N3-C2-N2	6.64	124.55	119.90
36	1	92	G	C5-C6-N1	6.64	114.82	111.50
1	6	1614	A	C5-N7-C8	-6.64	100.58	103.90
36	1	2661	G	O5'-P-OP1	-6.64	99.72	105.70
36	1	1150	A	O5'-P-OP2	-6.64	99.73	105.70
36	5	2931	C	N1-C2-O2	-6.64	114.92	118.90
17	c5	36	LEU	CA-CB-CG	6.63	130.56	115.30
36	1	996	A	N1-C6-N6	-6.63	114.62	118.60
36	1	2379	U	N1-C2-O2	-6.63	118.16	122.80
36	5	2166	A	C8-N9-C4	6.63	108.45	105.80
1	2	1082	C	N3-C2-O2	-6.63	117.26	121.90
36	1	1428	A	N1-C6-N6	6.63	122.58	118.60
36	1	979	U	O4'-C1'-N1	6.62	113.50	108.20
36	1	981	U	C5-C6-N1	6.62	126.01	122.70
36	5	2350	C	OP1-P-OP2	-6.62	109.66	119.60
36	1	2836	C	C5-C6-N1	-6.62	117.69	121.00
36	1	1363	A	O5'-P-OP2	-6.62	99.74	105.70
36	1	960	U	N3-C4-O4	-6.62	114.77	119.40
36	1	701	G	N1-C6-O6	6.62	123.87	119.90
36	1	718	G	C6-C5-N7	-6.62	126.43	130.40
1	2	1487	A	O5'-P-OP1	-6.61	99.75	105.70
36	1	2846	U	N1-C2-O2	6.61	127.43	122.80
36	5	1868	G	C4-C5-N7	6.61	113.44	110.80
36	5	2116	G	C6-C5-N7	-6.61	126.43	130.40
37	7	117	A	C2-N3-C4	-6.61	107.30	110.60
36	1	1366	A	O5'-P-OP2	-6.61	99.75	105.70
36	5	2371	G	N3-C2-N2	6.61	124.53	119.90
38	8	33	A	N9-C4-C5	-6.61	103.16	105.80
70	O4	8	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	2	1596	C	N3-C2-O2	-6.60	117.28	121.90
36	1	3311	C	O5'-P-OP1	-6.60	99.76	105.70
38	8	8	C	C6-N1-C2	-6.60	117.66	120.30
1	6	364	G	C8-N9-C4	6.60	109.04	106.40
36	5	437	G	N7-C8-N9	6.60	116.40	113.10
64	n8	73	LEU	CA-CB-CG	6.60	130.48	115.30
1	6	453	U	C6-N1-C2	-6.60	117.04	121.00
1	6	453	U	N1-C2-O2	6.60	127.42	122.80
36	5	2870	C	C6-N1-C1'	6.60	128.72	120.80
36	5	2162	U	C5-C6-N1	-6.59	119.40	122.70
36	5	2372	A	N3-C4-C5	-6.59	122.19	126.80
36	1	815	G	C4-C5-N7	6.59	113.44	110.80
1	6	1654	G	C4-C5-N7	6.59	113.43	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2353	G	C5-C6-O6	-6.58	124.65	128.60
1	6	382	C	C2-N3-C4	-6.58	116.61	119.90
54	M8	178	ARG	NE-CZ-NH1	-6.58	117.01	120.30
36	1	1450	G	C5-C6-O6	-6.58	124.65	128.60
36	1	2377	G	N3-C2-N2	6.58	124.51	119.90
36	1	3277	U	N3-C2-O2	-6.58	117.59	122.20
1	6	647	G	N3-C2-N2	-6.58	115.30	119.90
36	5	2932	U	N3-C2-O2	-6.58	117.60	122.20
36	1	1008	U	C5-C4-O4	6.58	129.85	125.90
36	1	2881	C	C6-N1-C2	6.58	122.93	120.30
36	1	3212	C	C5-C6-N1	-6.58	117.71	121.00
36	1	283	G	C4-C5-N7	6.57	113.43	110.80
36	5	546	C	N1-C2-O2	6.57	122.84	118.90
1	2	1490	C	C6-N1-C2	-6.57	117.67	120.30
36	5	622	A	N1-C6-N6	6.57	122.54	118.60
36	1	648	C	C6-N1-C1'	-6.56	112.92	120.80
1	2	1600	A	C2-N3-C4	-6.56	107.32	110.60
36	1	1164	G	N1-C6-O6	-6.56	115.96	119.90
36	5	883	A	C8-N9-C4	6.56	108.42	105.80
36	5	2978	U	O4'-C1'-N1	6.56	113.45	108.20
77	Q1	13	LEU	CA-CB-CG	6.56	130.39	115.30
36	5	669	U	N1-C2-N3	6.56	118.84	114.90
36	1	2617	U	C5-C6-N1	-6.56	119.42	122.70
36	5	2358	A	C8-N9-C4	6.56	108.42	105.80
36	1	2983	C	C4-C5-C6	6.55	120.68	117.40
36	5	1124	U	C4-C5-C6	-6.55	115.77	119.70
36	5	2815	G	C8-N9-C4	6.55	109.02	106.40
37	7	92	A	N1-C2-N3	-6.55	126.02	129.30
36	1	397	A	N1-C6-N6	-6.55	114.67	118.60
1	6	364	G	N3-C4-N9	6.55	129.93	126.00
36	1	2724	U	N3-C2-O2	-6.55	117.61	122.20
36	1	2943	G	C4-C5-N7	6.55	113.42	110.80
36	5	340	C	C5-C6-N1	-6.55	117.72	121.00
36	1	1447	G	N1-C6-O6	-6.55	115.97	119.90
36	5	717	C	N1-C2-O2	-6.55	114.97	118.90
37	7	92	A	N1-C6-N6	6.55	122.53	118.60
36	1	1192	C	C6-N1-C2	-6.55	117.68	120.30
36	5	2980	U	N1-C2-N3	6.54	118.83	114.90
36	1	1595	U	N3-C2-O2	6.54	126.78	122.20
36	5	682	U	O5'-P-OP1	-6.54	99.81	105.70
36	5	412	G	N3-C4-C5	-6.54	125.33	128.60
36	1	803	C	O5'-P-OP1	6.54	118.55	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	13	A	O5'-P-OP1	-6.54	99.81	105.70
1	2	1339	C	P-O3'-C3'	6.54	127.54	119.70
36	1	1148	G	N9-C4-C5	-6.53	102.79	105.40
36	5	1152	G	N1-C2-N2	6.53	122.08	116.20
37	7	87	G	N1-C6-O6	6.53	123.82	119.90
36	1	2400	G	N1-C6-O6	6.53	123.82	119.90
36	1	2946	A	N1-C6-N6	6.53	122.52	118.60
36	5	395	A	N1-C6-N6	6.52	122.51	118.60
36	5	644	G	N9-C4-C5	6.52	108.01	105.40
36	1	1906	G	N1-C6-O6	6.52	123.81	119.90
36	5	217	U	C5-C6-N1	-6.52	119.44	122.70
36	5	1895	A	N1-C6-N6	-6.52	114.69	118.60
36	5	3098	G	N3-C4-C5	-6.52	125.34	128.60
56	n0	155	ARG	NE-CZ-NH2	6.52	123.56	120.30
37	7	83	U	O5'-P-OP2	-6.51	99.84	105.70
42	L5	146	LEU	CA-CB-CG	6.51	130.27	115.30
1	6	334	G	C5-C6-N1	6.51	114.75	111.50
36	1	1150	A	N1-C6-N6	-6.51	114.69	118.60
36	5	2142	A	OP1-P-O3'	6.51	119.52	105.20
1	6	647	G	N3-C4-C5	6.51	131.85	128.60
36	5	346	C	N3-C2-O2	-6.51	117.35	121.90
36	5	1004	U	N1-C2-O2	6.51	127.36	122.80
36	1	3362	A	C6-C5-N7	-6.50	127.75	132.30
36	1	2377	G	C2-N3-C4	-6.50	108.65	111.90
1	6	144	U	C6-N1-C2	-6.50	117.10	121.00
36	5	2719	U	C2-N1-C1'	-6.50	109.89	117.70
36	1	933	A	N1-C2-N3	6.50	132.55	129.30
36	1	2550	U	N3-C2-O2	-6.50	117.65	122.20
36	5	1938	U	C5-C6-N1	-6.50	119.45	122.70
1	2	1280	C	C6-N1-C2	-6.50	117.70	120.30
36	1	3097	C	O5'-P-OP2	-6.50	99.86	105.70
36	5	1113	G	C2-N3-C4	-6.50	108.65	111.90
36	5	682	U	C5-C4-O4	6.49	129.80	125.90
36	5	923	C	N3-C2-O2	-6.49	117.36	121.90
36	5	1716	U	P-O3'-C3'	6.49	127.49	119.70
36	5	2372	A	P-O3'-C3'	6.49	127.49	119.70
36	1	2257	C	C2-N1-C1'	6.49	125.94	118.80
36	5	2944	U	N3-C2-O2	-6.49	117.66	122.20
36	5	3181	C	C5-C6-N1	6.49	124.24	121.00
36	5	2639	G	C4-C5-C6	6.49	122.69	118.80
36	5	3136	G	N1-C2-N3	6.49	127.79	123.90
36	1	948	C	C4-C5-C6	6.48	120.64	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1662	G	C4-C5-N7	6.48	113.39	110.80
1	6	56	U	C5-C6-N1	-6.48	119.46	122.70
1	2	728	U	N1-C2-O2	6.48	127.34	122.80
1	6	1634	C	C6-N1-C2	-6.48	117.71	120.30
36	1	111	C	C6-N1-C2	6.48	122.89	120.30
36	1	1396	C	C5-C4-N4	-6.48	115.67	120.20
36	1	3362	A	N1-C6-N6	6.48	122.49	118.60
38	4	23	U	N1-C2-O2	-6.48	118.27	122.80
36	1	2172	A	C8-N9-C4	6.48	108.39	105.80
36	1	2617	U	C4-C5-C6	6.47	123.58	119.70
36	1	644	G	C2-N3-C4	-6.47	108.66	111.90
36	1	2948	C	N3-C4-C5	6.47	124.49	121.90
38	4	113	U	C5-C6-N1	-6.47	119.46	122.70
36	5	421	G	C4-N9-C1'	6.47	134.91	126.50
36	1	1365	G	C6-C5-N7	-6.47	126.52	130.40
36	1	1269	U	C2-N1-C1'	6.46	125.46	117.70
36	1	2719	U	N1-C2-O2	-6.46	118.28	122.80
36	1	2417	U	N1-C2-N3	6.46	118.78	114.90
36	5	960	U	N3-C2-O2	-6.46	117.68	122.20
36	5	1081	U	C2-N1-C1'	6.46	125.46	117.70
36	5	1428	A	C8-N9-C4	6.46	108.38	105.80
36	1	730	C	N3-C4-C5	6.46	124.48	121.90
36	1	1481	A	N1-C6-N6	6.46	122.47	118.60
1	6	119	A	C2-N3-C4	-6.46	107.37	110.60
36	5	2943	G	C5-C6-O6	-6.46	124.73	128.60
36	5	3382	U	C2-N1-C1'	6.46	125.44	117.70
36	1	908	G	N1-C6-O6	6.45	123.77	119.90
36	1	1047	A	O5'-P-OP2	-6.45	99.90	105.70
36	5	1907	C	N1-C2-N3	6.44	123.71	119.20
36	1	1365	G	N3-C2-N2	6.44	124.41	119.90
36	5	669	U	C2-N3-C4	-6.44	123.14	127.00
36	5	2816	G	C4-C5-N7	6.44	113.38	110.80
36	1	2984	C	N1-C2-N3	6.44	123.71	119.20
36	1	3175	U	O5'-P-OP2	-6.44	99.90	105.70
36	5	2215	A	N9-C4-C5	-6.44	103.22	105.80
36	5	2689	A	C4-C5-C6	6.44	120.22	117.00
37	7	27	A	C8-N9-C4	-6.44	103.22	105.80
36	1	1367	G	N1-C6-O6	6.44	123.76	119.90
36	5	1620	U	N3-C2-O2	-6.44	117.69	122.20
36	1	3181	C	N3-C2-O2	-6.44	117.39	121.90
36	5	3181	C	C6-N1-C2	-6.44	117.72	120.30
1	2	328	A	N1-C6-N6	6.43	122.46	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	628	A	C8-N9-C4	6.43	108.37	105.80
36	5	2833	A	N1-C2-N3	6.43	132.52	129.30
36	5	2884	C	N1-C2-O2	-6.43	115.04	118.90
36	5	1139	G	C5-C6-O6	6.43	132.46	128.60
36	5	3327	G	C6-C5-N7	-6.43	126.54	130.40
36	1	2984	C	N3-C4-N4	-6.42	113.50	118.00
36	5	1303	A	N1-C6-N6	6.42	122.45	118.60
36	5	3022	G	O4'-C1'-N9	6.42	113.34	108.20
36	5	2305	G	C8-N9-C4	-6.42	103.83	106.40
36	5	1322	U	C5-C4-O4	-6.42	122.05	125.90
36	1	939	U	C2-N3-C4	-6.42	123.15	127.00
35	sM	167	PRO	N-CA-CB	6.42	111.00	103.30
36	5	2704	A	OP1-P-OP2	6.41	129.22	119.60
38	8	104	A	C2-N3-C4	-6.41	107.39	110.60
36	1	282	G	N1-C6-O6	-6.41	116.05	119.90
36	1	1931	U	C2-N1-C1'	-6.41	110.00	117.70
36	1	3275	U	OP1-P-O3'	6.41	119.31	105.20
36	5	3207	U	N1-C2-O2	-6.41	118.31	122.80
36	5	2830	G	C6-N1-C2	-6.41	121.25	125.10
36	5	2145	A	C5-C6-N1	6.41	120.90	117.70
36	5	2383	C	N1-C2-O2	-6.41	115.06	118.90
36	5	2873	U	C4-C5-C6	6.41	123.54	119.70
36	1	295	A	N7-C8-N9	6.41	117.00	113.80
36	5	1863	G	C5-C6-N1	6.41	114.70	111.50
36	1	1180	A	O4'-C1'-N9	-6.40	103.08	108.20
36	5	2880	U	C5-C4-O4	6.40	129.74	125.90
36	1	608	A	N9-C4-C5	-6.40	103.24	105.80
36	5	2726	C	N3-C4-N4	-6.40	113.52	118.00
1	6	639	U	N1-C2-O2	6.40	127.28	122.80
1	2	1560	U	C5-C4-O4	6.40	129.74	125.90
36	1	2758	A	N1-C2-N3	-6.40	126.10	129.30
36	5	873	C	OP2-P-O3'	6.40	119.28	105.20
36	1	286	U	N3-C2-O2	-6.40	117.72	122.20
36	5	1904	C	C6-N1-C2	-6.40	117.74	120.30
36	1	2646	C	C5-C6-N1	-6.39	117.80	121.00
36	5	842	G	C5-C6-O6	-6.39	124.76	128.60
36	5	3351	U	N3-C2-O2	-6.39	117.72	122.20
1	6	630	A	C2-N3-C4	-6.39	107.40	110.60
36	5	2830	G	N3-C4-N9	6.39	129.84	126.00
36	5	2371	G	N1-C2-N2	-6.39	110.45	116.20
36	1	1146	C	N1-C2-O2	6.39	122.73	118.90
36	1	2827	U	N3-C2-O2	-6.39	117.73	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	3	5	G	N3-C4-C5	6.39	131.79	128.60
36	1	2599	U	C6-N1-C2	-6.39	117.17	121.00
36	1	1489	A	C5-C6-N6	-6.38	118.59	123.70
36	1	2836	C	N3-C4-N4	-6.38	113.53	118.00
36	5	2819	A	N9-C4-C5	6.38	108.35	105.80
36	1	1838	G	C6-C5-N7	-6.38	126.57	130.40
36	1	3362	A	N1-C2-N3	6.38	132.49	129.30
64	N8	116	GLY	N-CA-C	6.38	129.05	113.10
1	6	316	A	C8-N9-C4	6.38	108.35	105.80
36	5	2392	C	C6-N1-C2	6.38	122.85	120.30
36	5	650	C	C5-C6-N1	-6.38	117.81	121.00
36	5	1536	G	N3-C2-N2	-6.38	115.44	119.90
36	5	2772	C	P-O3'-C3'	6.38	127.35	119.70
36	5	894	G	N3-C4-N9	6.37	129.82	126.00
36	5	2931	C	N3-C2-O2	6.37	126.36	121.90
36	5	3306	U	N3-C4-C5	6.37	118.42	114.60
36	1	192	C	C6-N1-C2	-6.37	117.75	120.30
36	1	2314	U	C6-N1-C1'	-6.37	112.28	121.20
37	3	53	U	N1-C2-O2	-6.37	118.34	122.80
36	5	1476	G	C8-N9-C4	6.37	108.95	106.40
36	5	2372	A	OP2-P-O3'	6.37	119.21	105.20
36	1	1406	A	N1-C6-N6	6.37	122.42	118.60
36	5	1440	G	N3-C4-N9	-6.37	122.18	126.00
36	5	2290	C	C6-N1-C2	6.37	122.85	120.30
36	1	2314	U	C4-C5-C6	-6.37	115.88	119.70
36	5	1592	G	C6-N1-C2	6.37	128.92	125.10
36	1	1902	G	C5-C6-O6	-6.37	124.78	128.60
1	6	1640	C	N1-C2-O2	6.37	122.72	118.90
36	1	1307	G	C2'-C3'-O3'	6.36	123.88	113.70
36	5	1889	G	N3-C4-N9	6.36	129.82	126.00
38	4	32	C	C2-N1-C1'	-6.36	111.81	118.80
36	5	1392	G	N9-C4-C5	-6.36	102.86	105.40
1	6	558	U	C2-N1-C1'	6.36	125.33	117.70
36	5	642	U	N3-C2-O2	-6.36	117.75	122.20
36	5	1160	C	C2-N1-C1'	-6.35	111.81	118.80
1	2	448	C	N3-C4-C5	-6.35	119.36	121.90
1	2	507	U	N3-C2-O2	-6.35	117.76	122.20
36	1	1848	G	N1-C6-O6	6.35	123.71	119.90
36	1	2281	A	O5'-P-OP2	-6.35	99.99	105.70
36	1	2996	U	C6-N1-C1'	-6.35	112.32	121.20
36	5	2931	C	N3-C4-N4	6.35	122.44	118.00
36	1	648	C	N1-C2-O2	6.34	122.71	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	337	G	N9-C4-C5	-6.34	102.86	105.40
36	1	2403	G	O5'-P-OP1	6.34	118.31	110.70
36	1	1157	G	O5'-P-OP2	-6.34	99.99	105.70
36	1	2948	C	N3-C4-N4	-6.34	113.56	118.00
1	6	1025	A	C8-N9-C4	6.34	108.34	105.80
36	5	1190	A	C8-N9-C4	-6.34	103.26	105.80
36	5	1370	G	N1-C6-O6	-6.34	116.10	119.90
36	5	2169	G	N1-C6-O6	-6.34	116.10	119.90
36	1	1453	A	C8-N9-C4	-6.34	103.27	105.80
36	1	2283	G	N1-C6-O6	6.34	123.70	119.90
1	6	1640	C	C2-N1-C1'	6.34	125.77	118.80
36	5	2639	G	N3-C4-C5	-6.33	125.43	128.60
36	5	3208	G	C6-C5-N7	-6.33	126.60	130.40
36	1	2927	C	N1-C2-O2	-6.33	115.10	118.90
1	2	440	U	N3-C4-O4	-6.33	114.97	119.40
1	2	1679	G	N1-C6-O6	-6.33	116.10	119.90
36	1	2899	C	N1-C2-O2	6.33	122.70	118.90
36	5	2199	G	C5-C6-O6	-6.33	124.80	128.60
36	5	2601	A	N1-C6-N6	-6.33	114.80	118.60
36	5	963	G	O5'-P-OP2	-6.33	100.01	105.70
36	1	974	G	C5-C6-O6	-6.32	124.81	128.60
41	L4	76	ARG	NE-CZ-NH1	-6.32	117.14	120.30
36	1	584	G	C5-C6-O6	6.32	132.39	128.60
36	5	41	G	OP2-P-O3'	6.32	119.10	105.20
1	2	39	A	O4'-C1'-N9	6.32	113.25	108.20
36	1	644	G	N1-C2-N2	-6.32	110.51	116.20
36	1	785	G	N3-C4-C5	-6.32	125.44	128.60
36	1	1305	U	C5-C4-O4	6.32	129.69	125.90
36	1	1396	C	N3-C2-O2	6.32	126.32	121.90
36	5	2775	U	C5-C4-O4	6.32	129.69	125.90
37	7	92	A	C4-C5-N7	6.32	113.86	110.70
1	2	1761	U	C6-N1-C2	-6.32	117.21	121.00
1	6	1039	A	O4'-C1'-N9	6.32	113.25	108.20
36	1	608	A	C4-C5-C6	6.31	120.16	117.00
36	1	2679	A	C2-N3-C4	-6.31	107.44	110.60
36	1	2984	C	C6-N1-C2	-6.31	117.77	120.30
36	1	49	A	C2-N3-C4	-6.31	107.44	110.60
36	5	1437	C	C2-N1-C1'	6.31	125.74	118.80
38	4	21	C	C6-N1-C2	6.31	122.82	120.30
36	5	838	G	N3-C4-N9	-6.31	122.22	126.00
1	2	1414	U	N1-C2-O2	6.30	127.21	122.80
36	1	2351	U	N1-C2-O2	6.30	127.21	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2694	A	O5'-P-OP2	-6.30	100.03	105.70
36	1	3244	A	O4'-C1'-N9	-6.30	103.16	108.20
36	5	866	A	C8-N9-C4	6.30	108.32	105.80
36	5	2320	A	C5-C6-N1	-6.30	114.55	117.70
36	1	645	A	C2-N3-C4	6.30	113.75	110.60
36	1	3362	A	C4-C5-N7	6.30	113.85	110.70
36	5	948	C	C6-N1-C2	6.30	122.82	120.30
36	5	3206	C	C6-N1-C1'	6.30	128.36	120.80
50	m4	72	LEU	CA-CB-CG	6.30	129.78	115.30
36	1	936	A	N1-C6-N6	6.30	122.38	118.60
36	1	1316	C	N1-C2-N3	6.30	123.61	119.20
36	5	1314	C	N3-C4-C5	6.30	124.42	121.90
36	5	2917	G	C6-N1-C2	-6.30	121.32	125.10
36	5	518	G	C6-C5-N7	-6.29	126.62	130.40
36	1	864	G	N1-C6-O6	-6.29	116.12	119.90
36	5	2319	U	N1-C2-O2	6.29	127.20	122.80
1	6	1484	G	O5'-P-OP1	-6.29	100.04	105.70
1	2	1096	C	C2-N1-C1'	6.29	125.72	118.80
36	5	218	G	O5'-P-OP1	-6.29	100.04	105.70
36	5	1869	C	N3-C4-C5	6.29	124.42	121.90
36	5	1928	G	N1-C6-O6	6.29	123.67	119.90
1	2	831	U	C6-N1-C2	-6.29	117.23	121.00
36	5	348	A	N1-C6-N6	6.28	122.37	118.60
36	5	3372	A	N1-C6-N6	-6.28	114.83	118.60
1	2	810	G	C4-N9-C1'	6.28	134.67	126.50
1	2	985	G	N3-C4-N9	6.28	129.77	126.00
36	5	794	U	O5'-P-OP2	-6.28	100.05	105.70
36	5	919	U	O5'-P-OP1	6.28	118.23	110.70
36	1	2200	U	N3-C4-O4	6.28	123.79	119.40
36	1	2758	A	C2-N3-C4	6.28	113.74	110.60
1	6	1473	U	C6-N1-C2	-6.28	117.23	121.00
36	5	3362	A	N1-C6-N6	6.28	122.37	118.60
1	6	1340	U	N1-C2-O2	6.28	127.19	122.80
36	5	901	G	C6-C5-N7	-6.28	126.64	130.40
36	1	613	G	N1-C6-O6	6.27	123.66	119.90
36	5	880	G	O4'-C1'-N9	6.27	113.22	108.20
36	1	2860	U	N1-C2-O2	-6.27	118.41	122.80
36	5	943	U	N1-C2-O2	-6.27	118.41	122.80
1	2	934	C	C2-N1-C1'	6.27	125.70	118.80
36	5	3362	A	O4'-C1'-N9	6.27	113.22	108.20
45	18	69	LEU	CA-CB-CG	6.27	129.72	115.30
36	1	1492	G	C5-N7-C8	6.27	107.43	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1420	C	C6-N1-C2	6.27	122.81	120.30
36	5	767	U	O4'-C1'-N1	6.27	113.21	108.20
36	1	2429	G	N1-C6-O6	-6.26	116.14	119.90
36	1	2129	U	N3-C2-O2	6.26	126.58	122.20
1	6	687	G	N3-C4-N9	-6.26	122.24	126.00
36	1	1103	A	P-O3'-C3'	6.26	127.21	119.70
36	1	1177	G	N3-C2-N2	-6.26	115.52	119.90
36	1	1298	C	O5'-P-OP1	-6.26	100.07	105.70
36	5	1481	A	P-O3'-C3'	6.26	127.21	119.70
36	5	2118	C	N1-C2-O2	6.26	122.65	118.90
36	1	2810	C	C5-C6-N1	-6.25	117.87	121.00
36	1	919	U	O5'-P-OP2	-6.25	100.07	105.70
36	1	1367	G	N3-C4-N9	6.25	129.75	126.00
36	5	216	G	N1-C6-O6	6.25	123.65	119.90
36	5	683	U	N1-C2-O2	-6.25	118.42	122.80
36	5	2937	G	C8-N9-C4	6.25	108.90	106.40
36	1	352	A	N1-C6-N6	6.25	122.35	118.60
36	1	1157	G	C5-C6-O6	6.25	132.35	128.60
36	5	857	G	C5-C6-N1	-6.25	108.37	111.50
36	5	2917	G	N3-C4-N9	6.25	129.75	126.00
36	5	3218	A	C5-N7-C8	-6.25	100.78	103.90
36	1	498	A	N1-C6-N6	-6.25	114.85	118.60
38	4	94	C	N3-C4-C5	6.25	124.40	121.90
36	1	1911	A	C5-C6-N1	6.24	120.82	117.70
70	O4	8	ARG	NE-CZ-NH2	-6.24	117.18	120.30
36	5	835	G	N9-C4-C5	-6.24	102.90	105.40
36	1	2572	C	C6-N1-C1'	-6.24	113.31	120.80
1	6	1280	C	N3-C4-C5	-6.24	119.40	121.90
36	5	2816	G	C8-N9-C4	6.24	108.90	106.40
1	2	581	U	C2-N1-C1'	6.24	125.19	117.70
36	1	2339	C	O4'-C1'-N1	-6.24	103.21	108.20
36	1	2352	A	C5-C6-N6	-6.24	118.71	123.70
36	1	3135	U	C5-C6-N1	-6.24	119.58	122.70
1	6	1478	G	C6-C5-N7	-6.24	126.66	130.40
36	1	3344	A	C8-N9-C4	-6.24	103.31	105.80
1	6	114	C	N1-C2-O2	6.24	122.64	118.90
36	5	384	A	C8-N9-C4	6.24	108.30	105.80
36	5	2213	A	N7-C8-N9	-6.24	110.68	113.80
1	2	158	U	P-O3'-C3'	6.23	127.18	119.70
36	1	2887	A	O5'-P-OP2	-6.23	100.09	105.70
36	5	2696	A	C6-N1-C2	6.23	122.34	118.60
36	1	1381	A	N1-C6-N6	6.23	122.34	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	104	A	O4'-C1'-N9	6.23	113.19	108.20
36	1	28	C	C5-C4-N4	-6.23	115.84	120.20
36	1	808	A	N1-C6-N6	-6.23	114.86	118.60
36	1	3101	G	C8-N9-C4	6.23	108.89	106.40
1	6	408	C	C6-N1-C2	-6.23	117.81	120.30
36	5	370	U	N3-C2-O2	-6.23	117.84	122.20
36	1	1595	U	C6-N1-C2	6.23	124.74	121.00
36	5	437	G	N3-C2-N2	-6.23	115.54	119.90
1	6	609	U	C5-C6-N1	-6.23	119.59	122.70
36	5	1151	U	N3-C4-O4	6.23	123.76	119.40
36	1	3228	C	C6-N1-C2	-6.23	117.81	120.30
36	5	581	U	C5-C6-N1	6.22	125.81	122.70
36	5	1085	A	N1-C6-N6	6.22	122.33	118.60
1	2	1481	C	C6-N1-C2	-6.22	117.81	120.30
1	6	600	U	O5'-P-OP2	-6.22	100.10	105.70
36	1	651	G	N1-C2-N2	-6.22	110.60	116.20
36	5	1495	U	C5-C6-N1	6.22	125.81	122.70
36	5	2761	G	N1-C6-O6	-6.22	116.17	119.90
36	1	283	G	C5-C6-O6	-6.22	124.87	128.60
36	1	1152	G	C6-C5-N7	-6.22	126.67	130.40
36	5	901	G	N3-C4-C5	-6.22	125.49	128.60
36	1	2719	U	N1-C2-N3	6.22	118.63	114.90
36	5	1170	A	N1-C6-N6	6.22	122.33	118.60
36	5	1193	A	N7-C8-N9	6.22	116.91	113.80
36	1	2314	U	C2-N1-C1'	6.22	125.16	117.70
36	5	2531	C	N1-C2-O2	6.21	122.63	118.90
36	5	2913	C	C4-C5-C6	6.21	120.51	117.40
1	2	1269	U	C2-N1-C1'	6.21	125.16	117.70
36	1	3382	U	C2-N1-C1'	6.21	125.16	117.70
1	6	609	U	N3-C4-O4	-6.21	115.05	119.40
36	1	587	U	C5-C4-O4	-6.21	122.17	125.90
36	1	2279	A	C5-C6-N6	-6.21	118.73	123.70
36	5	2235	C	C6-N1-C2	6.21	122.78	120.30
36	5	2777	G	C5-C6-O6	6.21	132.33	128.60
36	1	197	G	C2-N3-C4	-6.21	108.80	111.90
1	2	1611	A	C8-N9-C4	-6.21	103.32	105.80
36	1	790	U	N3-C2-O2	-6.21	117.86	122.20
36	1	350	C	N3-C2-O2	-6.21	117.56	121.90
1	2	765	G	O4'-C1'-N9	-6.20	103.24	108.20
1	2	1730	A	C8-N9-C4	6.20	108.28	105.80
36	1	651	G	N1-C6-O6	-6.20	116.18	119.90
36	5	2608	G	OP2-P-O3'	6.20	118.84	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	33	U	N3-C2-O2	-6.20	117.86	122.20
36	5	2607	G	N7-C8-N9	6.20	116.20	113.10
36	1	1835	A	C2-N3-C4	-6.20	107.50	110.60
1	6	1192	C	N1-C2-O2	6.20	122.62	118.90
1	6	1782	A	C8-N9-C4	-6.20	103.32	105.80
36	5	73	C	C6-N1-C2	6.20	122.78	120.30
36	5	877	C	C5-C4-N4	-6.20	115.86	120.20
36	1	2640	A	N1-C2-N3	6.20	132.40	129.30
1	6	1072	C	C6-N1-C2	-6.20	117.82	120.30
1	2	570	A	N1-C6-N6	6.19	122.32	118.60
36	1	2981	U	N3-C2-O2	-6.19	117.86	122.20
36	5	3269	U	P-O3'-C3'	6.19	127.13	119.70
1	2	507	U	C2-N1-C1'	6.19	125.13	117.70
1	6	163	G	N3-C4-C5	6.19	131.70	128.60
36	5	1161	G	C6-C5-N7	6.19	134.12	130.40
36	5	1304	A	C2-N3-C4	6.19	113.70	110.60
36	5	2191	U	N3-C2-O2	-6.19	117.86	122.20
1	2	1611	A	N7-C8-N9	6.19	116.90	113.80
36	1	2121	G	N3-C4-C5	-6.19	125.50	128.60
36	5	1116	G	C2-N3-C4	6.19	115.00	111.90
36	5	1342	C	C5-C6-N1	-6.19	117.90	121.00
36	5	1452	A	C4-C5-N7	6.19	113.80	110.70
36	1	1331	U	C5-C6-N1	-6.19	119.61	122.70
1	6	353	A	C2-N3-C4	6.19	113.69	110.60
1	6	542	A	O4'-C1'-N9	6.19	113.15	108.20
36	1	2649	A	C5-C6-N1	6.18	120.79	117.70
36	5	1326	A	O5'-P-OP2	-6.18	100.14	105.70
36	5	2604	U	C5-C4-O4	6.18	129.61	125.90
50	m4	77	ARG	NE-CZ-NH1	-6.18	117.21	120.30
38	8	86	U	C5-C6-N1	6.18	125.79	122.70
36	1	1385	C	C6-N1-C2	6.18	122.77	120.30
1	6	1119	G	N1-C2-N2	-6.18	110.64	116.20
1	2	1749	A	N3-C4-C5	6.18	131.12	126.80
36	1	3079	U	N1-C2-O2	-6.18	118.48	122.80
36	5	941	G	C8-N9-C4	-6.17	103.93	106.40
1	2	736	C	C5-C6-N1	6.17	124.09	121.00
36	1	682	U	C6-N1-C1'	6.17	129.84	121.20
1	6	1600	A	C2-N3-C4	-6.17	107.52	110.60
36	5	2700	G	C4-C5-N7	6.17	113.27	110.80
1	2	810	G	C4-C5-N7	6.17	113.27	110.80
36	1	770	G	O4'-C1'-N9	6.17	113.13	108.20
36	5	857	G	C4-C5-C6	6.17	122.50	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	39	A	N3-C4-C5	6.16	131.11	126.80
36	1	2658	G	C8-N9-C4	6.16	108.86	106.40
1	6	158	U	P-O3'-C3'	6.16	127.10	119.70
36	5	2135	U	N3-C4-C5	6.16	118.30	114.60
36	5	2283	G	C5-C6-O6	-6.16	124.90	128.60
36	5	3093	C	C2-N3-C4	-6.16	116.82	119.90
36	1	1113	G	N7-C8-N9	6.16	116.18	113.10
1	2	402	C	C2-N1-C1'	-6.16	112.02	118.80
36	1	1113	G	N3-C2-N2	-6.16	115.59	119.90
36	1	2884	C	C6-N1-C2	6.16	122.77	120.30
36	5	2887	A	C4-C5-C6	6.16	120.08	117.00
36	1	2914	G	O5'-P-OP2	-6.16	100.16	105.70
36	5	914	A	N9-C4-C5	-6.16	103.34	105.80
36	1	1152	G	C5-C6-O6	-6.16	124.91	128.60
54	M8	174	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	2	864	U	N3-C2-O2	-6.15	117.89	122.20
1	2	1305	U	C5-C4-O4	6.15	129.59	125.90
36	5	2185	G	N3-C2-N2	-6.15	115.59	119.90
36	5	2874	G	C5-C6-O6	6.15	132.29	128.60
36	1	2943	G	C5-C6-O6	-6.15	124.91	128.60
36	1	3207	U	C5-C6-N1	-6.15	119.62	122.70
36	5	205	C	O5'-P-OP1	-6.15	100.17	105.70
36	5	2953	U	N3-C4-C5	-6.15	110.91	114.60
1	2	507	U	N1-C2-O2	6.15	127.11	122.80
36	5	2625	C	N3-C4-C5	6.15	124.36	121.90
36	5	1124	U	C5-C4-O4	-6.15	122.21	125.90
36	1	2404	A	O5'-P-OP2	-6.14	100.17	105.70
36	1	2945	G	C5-C6-O6	-6.14	124.91	128.60
1	2	728	U	N3-C2-O2	-6.14	117.90	122.20
36	1	2815	G	N7-C8-N9	-6.14	110.03	113.10
36	5	2718	U	N3-C2-O2	-6.14	117.90	122.20
36	1	2194	G	N1-C6-O6	6.14	123.58	119.90
36	5	2191	U	C5-C4-O4	6.14	129.58	125.90
1	6	933	A	N1-C6-N6	-6.13	114.92	118.60
36	5	2917	G	N3-C4-C5	-6.13	125.53	128.60
10	s8	29	LEU	CB-CG-CD2	6.13	121.43	111.00
36	1	1433	A	O4'-C1'-N9	-6.13	103.30	108.20
36	1	2606	G	N1-C2-N2	-6.13	110.68	116.20
36	1	2755	C	O5'-P-OP1	-6.13	100.18	105.70
36	5	3142	A	O5'-P-OP1	-6.13	100.18	105.70
1	2	158	U	C2-N1-C1'	6.13	125.05	117.70
36	5	630	A	N1-C2-N3	6.13	132.37	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1452	A	C5-C6-N6	-6.13	118.80	123.70
36	1	2284	C	C6-N1-C2	-6.13	117.85	120.30
36	1	3369	G	C5-C6-O6	-6.13	124.92	128.60
36	1	1307	G	N1-C6-O6	-6.12	116.22	119.90
36	1	1517	G	C8-N9-C4	6.12	108.85	106.40
36	1	1381	A	O5'-P-OP1	-6.12	100.19	105.70
1	2	554	C	C5-C6-N1	6.12	124.06	121.00
36	1	2725	U	C5-C6-N1	-6.12	119.64	122.70
36	5	222	A	O5'-P-OP2	-6.12	100.19	105.70
36	5	931	C	N3-C4-C5	6.12	124.35	121.90
1	2	49	C	C6-N1-C2	-6.12	117.85	120.30
36	5	986	U	N1-C2-O2	6.12	127.08	122.80
36	5	2699	G	N1-C2-N2	6.12	121.71	116.20
36	1	794	U	N1-C2-O2	-6.12	118.52	122.80
36	1	2821	C	O5'-P-OP1	-6.12	100.19	105.70
9	s7	131	PHE	C-N-CD	6.12	141.25	128.40
36	5	637	C	N1-C2-O2	-6.12	115.23	118.90
36	1	651	G	C8-N9-C1'	-6.12	119.05	127.00
36	1	3143	C	N3-C2-O2	6.12	126.18	121.90
36	5	2190	U	N1-C2-N3	6.12	118.57	114.90
36	1	642	U	C5-C6-N1	-6.12	119.64	122.70
36	1	2200	U	C5-C6-N1	6.12	125.76	122.70
36	1	2337	C	C6-N1-C2	-6.12	117.85	120.30
36	5	2950	G	C4-C5-N7	6.12	113.25	110.80
36	1	1149	G	C5-C6-N1	-6.11	108.44	111.50
1	2	685	A	P-O3'-C3'	6.11	127.03	119.70
36	1	2760	C	N1-C2-O2	-6.11	115.23	118.90
1	6	194	U	N1-C2-O2	6.11	127.08	122.80
36	1	3208	G	N3-C4-N9	-6.11	122.33	126.00
36	5	890	C	N1-C2-O2	6.11	122.57	118.90
38	8	44	A	N9-C4-C5	-6.11	103.36	105.80
36	1	3228	C	C2-N1-C1'	6.11	125.52	118.80
37	7	12	U	C5-C4-O4	-6.11	122.23	125.90
1	2	378	A	N1-C6-N6	6.11	122.26	118.60
1	6	90	C	N3-C2-O2	-6.11	117.63	121.90
36	5	2792	A	C8-N9-C4	-6.11	103.36	105.80
36	5	2372	A	N9-C4-C5	6.10	108.24	105.80
36	1	584	G	N9-C4-C5	6.10	107.84	105.40
36	1	941	G	C8-N9-C4	-6.10	103.96	106.40
36	1	2831	G	C6-C5-N7	-6.10	126.74	130.40
1	6	601	A	N1-C6-N6	-6.10	114.94	118.60
36	5	2211	U	C5-C4-O4	6.10	129.56	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1114	U	N3-C4-O4	-6.10	115.13	119.40
36	1	1335	C	N1-C2-O2	6.10	122.56	118.90
36	1	2399	A	C5-C6-N6	-6.10	118.82	123.70
36	5	3309	G	N1-C6-O6	-6.10	116.24	119.90
36	5	1439	U	O5'-P-OP2	6.10	118.02	110.70
36	5	1561	G	O4'-C1'-N9	6.09	113.08	108.20
36	5	1931	U	N3-C4-O4	-6.09	115.14	119.40
36	5	2512	C	C2-N1-C1'	6.09	125.50	118.80
36	1	647	A	C8-N9-C4	6.09	108.24	105.80
1	6	89	G	N1-C6-O6	6.09	123.55	119.90
1	6	139	C	P-O3'-C3'	6.09	127.01	119.70
36	5	3125	U	N3-C4-O4	-6.09	115.14	119.40
37	7	13	A	C5-C6-N1	6.09	120.75	117.70
36	1	48	A	N1-C2-N3	6.09	132.34	129.30
36	5	846	A	O5'-P-OP2	-6.09	100.22	105.70
36	5	3245	A	C4-C5-C6	6.09	120.05	117.00
36	1	937	G	O5'-P-OP2	-6.09	100.22	105.70
36	5	2833	A	C6-N1-C2	-6.09	114.95	118.60
36	1	901	G	N1-C6-O6	6.09	123.55	119.90
36	1	1149	G	C5-C6-O6	-6.09	124.95	128.60
36	1	2550	U	N1-C2-N3	6.09	118.55	114.90
1	6	1079	U	N3-C2-O2	-6.09	117.94	122.20
36	5	1719	G	N9-C4-C5	-6.09	102.97	105.40
36	5	1897	G	N3-C4-C5	6.09	131.64	128.60
36	1	925	A	O5'-P-OP1	-6.08	100.22	105.70
36	1	339	C	C5-C4-N4	6.08	124.46	120.20
36	1	986	U	C6-N1-C2	-6.08	117.35	121.00
1	6	1414	U	N3-C4-O4	-6.08	115.14	119.40
36	5	1480	G	O4'-C1'-N9	6.08	113.07	108.20
36	5	942	U	N1-C2-O2	-6.08	118.54	122.80
39	12	237	LEU	CA-CB-CG	-6.08	101.31	115.30
36	1	530	G	N1-C6-O6	-6.08	116.25	119.90
36	5	3215	A	C2-N3-C4	-6.08	107.56	110.60
37	3	84	A	OP1-P-O3'	6.08	118.57	105.20
1	6	988	A	O5'-P-OP2	-6.08	100.23	105.70
36	1	2641	U	C6-N1-C2	6.07	124.64	121.00
36	1	2641	U	C5-C6-N1	-6.07	119.66	122.70
36	1	1001	G	N1-C6-O6	6.07	123.54	119.90
36	1	282	G	C2'-C3'-O3'	6.07	123.41	113.70
36	1	3244	A	C5-C6-N6	-6.07	118.84	123.70
36	1	2599	U	N3-C2-O2	-6.07	117.95	122.20
41	L4	139	GLY	N-CA-C	-6.07	97.93	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	n9	23	LYS	C-N-CD	6.07	141.14	128.40
1	2	810	G	C8-N9-C1'	-6.07	119.11	127.00
36	5	1192	C	C5-C4-N4	-6.07	115.95	120.20
36	5	1305	U	C5-C4-O4	-6.07	122.26	125.90
1	2	811	A	C8-N9-C4	-6.06	103.38	105.80
1	6	1	U	N3-C2-O2	-6.06	117.96	122.20
36	5	211	A	N1-C6-N6	-6.06	114.96	118.60
36	5	327	A	C8-N9-C4	6.06	108.22	105.80
36	5	2765	C	C5-C6-N1	6.06	124.03	121.00
36	5	2952	G	N3-C2-N2	6.06	124.14	119.90
36	1	1177	G	C5-C6-O6	-6.06	124.96	128.60
36	1	1480	G	N3-C4-C5	6.06	131.63	128.60
36	1	1556	C	C2-N1-C1'	6.06	125.47	118.80
1	6	512	A	N1-C6-N6	6.06	122.24	118.60
36	5	922	U	N3-C4-O4	-6.06	115.16	119.40
36	5	2257	C	C6-N1-C2	-6.06	117.88	120.30
36	1	2945	G	N1-C6-O6	6.06	123.54	119.90
36	5	1171	G	N1-C2-N2	-6.06	110.75	116.20
1	2	393	C	C6-N1-C2	6.06	122.72	120.30
36	1	1489	A	C8-N9-C4	6.06	108.22	105.80
36	1	291	C	OP2-P-O3'	6.06	118.52	105.20
36	1	2273	G	C8-N9-C4	6.06	108.82	106.40
1	6	1796	C	C5-C6-N1	-6.05	117.97	121.00
36	5	1116	G	C8-N9-C4	-6.05	103.98	106.40
36	5	1695	U	N3-C2-O2	-6.05	117.96	122.20
36	5	1879	A	N1-C6-N6	6.05	122.23	118.60
36	5	2917	G	O5'-P-OP2	-6.05	100.25	105.70
36	1	439	C	N1-C2-O2	6.05	122.53	118.90
44	17	83	LEU	CA-CB-CG	6.05	129.22	115.30
36	5	661	G	C6-C5-N7	-6.05	126.77	130.40
36	5	2133	U	N3-C4-O4	-6.05	115.16	119.40
36	1	304	G	N9-C4-C5	6.05	107.82	105.40
36	5	1099	A	N1-C6-N6	6.05	122.23	118.60
36	5	2371	G	C8-N9-C4	6.05	108.82	106.40
36	5	2993	G	C5-C6-O6	-6.05	124.97	128.60
36	1	343	U	N1-C2-O2	-6.05	118.57	122.80
36	1	1313	G	C4-C5-N7	6.05	113.22	110.80
36	1	1919	G	C5-C6-O6	6.05	132.23	128.60
36	5	518	G	N1-C6-O6	6.05	123.53	119.90
38	8	100	U	C2-N1-C1'	6.05	124.96	117.70
36	5	2728	G	O4'-C1'-N9	6.04	113.04	108.20
36	1	298	U	N3-C2-O2	-6.04	117.97	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	48	G	C8-N9-C4	6.04	108.82	106.40
36	5	506	U	O5'-P-OP2	-6.04	100.26	105.70
36	5	649	A	C8-N9-C4	-6.04	103.38	105.80
36	1	1881	A	C8-N9-C4	6.04	108.22	105.80
36	5	419	G	O5'-P-OP2	-6.04	100.27	105.70
18	C6	40	GLU	C-N-CD	-6.04	107.32	120.60
1	2	73	U	OP1-P-O3'	6.04	118.48	105.20
1	2	132	U	OP2-P-O3'	6.04	118.48	105.20
36	1	650	C	C2-N3-C4	-6.04	116.88	119.90
36	5	715	A	P-O3'-C3'	6.04	126.94	119.70
36	5	1606	U	O4'-C1'-N1	6.04	113.03	108.20
48	m1	30	LEU	CA-CB-CG	6.04	129.18	115.30
1	6	630	A	O5'-P-OP2	-6.03	100.27	105.70
36	1	1349	G	N3-C4-C5	-6.03	125.58	128.60
1	6	965	U	N1-C2-O2	6.03	127.02	122.80
36	5	31	C	N1-C2-O2	6.03	122.52	118.90
36	5	954	U	C6-N1-C2	-6.03	117.38	121.00
36	5	2792	A	N1-C6-N6	6.03	122.22	118.60
36	5	425	G	N9-C4-C5	-6.03	102.99	105.40
36	5	874	U	O5'-P-OP1	-6.03	100.28	105.70
36	5	1499	C	C2-N1-C1'	-6.03	112.17	118.80
38	8	80	A	N7-C8-N9	6.03	116.81	113.80
36	5	2607	G	C8-N9-C4	-6.03	103.99	106.40
36	5	2931	C	C5-C4-N4	-6.03	115.98	120.20
36	1	2257	C	C6-N1-C2	-6.02	117.89	120.30
36	1	3023	U	O5'-P-OP1	-6.02	100.28	105.70
1	6	354	C	N3-C4-C5	6.02	124.31	121.90
1	2	1486	G	N7-C8-N9	6.02	116.11	113.10
36	1	44	U	C6-N1-C2	6.02	124.61	121.00
36	1	2114	C	O5'-P-OP2	-6.02	100.28	105.70
36	1	2377	G	N9-C4-C5	-6.02	102.99	105.40
1	6	639	U	C2-N1-C1'	6.02	124.92	117.70
36	5	912	G	C5-C6-O6	6.02	132.21	128.60
36	5	3309	G	N3-C4-C5	-6.02	125.59	128.60
38	4	20	U	C5-C6-N1	-6.02	119.69	122.70
1	6	75	U	C2-N1-C1'	6.02	124.92	117.70
1	6	1478	G	C8-N9-C1'	-6.02	119.17	127.00
36	5	659	G	C5-C6-O6	-6.02	124.99	128.60
36	5	1300	G	C5-C6-O6	-6.02	124.99	128.60
36	1	317	A	C2-N3-C4	-6.02	107.59	110.60
36	1	867	G	C5-C6-O6	6.02	132.21	128.60
36	1	1435	A	OP1-P-OP2	-6.02	110.58	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2860	U	C6-N1-C2	6.02	124.61	121.00
36	1	416	A	C8-N9-C4	6.01	108.21	105.80
36	5	2393	G	C6-C5-N7	-6.01	126.79	130.40
36	5	3215	A	N1-C6-N6	6.01	122.21	118.60
36	1	2370	G	N1-C2-N3	6.01	127.51	123.90
36	1	189	G	C5-C6-O6	-6.01	124.99	128.60
36	1	1795	U	C5-C4-O4	-6.01	122.29	125.90
36	5	2812	C	N3-C4-C5	6.01	124.30	121.90
79	Q3	17	ARG	NE-CZ-NH1	-6.01	117.30	120.30
1	6	1474	G	N3-C4-C5	-6.01	125.59	128.60
36	5	92	G	N3-C4-N9	6.01	129.61	126.00
36	5	3197	G	N3-C4-N9	-6.01	122.39	126.00
36	1	109	A	OP1-P-O3'	6.01	118.42	105.20
36	5	515	C	N1-C2-O2	-6.00	115.30	118.90
36	5	715	A	O4'-C1'-N9	6.00	113.00	108.20
1	6	1180	C	C6-N1-C2	-6.00	117.90	120.30
36	5	1704	A	C2-N3-C4	-6.00	107.60	110.60
36	1	894	G	N9-C4-C5	6.00	107.80	105.40
36	1	1340	G	OP1-P-OP2	6.00	128.60	119.60
36	5	2411	U	N3-C4-O4	-6.00	115.20	119.40
1	2	1698	G	P-O3'-C3'	6.00	126.90	119.70
73	O7	21	ARG	NE-CZ-NH2	-6.00	117.30	120.30
36	1	2796	G	N1-C2-N3	6.00	127.50	123.90
1	2	334	G	C4-N9-C1'	-5.99	118.71	126.50
36	1	3344	A	C5-N7-C8	-5.99	100.90	103.90
36	5	1719	G	N1-C6-O6	5.99	123.50	119.90
36	5	2764	C	C6-N1-C2	5.99	122.70	120.30
37	7	13	A	C2-N3-C4	5.99	113.60	110.60
36	1	2572	C	N3-C2-O2	-5.99	117.71	121.90
1	6	1072	C	C5-C6-N1	5.99	124.00	121.00
36	5	1049	C	C6-N1-C2	-5.99	117.91	120.30
36	5	1176	C	C4-C5-C6	5.99	120.39	117.40
36	5	1179	A	OP1-P-O3'	5.99	118.38	105.20
36	5	1878	G	C4-N9-C1'	5.99	134.28	126.50
36	5	2129	U	C5-C4-O4	5.99	129.49	125.90
38	4	50	C	C6-N1-C2	-5.99	117.91	120.30
36	1	3195	U	O4'-C1'-N1	5.98	112.99	108.20
70	O4	51	LEU	CA-CB-CG	5.98	129.06	115.30
1	2	1258	U	N3-C2-O2	-5.98	118.01	122.20
36	5	1456	A	OP2-P-O3'	-5.98	92.04	105.20
36	1	321	C	N1-C2-O2	5.98	122.49	118.90
36	5	2929	C	C5-C6-N1	-5.98	118.01	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	350	U	N1-C2-N3	5.98	118.49	114.90
36	1	1160	C	N3-C4-C5	-5.98	119.51	121.90
36	1	2634	U	C5-C6-N1	-5.98	119.71	122.70
36	1	1879	A	O4'-C1'-N9	5.97	112.98	108.20
38	4	65	A	C2-N3-C4	-5.97	107.61	110.60
1	6	542	A	P-O3'-C3'	5.97	126.87	119.70
1	6	977	A	N1-C6-N6	5.97	122.18	118.60
37	7	28	C	C6-N1-C2	5.97	122.69	120.30
36	1	701	G	N3-C2-N2	-5.97	115.72	119.90
36	1	859	G	N9-C4-C5	-5.97	103.01	105.40
36	1	1349	G	N3-C4-N9	5.97	129.58	126.00
36	1	2706	G	N3-C4-N9	5.97	129.58	126.00
36	5	818	C	N1-C2-O2	-5.97	115.32	118.90
36	5	2608	G	N7-C8-N9	-5.97	110.12	113.10
79	q3	17	ARG	NE-CZ-NH1	-5.97	117.32	120.30
36	1	1331	U	C2-N3-C4	-5.97	123.42	127.00
36	5	914	A	C5-C6-N6	-5.97	118.92	123.70
36	1	2872	A	C6-N1-C2	-5.97	115.02	118.60
1	6	163	G	N7-C8-N9	5.97	116.08	113.10
1	2	1489	U	N3-C2-O2	-5.96	118.03	122.20
36	1	1891	A	O5'-P-OP2	-5.96	100.33	105.70
1	6	1456	C	C4-C5-C6	5.96	120.38	117.40
36	5	3318	G	N1-C6-O6	-5.96	116.32	119.90
61	n5	34	LEU	CA-CB-CG	5.96	129.02	115.30
36	1	1923	C	C6-N1-C2	5.96	122.69	120.30
1	2	1051	G	P-O3'-C3'	5.96	126.85	119.70
1	2	1291	G	C5-N7-C8	-5.96	101.32	104.30
36	1	1747	G	N1-C6-O6	5.96	123.48	119.90
36	1	2265	C	C6-N1-C2	-5.96	117.92	120.30
36	5	88	A	C2-N3-C4	-5.96	107.62	110.60
1	6	593	U	C6-N1-C2	-5.96	117.42	121.00
36	5	2980	U	O5'-P-OP2	-5.96	100.34	105.70
36	1	2373	A	C8-N9-C4	-5.96	103.42	105.80
36	5	2913	C	N1-C2-N3	5.96	123.37	119.20
1	2	554	C	N3-C4-C5	-5.96	119.52	121.90
36	1	2379	U	C5-C6-N1	5.96	125.68	122.70
1	6	1218	G	C4-N9-C1'	-5.96	118.76	126.50
36	5	2892	A	O5'-P-OP2	-5.96	100.34	105.70
36	1	517	G	N3-C4-C5	-5.95	125.62	128.60
36	1	1160	C	O5'-P-OP1	-5.95	100.34	105.70
1	6	144	U	N1-C2-N3	5.95	118.47	114.90
36	1	2129	U	N1-C2-O2	-5.95	118.64	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2321	A	C8-N9-C4	5.95	108.18	105.80
36	1	1152	G	N1-C6-O6	5.95	123.47	119.90
36	1	1361	U	O5'-P-OP1	-5.95	100.34	105.70
36	1	2393	G	O5'-P-OP2	-5.95	100.35	105.70
36	1	2410	U	C5-C4-O4	-5.95	122.33	125.90
1	2	961	U	C6-N1-C2	-5.95	117.43	121.00
36	1	864	G	C5-C6-O6	5.95	132.17	128.60
36	1	1447	G	C5-C6-N1	5.95	114.47	111.50
1	6	1614	A	C4-C5-N7	5.95	113.67	110.70
36	5	271	C	N3-C2-O2	-5.95	117.74	121.90
36	5	888	A	OP2-P-O3'	5.95	118.28	105.20
36	5	2403	G	C2-N3-C4	5.95	114.87	111.90
38	8	32	C	C6-N1-C2	5.95	122.68	120.30
36	5	3266	G	C8-N9-C4	-5.94	104.02	106.40
36	1	1445	U	N1-C2-O2	-5.94	118.64	122.80
36	1	2948	C	C6-N1-C2	5.94	122.68	120.30
36	1	28	C	C6-N1-C2	5.94	122.68	120.30
36	1	1798	A	C2-N3-C4	-5.94	107.63	110.60
36	1	2163	C	C5-C6-N1	-5.94	118.03	121.00
36	1	3382	U	N1-C2-O2	5.94	126.96	122.80
36	5	342	A	C5-N7-C8	-5.94	100.93	103.90
36	5	1336	U	O5'-P-OP2	-5.94	100.35	105.70
36	5	1910	A	N9-C4-C5	-5.94	103.42	105.80
36	5	2831	G	N1-C6-O6	-5.94	116.34	119.90
36	1	192	C	N3-C2-O2	-5.94	117.74	121.90
36	1	3181	C	C5-C4-N4	5.94	124.36	120.20
36	1	25	U	C6-N1-C2	-5.94	117.44	121.00
36	1	986	U	N3-C2-O2	-5.94	118.04	122.20
36	1	1556	C	N3-C2-O2	-5.94	117.74	121.90
36	5	1858	A	C8-N9-C4	-5.94	103.42	105.80
36	5	2371	G	N9-C4-C5	-5.94	103.03	105.40
12	c0	83	PRO	N-CA-CB	5.94	110.42	103.30
36	5	2634	U	N1-C2-N3	5.93	118.46	114.90
36	5	2849	C	OP1-P-OP2	5.93	128.50	119.60
36	1	2958	A	C5-C6-N6	5.93	128.45	123.70
36	5	3309	G	C5-C6-O6	5.93	132.16	128.60
36	5	2403	G	N3-C4-N9	5.93	129.56	126.00
36	1	1306	G	N9-C4-C5	-5.93	103.03	105.40
36	5	918	C	C6-N1-C2	5.93	122.67	120.30
36	5	3218	A	N1-C6-N6	5.93	122.16	118.60
36	1	1406	A	C5-C6-N6	-5.92	118.96	123.70
36	1	1897	G	C5-C6-N1	-5.92	108.54	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1325	U	C5-C4-O4	5.92	129.45	125.90
36	5	2797	C	N3-C4-C5	-5.92	119.53	121.90
36	1	714	G	OP2-P-O3'	5.92	118.23	105.20
36	5	221	A	C8-N9-C4	5.92	108.17	105.80
36	5	2805	G	C5-C6-O6	-5.92	125.05	128.60
36	1	1902	G	C6-C5-N7	-5.92	126.85	130.40
36	1	3119	U	N1-C2-O2	5.92	126.94	122.80
1	6	638	U	N1-C2-O2	5.92	126.94	122.80
36	5	1868	G	N1-C6-O6	5.92	123.45	119.90
53	m7	135	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	6	477	A	N1-C6-N6	5.92	122.15	118.60
36	5	688	G	N1-C6-O6	5.92	123.45	119.90
36	5	2134	G	N3-C4-C5	-5.92	125.64	128.60
36	5	2179	C	C6-N1-C2	5.92	122.67	120.30
36	5	2935	U	O5'-P-OP2	-5.92	100.37	105.70
1	6	407	A	OP2-P-O3'	5.92	118.22	105.20
36	5	1152	G	C5-C6-O6	-5.92	125.05	128.60
36	5	2728	G	N3-C2-N2	-5.92	115.76	119.90
1	2	1114	G	O4'-C1'-N9	5.92	112.93	108.20
36	5	2187	G	N3-C4-N9	5.92	129.55	126.00
36	5	2869	U	N3-C4-O4	-5.92	115.26	119.40
36	5	406	G	N1-C6-O6	-5.91	116.35	119.90
36	5	644	G	C4-C5-N7	-5.91	108.43	110.80
36	5	682	U	C5-C6-N1	-5.91	119.74	122.70
36	5	3040	A	C8-N9-C4	5.91	108.17	105.80
36	1	1724	U	O4'-C1'-N1	5.91	112.93	108.20
36	1	582	G	N9-C4-C5	5.91	107.76	105.40
36	1	788	C	C5-C6-N1	-5.91	118.05	121.00
36	1	1316	C	N3-C4-C5	-5.91	119.54	121.90
36	1	2349	U	N3-C2-O2	-5.91	118.06	122.20
36	5	2696	A	C5-C6-N1	-5.91	114.75	117.70
36	1	49	A	C8-N9-C4	5.91	108.16	105.80
36	1	2895	G	N1-C6-O6	-5.91	116.36	119.90
36	1	2944	U	C5-C4-O4	-5.91	122.36	125.90
36	5	2964	G	C8-N9-C4	5.91	108.76	106.40
36	1	1308	A	N9-C4-C5	5.90	108.16	105.80
36	1	2914	G	N1-C6-O6	-5.90	116.36	119.90
36	1	3368	U	C2-N1-C1'	-5.90	110.62	117.70
36	5	2811	A	C2-N3-C4	-5.90	107.65	110.60
36	1	97	U	N1-C2-O2	-5.90	118.67	122.80
36	1	946	U	OP1-P-OP2	5.90	128.45	119.60
38	4	103	G	N1-C6-O6	-5.90	116.36	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1277	G	N3-C4-N9	-5.90	122.46	126.00
1	6	151	G	N3-C2-N2	-5.90	115.77	119.90
36	5	2640	A	OP1-P-OP2	-5.90	110.75	119.60
36	1	1365	G	N3-C4-C5	-5.90	125.65	128.60
36	5	1719	G	C5-C6-O6	-5.90	125.06	128.60
36	1	704	U	C4-C5-C6	5.90	123.24	119.70
36	1	933	A	C6-C5-N7	-5.89	128.17	132.30
36	1	2929	C	C2-N3-C4	-5.89	116.95	119.90
36	1	3375	A	N1-C2-N3	5.89	132.25	129.30
1	6	1097	U	P-O3'-C3'	5.89	126.77	119.70
36	5	1370	G	N3-C4-C5	-5.89	125.65	128.60
36	1	2323	G	N3-C4-N9	5.89	129.53	126.00
1	6	1000	C	N3-C2-O2	-5.89	117.78	121.90
36	1	676	G	C6-C5-N7	-5.89	126.86	130.40
36	1	2249	G	P-O3'-C3'	5.89	126.77	119.70
13	c1	5	LEU	CA-CB-CG	5.89	128.85	115.30
36	5	1907	C	C6-N1-C2	-5.89	117.94	120.30
36	5	2627	C	C2-N3-C4	-5.89	116.95	119.90
36	5	2726	C	N3-C4-C5	-5.89	119.54	121.90
1	2	1196	A	P-O3'-C3'	5.89	126.77	119.70
36	1	66	A	O5'-P-OP1	-5.89	100.40	105.70
36	5	3188	G	N1-C6-O6	-5.89	116.37	119.90
36	5	3343	G	N3-C4-N9	5.89	129.53	126.00
36	1	189	G	C6-C5-N7	-5.88	126.87	130.40
36	1	2138	A	N1-C6-N6	5.88	122.13	118.60
36	1	718	G	N7-C8-N9	5.88	116.04	113.10
1	6	1473	U	C5-C4-O4	5.88	129.43	125.90
1	2	1022	C	N3-C4-C5	5.88	124.25	121.90
1	6	1537	C	N1-C2-O2	-5.88	115.37	118.90
36	5	2777	G	C4-C5-N7	-5.88	108.45	110.80
36	1	3180	A	C2-N3-C4	-5.88	107.66	110.60
36	5	656	A	N1-C6-N6	5.88	122.13	118.60
36	1	2312	A	N1-C6-N6	-5.88	115.07	118.60
36	1	2374	C	N1-C2-N3	5.88	123.31	119.20
1	6	1640	C	C5-C4-N4	-5.88	116.09	120.20
36	5	146	U	C5-C6-N1	-5.88	119.76	122.70
36	5	2851	A	C2-N3-C4	-5.88	107.66	110.60
36	5	116	A	O4'-C1'-N9	5.88	112.90	108.20
36	5	2710	C	N1-C2-O2	-5.88	115.38	118.90
14	C2	103	LEU	CA-CB-CG	5.87	128.81	115.30
36	1	2395	G	O5'-P-OP2	-5.87	100.42	105.70
1	6	396	G	C8-N9-C4	-5.87	104.05	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2319	U	N3-C2-O2	-5.87	118.09	122.20
36	1	386	A	N1-C6-N6	5.87	122.12	118.60
36	1	2763	U	C6-N1-C2	5.87	124.52	121.00
1	2	1486	G	C6-C5-N7	-5.87	126.88	130.40
36	5	1056	U	C5-C6-N1	5.87	125.63	122.70
36	5	2150	G	N7-C8-N9	5.87	116.03	113.10
1	2	159	U	C2-N1-C1'	-5.87	110.66	117.70
1	6	1657	U	N1-C2-O2	5.87	126.91	122.80
36	1	212	G	N3-C4-N9	5.87	129.52	126.00
36	1	318	A	O5'-P-OP1	-5.87	100.42	105.70
36	5	3243	A	O4'-C1'-N9	-5.87	103.51	108.20
36	1	1481	A	C5-N7-C8	-5.86	100.97	103.90
36	5	838	G	C6-C5-N7	5.86	133.92	130.40
36	5	1900	A	C5-C6-N1	5.86	120.63	117.70
36	1	210	U	C5-C4-O4	-5.86	122.38	125.90
36	5	297	G	O4'-C1'-N9	5.86	112.89	108.20
36	5	3056	U	N3-C2-O2	5.86	126.30	122.20
36	5	3329	U	C5-C4-O4	5.86	129.42	125.90
1	6	864	U	N3-C2-O2	-5.86	118.10	122.20
36	1	1495	U	C6-N1-C1'	5.86	129.40	121.20
36	1	2403	G	C6-C5-N7	-5.86	126.89	130.40
1	6	47	A	O5'-P-OP1	-5.86	100.43	105.70
36	5	2730	G	C4-C5-N7	5.86	113.14	110.80
36	1	78	U	C4-C5-C6	5.86	123.21	119.70
38	4	60	U	N1-C2-N3	5.86	118.41	114.90
36	1	1113	G	C8-N9-C4	-5.85	104.06	106.40
36	1	3306	U	N1-C2-O2	5.85	126.90	122.80
36	5	1316	C	N1-C2-O2	-5.85	115.39	118.90
36	5	1637	A	N1-C6-N6	-5.85	115.09	118.60
36	1	1192	C	C6-N1-C1'	-5.85	113.78	120.80
36	5	934	G	C4-N9-C1'	5.85	134.11	126.50
36	5	1149	G	N3-C2-N2	-5.85	115.80	119.90
36	5	2409	G	O5'-P-OP2	-5.85	100.43	105.70
36	5	1113	G	C5-C6-N1	-5.85	108.58	111.50
37	7	83	U	C5-C6-N1	-5.85	119.77	122.70
1	6	1137	A	C8-N9-C4	5.85	108.14	105.80
36	5	953	G	C5-C6-O6	-5.85	125.09	128.60
36	5	2368	A	C2-N3-C4	5.85	113.53	110.60
1	6	1175	U	N3-C2-O2	-5.85	118.11	122.20
1	2	42	G	C8-N9-C4	5.85	108.74	106.40
18	C6	53	LEU	CA-CB-CG	-5.85	101.85	115.30
36	1	2379	U	C6-N1-C2	-5.85	117.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1761	U	N1-C2-N3	5.84	118.41	114.90
37	3	116	C	C6-N1-C2	-5.84	117.96	120.30
36	5	283	G	O4'-C1'-N9	-5.84	103.53	108.20
36	1	608	A	N3-C4-N9	5.84	132.07	127.40
36	1	1127	G	C5-C6-N1	5.84	114.42	111.50
36	1	1182	A	O5'-P-OP1	-5.84	100.44	105.70
36	1	2887	A	C6-C5-N7	-5.84	128.21	132.30
36	5	92	G	N3-C4-C5	-5.84	125.68	128.60
1	6	609	U	N3-C2-O2	-5.84	118.11	122.20
38	8	42	G	C5-C6-O6	5.84	132.10	128.60
1	2	334	G	N3-C4-C5	5.84	131.52	128.60
36	5	666	A	O5'-P-OP1	-5.84	100.45	105.70
36	5	3154	C	C6-N1-C2	-5.84	117.97	120.30
36	1	1849	C	N1-C2-O2	-5.84	115.40	118.90
36	1	155	G	N3-C4-C5	-5.83	125.68	128.60
36	1	701	G	C5-C6-O6	-5.83	125.10	128.60
36	1	2359	C	N3-C4-C5	5.83	124.23	121.90
36	1	2808	A	O4'-C1'-N9	-5.83	103.53	108.20
36	1	2887	A	C5-C6-N6	-5.83	119.03	123.70
1	6	1072	C	N3-C4-N4	5.83	122.08	118.00
36	1	1146	C	N3-C2-O2	-5.83	117.82	121.90
36	1	1716	U	P-O3'-C3'	5.83	126.70	119.70
38	4	90	U	C5-C6-N1	-5.83	119.78	122.70
1	6	1340	U	N3-C2-O2	-5.83	118.12	122.20
36	5	116	A	O5'-P-OP1	-5.83	100.45	105.70
36	5	1292	C	N3-C4-C5	5.83	124.23	121.90
36	5	1428	A	C4-C5-C6	-5.83	114.09	117.00
36	5	2830	G	C8-N9-C1'	-5.83	119.42	127.00
36	1	2413	A	C4-C5-C6	-5.83	114.09	117.00
1	2	1082	C	N1-C2-O2	5.83	122.39	118.90
1	2	1327	C	C6-N1-C2	-5.83	117.97	120.30
36	1	229	G	N3-C2-N2	-5.83	115.82	119.90
36	5	2187	G	C6-C5-N7	-5.82	126.91	130.40
36	1	1307	G	C5-C6-O6	5.82	132.09	128.60
36	5	986	U	N3-C4-O4	-5.82	115.33	119.40
1	2	549	G	O5'-P-OP1	-5.82	100.46	105.70
36	1	745	C	N1-C2-O2	-5.82	115.41	118.90
36	1	1581	C	N1-C2-O2	5.82	122.39	118.90
36	1	3115	C	N1-C2-O2	-5.82	115.41	118.90
1	6	1414	U	C5-C4-O4	5.82	129.39	125.90
36	5	1308	A	OP1-P-OP2	-5.82	110.87	119.60
36	1	85	A	C2-N3-C4	-5.82	107.69	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3228	C	N1-C2-O2	5.82	122.39	118.90
36	5	150	A	C5-C6-N6	-5.82	119.05	123.70
36	5	881	C	C4-C5-C6	-5.82	114.49	117.40
36	1	638	C	N3-C2-O2	-5.82	117.83	121.90
38	4	125	U	N3-C2-O2	-5.82	118.13	122.20
1	6	1	U	C6-N1-C2	-5.81	117.51	121.00
36	1	684	G	C4-C5-N7	5.81	113.12	110.80
36	1	1834	U	C4-C5-C6	5.81	123.19	119.70
36	5	834	U	N3-C4-C5	5.81	118.09	114.60
36	5	835	G	C8-N9-C4	5.81	108.72	106.40
36	5	1556	C	C6-N1-C2	-5.81	117.97	120.30
36	5	2875	U	C5-C6-N1	-5.81	119.79	122.70
36	1	421	G	N3-C4-N9	5.81	129.49	126.00
36	1	3036	G	N3-C4-C5	-5.81	125.69	128.60
36	5	1405	U	C5-C6-N1	-5.81	119.80	122.70
36	5	2415	C	N3-C4-C5	5.81	124.22	121.90
36	1	1269	U	N1-C2-O2	5.81	126.87	122.80
36	1	1646	G	C4-C5-N7	5.81	113.12	110.80
37	3	81	U	C5-C4-O4	-5.81	122.42	125.90
36	5	3206	C	C2-N1-C1'	-5.81	112.41	118.80
1	2	1022	C	C6-N1-C2	5.81	122.62	120.30
12	c0	97	PRO	N-CA-CB	5.81	110.27	103.30
1	2	933	A	C8-N9-C4	-5.80	103.48	105.80
36	1	2298	U	O4'-C1'-N1	5.80	112.84	108.20
1	6	387	A	C4-C5-N7	-5.80	107.80	110.70
36	1	2399	A	N1-C6-N6	5.80	122.08	118.60
36	5	620	U	N1-C2-O2	5.80	126.86	122.80
36	5	2350	C	O5'-P-OP1	5.80	117.66	110.70
36	1	2938	G	OP1-P-OP2	5.80	128.30	119.60
1	6	359	A	N3-C4-C5	5.80	130.86	126.80
36	5	659	G	N1-C6-O6	5.80	123.38	119.90
36	5	1488	G	N1-C6-O6	-5.80	116.42	119.90
36	5	1332	A	N1-C2-N3	5.80	132.20	129.30
36	1	1334	U	C6-N1-C2	-5.80	117.52	121.00
36	1	1475	A	C8-N9-C4	5.80	108.12	105.80
36	5	645	A	N1-C2-N3	5.80	132.20	129.30
1	2	1486	G	C4-C5-N7	5.79	113.12	110.80
36	1	893	C	N3-C2-O2	-5.79	117.84	121.90
1	2	647	G	N3-C4-N9	-5.79	122.52	126.00
36	1	2811	A	N1-C6-N6	-5.79	115.12	118.60
1	2	1200	G	C5-C6-N1	-5.79	108.61	111.50
36	1	50	U	C5-C4-O4	5.79	129.38	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	53	A	C2-N3-C4	5.79	113.50	110.60
36	1	2942	C	N3-C4-C5	5.79	124.22	121.90
1	2	1241	G	N7-C8-N9	5.79	115.99	113.10
36	1	111	C	N3-C4-C5	5.79	124.22	121.90
36	1	2385	G	N3-C4-C5	5.79	131.49	128.60
36	5	1161	G	C5-C6-N1	5.79	114.39	111.50
36	5	1445	U	N1-C2-O2	-5.79	118.75	122.80
1	2	1459	C	O5'-P-OP2	-5.79	100.49	105.70
1	2	1389	C	N1-C2-O2	5.79	122.37	118.90
36	1	2313	A	O5'-P-OP1	-5.79	100.49	105.70
36	5	1159	A	OP2-P-O3'	5.79	117.93	105.20
36	5	1367	G	OP1-P-O3'	5.79	117.93	105.20
36	1	1163	A	N1-C2-N3	5.78	132.19	129.30
36	1	2333	C	O5'-P-OP1	-5.78	100.50	105.70
36	5	41	G	OP1-P-O3'	-5.78	92.48	105.20
36	5	1837	U	C5-C4-O4	-5.78	122.43	125.90
36	1	25	U	N3-C4-O4	5.78	123.45	119.40
36	1	1400	G	N3-C4-N9	5.78	129.47	126.00
36	5	2406	C	N3-C2-O2	5.78	125.95	121.90
36	1	784	A	C8-N9-C4	-5.78	103.49	105.80
36	1	518	G	O4'-C1'-N9	5.78	112.82	108.20
1	6	394	C	C6-N1-C2	-5.78	117.99	120.30
1	6	1765	A	O5'-P-OP1	-5.78	100.50	105.70
36	5	1116	G	N1-C2-N3	5.78	127.37	123.90
36	5	1169	A	C4-C5-C6	5.78	119.89	117.00
1	6	59	C	N1-C2-O2	5.78	122.36	118.90
36	5	2292	U	N1-C2-O2	5.77	126.84	122.80
36	1	402	A	N7-C8-N9	-5.77	110.91	113.80
36	1	902	G	C8-N9-C4	-5.77	104.09	106.40
36	1	1450	G	C4-C5-N7	5.77	113.11	110.80
36	1	2883	U	O5'-P-OP2	-5.77	100.51	105.70
36	1	2884	C	O5'-P-OP1	-5.77	100.51	105.70
36	5	1450	G	C5-C6-O6	-5.77	125.14	128.60
36	1	1589	A	C6-N1-C2	-5.77	115.14	118.60
36	5	910	G	C5-C6-N1	5.77	114.39	111.50
36	1	99	A	C8-N9-C4	-5.77	103.49	105.80
36	1	942	U	C4-C5-C6	5.77	123.16	119.70
36	1	1476	G	C5-C6-O6	5.77	132.06	128.60
36	5	2991	A	C8-N9-C4	-5.77	103.49	105.80
36	1	1160	C	C2-N3-C4	5.76	122.78	119.90
36	5	3377	G	C5-C6-O6	-5.76	125.14	128.60
36	1	949	C	N1-C2-O2	-5.76	115.44	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2165	G	C5-C6-O6	-5.76	125.14	128.60
36	1	3369	G	C4-C5-N7	5.76	113.11	110.80
36	5	1456	A	OP1-P-O3'	5.76	117.88	105.20
36	1	3266	G	N9-C4-C5	5.76	107.70	105.40
45	18	236	GLY	N-CA-C	-5.76	98.70	113.10
36	1	1128	U	N1-C2-N3	5.76	118.36	114.90
36	1	1365	G	N3-C4-N9	5.76	129.46	126.00
36	1	3319	U	P-O3'-C3'	5.76	126.61	119.70
38	4	55	U	N3-C2-O2	-5.76	118.17	122.20
1	6	1421	A	C8-N9-C4	5.76	108.10	105.80
36	5	2377	G	C4-C5-N7	-5.76	108.50	110.80
36	5	2805	G	N3-C4-C5	-5.76	125.72	128.60
36	5	197	G	C5-C6-O6	-5.75	125.15	128.60
36	1	979	U	N3-C2-O2	-5.75	118.17	122.20
1	6	335	U	N3-C2-O2	-5.75	118.17	122.20
36	5	329	U	C6-N1-C2	5.75	124.45	121.00
36	5	669	U	C4-C5-C6	5.75	123.15	119.70
36	1	2393	G	N3-C2-N2	-5.75	115.88	119.90
36	5	1589	A	C5-C6-N6	-5.75	119.10	123.70
36	5	2767	U	N3-C4-O4	-5.75	115.38	119.40
37	7	112	G	O5'-P-OP2	-5.75	100.53	105.70
24	D2	65	LEU	CA-CB-CG	5.75	128.52	115.30
36	1	2726	C	N1-C2-N3	5.75	123.22	119.20
36	5	1372	C	C6-N1-C2	5.75	122.60	120.30
1	2	571	G	C4-C5-N7	-5.75	108.50	110.80
36	5	3098	G	N3-C4-N9	5.75	129.45	126.00
1	2	378	A	C5-C6-N6	-5.74	119.11	123.70
1	2	1198	G	C8-N9-C4	-5.74	104.10	106.40
36	1	1142	G	C5-C6-O6	-5.74	125.15	128.60
36	1	2830	G	N3-C2-N2	-5.74	115.88	119.90
1	6	400	A	N1-C6-N6	5.74	122.05	118.60
37	7	25	G	O5'-P-OP2	-5.74	100.53	105.70
36	1	2114	C	OP1-P-OP2	5.74	128.21	119.60
36	1	2823	G	C5-N7-C8	5.74	107.17	104.30
36	1	1458	U	O5'-P-OP2	-5.74	100.53	105.70
36	5	114	A	N1-C6-N6	5.74	122.04	118.60
36	5	835	G	N1-C6-O6	5.74	123.34	119.90
36	5	1181	U	C5-C6-N1	-5.74	119.83	122.70
36	5	1534	A	N3-C4-C5	-5.74	122.78	126.80
36	5	3306	U	O5'-P-OP2	-5.74	100.53	105.70
1	2	16	G	N3-C4-N9	5.74	129.44	126.00
36	1	810	A	C8-N9-C4	-5.74	103.50	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1326	A	C8-N9-C4	5.74	108.09	105.80
1	6	194	U	C5-C6-N1	5.74	125.57	122.70
36	5	283	G	C8-N9-C1'	-5.74	119.54	127.00
36	5	2981	U	C2-N1-C1'	5.74	124.59	117.70
36	5	3151	U	C6-N1-C2	5.74	124.44	121.00
1	6	272	U	P-O3'-C3'	5.74	126.58	119.70
36	5	2938	G	C5-C6-N1	5.74	114.37	111.50
1	2	443	C	C6-N1-C2	-5.74	118.01	120.30
36	1	142	C	C5-C6-N1	5.74	123.87	121.00
36	1	819	U	OP2-P-O3'	5.74	117.82	105.20
1	6	75	U	N1-C2-O2	5.74	126.81	122.80
36	5	2818	U	C5'-C4'-O4'	-5.74	102.22	109.10
1	6	1058	U	P-O3'-C3'	5.73	126.58	119.70
36	5	651	G	N1-C6-O6	-5.73	116.46	119.90
36	5	934	G	C8-N9-C1'	-5.73	119.55	127.00
36	5	2340	U	O5'-P-OP1	-5.73	100.54	105.70
1	2	966	A	N7-C8-N9	-5.73	110.93	113.80
36	1	1592	G	N3-C4-C5	-5.73	125.73	128.60
36	5	313	A	C8-N9-C4	-5.73	103.51	105.80
36	5	2932	U	C5-C6-N1	-5.73	119.83	122.70
37	7	49	G	C5-C6-O6	-5.73	125.16	128.60
1	6	696	C	C2-N1-C1'	-5.73	112.50	118.80
36	5	1178	G	C5-C6-O6	-5.73	125.16	128.60
36	1	1481	A	C4-C5-N7	5.73	113.56	110.70
1	2	704	C	N1-C2-O2	5.73	122.34	118.90
36	1	949	C	C4-C5-C6	5.73	120.26	117.40
36	1	1116	G	N3-C4-C5	-5.73	125.74	128.60
36	5	2703	A	O5'-P-OP2	-5.73	100.55	105.70
38	8	55	U	C6-N1-C2	-5.73	117.56	121.00
36	1	867	G	C4-C5-N7	-5.72	108.51	110.80
36	1	1919	G	N1-C6-O6	-5.72	116.47	119.90
36	5	1392	G	N7-C8-N9	-5.72	110.24	113.10
36	5	1437	C	N3-C2-O2	-5.72	117.89	121.90
36	1	2616	C	O5'-P-OP1	-5.72	100.55	105.70
1	6	1634	C	C5-C6-N1	5.72	123.86	121.00
36	5	807	A	C8-N9-C4	-5.72	103.51	105.80
36	5	878	G	C4-C5-N7	5.72	113.09	110.80
36	5	1375	G	C2-N3-C4	5.72	114.76	111.90
36	1	1492	G	C4-C5-N7	-5.72	108.51	110.80
1	2	571	G	N3-C4-N9	-5.72	122.57	126.00
21	c9	57	ARG	NE-CZ-NH1	5.72	123.16	120.30
36	5	518	G	C4-C5-N7	5.72	113.09	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	24	G	C8-N9-C4	5.72	108.69	106.40
36	5	2994	A	C6-C5-N7	-5.72	128.30	132.30
36	1	2401	A	C4-N9-C1'	-5.72	116.01	126.30
36	1	2878	G	C8-N9-C4	5.72	108.69	106.40
1	6	610	G	C8-N9-C1'	-5.72	119.57	127.00
36	5	428	A	N1-C6-N6	5.72	122.03	118.60
36	5	1592	G	C8-N9-C4	-5.72	104.11	106.40
1	2	1246	C	N3-C2-O2	-5.71	117.90	121.90
37	7	50	U	C5-C6-N1	5.71	125.56	122.70
36	5	1725	C	C5'-C4'-O4'	5.71	115.95	109.10
36	5	1902	G	C4-N9-C1'	5.71	133.93	126.50
36	5	844	G	C8-N9-C4	5.71	108.69	106.40
36	5	1155	C	C2-N1-C1'	5.71	125.08	118.80
36	5	1724	U	O4'-C1'-N1	5.71	112.77	108.20
36	5	2385	G	N1-C6-O6	5.71	123.33	119.90
62	N6	57	LEU	CA-CB-CG	5.71	128.43	115.30
36	1	676	G	N1-C6-O6	5.71	123.33	119.90
36	1	1152	G	O4'-C1'-N9	5.71	112.77	108.20
36	1	2384	A	C4-C5-C6	5.71	119.86	117.00
36	5	1797	A	O5'-P-OP1	-5.71	100.56	105.70
36	5	2632	G	O5'-P-OP1	-5.71	100.56	105.70
36	5	3092	C	N1-C2-O2	5.71	122.33	118.90
36	1	1136	A	C8-N9-C4	-5.71	103.52	105.80
36	1	2885	C	C5-C6-N1	-5.71	118.15	121.00
1	6	1770	U	N1-C2-O2	5.71	126.79	122.80
36	5	648	C	C5-C4-N4	-5.71	116.21	120.20
36	5	806	A	O5'-P-OP1	-5.71	100.56	105.70
36	5	1421	G	C8-N9-C4	5.71	108.68	106.40
36	5	1200	A	C5-C6-N6	-5.71	119.14	123.70
36	1	1469	C	OP1-P-OP2	5.70	128.15	119.60
36	1	3204	C	C6-N1-C2	-5.70	118.02	120.30
36	5	1193	A	C4-N9-C1'	5.70	136.57	126.30
36	5	1837	U	N3-C4-O4	5.70	123.39	119.40
1	2	1081	A	O4'-C1'-N9	5.70	112.76	108.20
36	5	546	C	N3-C2-O2	-5.70	117.91	121.90
36	5	926	A	N1-C6-N6	5.70	122.02	118.60
36	5	559	A	C8-N9-C4	-5.70	103.52	105.80
36	5	2878	G	OP1-P-OP2	-5.70	111.05	119.60
36	1	918	C	N1-C2-O2	-5.70	115.48	118.90
36	1	1366	A	C8-N9-C4	-5.70	103.52	105.80
36	1	1140	G	C5-C6-O6	5.69	132.02	128.60
36	1	1433	A	N1-C6-N6	5.69	122.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	625	C	C5-C4-N4	-5.69	116.21	120.20
36	5	847	A	C8-N9-C4	5.69	108.08	105.80
36	5	3018	C	O5'-P-OP2	-5.69	100.58	105.70
37	7	44	C	N3-C4-C5	-5.69	119.62	121.90
1	2	1033	C	C5-C6-N1	-5.69	118.15	121.00
36	1	1142	G	C5-C6-N1	5.69	114.35	111.50
38	4	21	C	C2-N1-C1'	-5.69	112.54	118.80
36	5	1855	U	N1-C2-N3	5.69	118.32	114.90
38	8	139	U	N3-C2-O2	-5.69	118.22	122.20
1	2	192	U	C2-N1-C1'	5.69	124.53	117.70
36	1	908	G	C4-N9-C1'	5.69	133.90	126.50
36	1	2983	C	N1-C2-N3	5.69	123.18	119.20
36	5	1381	A	C2-N3-C4	-5.69	107.75	110.60
36	5	3218	A	C4-C5-N7	5.69	113.55	110.70
36	1	1442	U	C5-C4-O4	-5.69	122.49	125.90
1	6	130	C	N1-C2-O2	5.69	122.31	118.90
1	6	1145	U	N1-C2-O2	-5.69	118.82	122.80
36	5	878	G	N3-C2-N2	5.69	123.88	119.90
36	5	2231	C	C6-N1-C1'	-5.69	113.98	120.80
36	5	3197	G	N3-C4-C5	5.69	131.44	128.60
36	1	938	C	N1-C2-N3	5.69	123.18	119.20
38	4	79	A	C8-N9-C4	-5.69	103.53	105.80
36	5	2292	U	N3-C2-O2	-5.69	118.22	122.20
36	5	2403	G	O5'-P-OP1	5.69	117.52	110.70
67	o1	90	PHE	CB-CA-C	-5.69	99.03	110.40
36	1	3219	G	O5'-P-OP1	-5.68	100.58	105.70
1	6	402	C	O5'-P-OP2	-5.68	100.58	105.70
36	5	721	G	C5-C6-O6	-5.68	125.19	128.60
36	5	2182	A	OP1-P-O3'	5.68	117.71	105.20
1	2	1291	G	N7-C8-N9	5.68	115.94	113.10
36	5	658	G	C6-C5-N7	-5.68	126.99	130.40
36	5	3093	C	N1-C2-O2	-5.68	115.49	118.90
36	1	639	G	C4-C5-N7	5.68	113.07	110.80
36	1	2798	C	N3-C4-C5	-5.68	119.63	121.90
36	5	1214	U	C6-N1-C2	-5.68	117.59	121.00
1	2	1389	C	C2-N1-C1'	5.68	125.05	118.80
1	2	1784	C	N3-C2-O2	-5.68	117.92	121.90
36	1	1606	U	C2-N1-C1'	-5.68	110.89	117.70
36	1	2679	A	O4'-C1'-N9	5.68	112.74	108.20
36	5	3142	A	N1-C6-N6	5.68	122.01	118.60
36	1	3022	G	C8-N9-C4	-5.68	104.13	106.40
36	1	1103	A	O5'-P-OP2	5.68	117.51	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2169	G	C5-C6-N1	5.68	114.34	111.50
36	5	75	G	N3-C4-C5	-5.68	125.76	128.60
36	5	1903	U	C5-C6-N1	5.68	125.54	122.70
36	5	2392	C	C5-C6-N1	-5.68	118.16	121.00
1	2	459	G	N1-C6-O6	5.67	123.31	119.90
36	1	1149	G	N3-C2-N2	-5.67	115.93	119.90
36	5	581	U	C5-C4-O4	-5.67	122.50	125.90
36	5	3103	A	C5-C6-N1	5.67	120.54	117.70
1	2	1745	G	C5-C6-N1	5.67	114.34	111.50
36	1	2628	A	O5'-P-OP2	-5.67	100.59	105.70
36	1	1405	U	C6-N1-C2	5.67	124.40	121.00
1	6	343	C	N1-C2-O2	-5.67	115.50	118.90
36	5	1494	U	N3-C4-O4	-5.67	115.43	119.40
36	5	3018	C	C6-N1-C2	-5.67	118.03	120.30
36	5	1868	G	N3-C4-N9	5.67	129.40	126.00
1	2	1762	A	N7-C8-N9	-5.67	110.97	113.80
36	1	347	G	C4-C5-N7	5.67	113.07	110.80
36	1	810	A	C5-C6-N1	5.67	120.53	117.70
36	1	888	A	N1-C6-N6	5.67	122.00	118.60
78	Q2	42	ARG	NE-CZ-NH1	5.67	123.13	120.30
36	5	2637	A	N9-C4-C5	-5.67	103.53	105.80
36	5	2796	G	N1-C6-O6	-5.67	116.50	119.90
36	1	1379	G	N1-C6-O6	-5.67	116.50	119.90
36	1	2163	C	C4-C5-C6	5.67	120.23	117.40
6	s4	38	LEU	CA-CB-CG	5.67	128.33	115.30
36	5	2409	G	C2-N3-C4	5.67	114.73	111.90
36	5	807	A	N7-C8-N9	5.67	116.63	113.80
36	1	1902	G	N1-C6-O6	5.66	123.30	119.90
36	5	1108	U	C5-C4-O4	5.66	129.30	125.90
36	5	2901	G	C8-N9-C4	-5.66	104.14	106.40
36	5	2584	G	C4-N9-C1'	5.66	133.86	126.50
1	2	1202	A	N1-C6-N6	-5.66	115.20	118.60
36	1	633	C	C4-C5-C6	5.66	120.23	117.40
36	1	1124	U	N3-C4-C5	5.66	118.00	114.60
36	1	1481	A	C6-C5-N7	-5.66	128.34	132.30
36	5	2792	A	C6-C5-N7	-5.66	128.34	132.30
1	2	730	G	C4-N9-C1'	5.66	133.85	126.50
36	5	856	G	N9-C4-C5	-5.66	103.14	105.40
36	5	1117	G	C5-C6-N1	5.66	114.33	111.50
36	5	3195	U	P-O3'-C3'	5.66	126.49	119.70
36	5	890	C	O5'-P-OP1	5.66	117.49	110.70
1	2	321	C	C6-N1-C2	-5.66	118.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1280	C	C4-C5-C6	5.66	120.23	117.40
36	1	409	A	O5'-P-OP2	-5.66	100.61	105.70
1	6	1537	C	O4'-C1'-N1	5.66	112.72	108.20
36	5	3218	A	P-O3'-C3'	5.66	126.49	119.70
36	1	1128	U	C5-C6-N1	-5.65	119.87	122.70
36	1	2142	A	C6-N1-C2	-5.65	115.21	118.60
36	5	2364	G	C5-C6-O6	5.65	131.99	128.60
36	1	3208	G	N9-C4-C5	5.65	107.66	105.40
36	5	2341	A	N7-C8-N9	-5.65	110.97	113.80
36	5	2964	G	N7-C8-N9	-5.65	110.27	113.10
36	1	503	C	N3-C4-N4	-5.65	114.05	118.00
1	6	1113	A	C2-N3-C4	-5.65	107.77	110.60
36	1	2718	U	N1-C2-N3	5.65	118.29	114.90
36	1	1368	U	OP2-P-O3'	5.65	117.62	105.20
36	1	1858	A	O5'-P-OP2	-5.65	100.62	105.70
36	5	1198	C	N3-C2-O2	-5.65	117.95	121.90
1	6	938	G	N1-C6-O6	5.65	123.29	119.90
36	5	871	U	N1-C2-N3	5.65	118.29	114.90
1	2	1200	G	C4-C5-C6	5.64	122.19	118.80
8	S6	76	LEU	CA-CB-CG	5.64	128.28	115.30
38	4	12	A	N1-C2-N3	-5.64	126.48	129.30
36	5	2930	A	N1-C6-N6	-5.64	115.21	118.60
36	1	2973	G	O5'-P-OP1	-5.64	100.62	105.70
36	5	1475	A	N1-C2-N3	5.64	132.12	129.30
36	1	2281	A	C2-N3-C4	-5.64	107.78	110.60
1	2	396	G	N9-C1'-C2'	-5.64	105.80	112.00
36	1	716	A	O5'-P-OP1	-5.64	100.62	105.70
36	5	1889	G	C2-N3-C4	5.64	114.72	111.90
36	5	3121	U	N3-C4-O4	-5.64	115.45	119.40
1	2	1007	C	C6-N1-C2	5.64	122.56	120.30
36	1	575	G	C5-C6-N1	5.64	114.32	111.50
36	1	2398	A	C8-N9-C4	5.64	108.06	105.80
1	2	1458	G	C4-N9-C1'	5.64	133.83	126.50
1	6	1700	C	N3-C2-O2	-5.64	117.95	121.90
36	5	2572	C	C6-N1-C2	-5.64	118.05	120.30
36	5	1081	U	C5-C6-N1	5.63	125.52	122.70
36	5	2639	G	C6-C5-N7	-5.63	127.02	130.40
36	5	2981	U	N3-C2-O2	-5.63	118.26	122.20
36	1	582	G	N3-C4-N9	-5.63	122.62	126.00
36	1	1122	U	N3-C4-C5	5.63	117.98	114.60
36	5	1342	C	C4-C5-C6	5.63	120.22	117.40
36	1	2315	G	C5-C6-O6	5.63	131.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1940	G	N3-C4-N9	5.63	129.38	126.00
37	7	73	C	N1-C2-O2	5.63	122.28	118.90
39	12	246	LEU	CA-CB-CG	5.63	128.25	115.30
48	m1	12	LEU	CA-CB-CG	5.63	128.25	115.30
1	2	1479	A	N1-C6-N6	5.63	121.98	118.60
36	1	873	C	P-O3'-C3'	5.63	126.46	119.70
1	6	351	C	N3-C4-N4	5.63	121.94	118.00
36	5	412	G	C8-N9-C4	-5.63	104.15	106.40
36	1	29	C	N3-C4-N4	5.63	121.94	118.00
36	1	663	C	C5-C4-N4	-5.63	116.26	120.20
1	6	961	U	C6-N1-C2	-5.63	117.62	121.00
36	5	1208	U	N1-C2-O2	5.63	126.74	122.80
36	1	44	U	C5-C6-N1	-5.63	119.89	122.70
36	1	267	G	N1-C6-O6	5.63	123.28	119.90
36	1	939	U	N1-C2-N3	5.63	118.28	114.90
1	6	92	A	C8-N9-C4	5.63	108.05	105.80
36	5	365	A	C5-C6-N6	-5.63	119.20	123.70
36	5	1889	G	C5-C6-O6	-5.63	125.22	128.60
36	5	3382	U	N1-C2-O2	5.63	126.74	122.80
36	1	225	C	N3-C4-N4	5.62	121.94	118.00
36	1	3263	G	C8-N9-C4	5.62	108.65	106.40
36	1	788	C	C6-N1-C2	5.62	122.55	120.30
36	1	2724	U	N1-C2-O2	5.62	126.74	122.80
36	5	2881	C	O5'-P-OP2	-5.62	100.64	105.70
38	8	100	U	N3-C4-O4	5.62	123.34	119.40
36	5	580	C	C6-N1-C2	-5.62	118.05	120.30
36	5	1474	A	N1-C6-N6	-5.62	115.23	118.60
36	5	2213	A	C8-N9-C4	5.62	108.05	105.80
36	1	1328	C	O5'-P-OP1	-5.62	100.64	105.70
36	1	2350	C	C2-N3-C4	-5.62	117.09	119.90
36	5	2207	A	O4'-C1'-N9	5.62	112.70	108.20
36	1	632	G	C8-N9-C4	5.62	108.65	106.40
36	1	695	C	N3-C4-C5	5.62	124.15	121.90
36	1	1820	U	OP2-P-O3'	5.62	117.56	105.20
61	N5	38	LEU	CA-CB-CG	5.62	128.22	115.30
36	5	1306	G	OP2-P-O3'	5.62	117.56	105.20
1	2	720	G	OP1-P-O3'	5.62	117.56	105.20
1	2	1081	A	P-O3'-C3'	5.62	126.44	119.70
36	1	1606	U	N3-C2-O2	5.62	126.13	122.20
36	5	1304	A	C5-C6-N1	5.62	120.51	117.70
36	5	3301	U	C6-N1-C2	5.62	124.37	121.00
1	2	1168	U	OP1-P-O3'	5.61	117.55	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2679	A	N1-C6-N6	5.61	121.97	118.60
36	5	2816	G	N1-C6-O6	5.61	123.27	119.90
36	1	2121	G	N1-C2-N2	-5.61	111.15	116.20
36	1	2805	G	C4-C5-N7	5.61	113.04	110.80
41	L4	327	LEU	CA-CB-CG	5.61	128.20	115.30
36	5	770	G	O4'-C1'-N9	5.61	112.69	108.20
36	5	2129	U	C6-N1-C2	-5.61	117.63	121.00
36	5	2211	U	N3-C2-O2	-5.61	118.27	122.20
37	7	13	A	N1-C6-N6	-5.61	115.23	118.60
36	1	56	G	O5'-P-OP1	-5.61	100.65	105.70
1	2	352	A	N7-C8-N9	-5.61	111.00	113.80
36	1	97	U	C5-C6-N1	-5.61	119.90	122.70
36	1	637	C	C5-C6-N1	-5.61	118.20	121.00
36	1	1158	A	C4-C5-C6	5.61	119.80	117.00
36	1	3120	C	N3-C2-O2	-5.61	117.97	121.90
36	1	351	A	C5-C6-N6	5.61	128.18	123.70
36	1	1128	U	N3-C2-O2	-5.61	118.28	122.20
36	1	1507	G	C4-C5-C6	5.61	122.16	118.80
36	1	2634	U	N3-C4-C5	5.61	117.96	114.60
36	5	1496	C	C2-N1-C1'	5.61	124.97	118.80
36	1	1336	U	O5'-P-OP1	5.60	117.42	110.70
36	5	940	G	N1-C2-N2	5.60	121.24	116.20
36	1	3055	U	N3-C4-C5	5.60	117.96	114.60
36	5	1364	C	OP2-P-O3'	5.60	117.53	105.20
36	5	2772	C	OP2-P-O3'	5.60	117.53	105.20
36	5	1160	C	C6-N1-C1'	5.60	127.52	120.80
36	1	1168	U	O5'-P-OP2	-5.60	100.66	105.70
36	1	3246	G	C6-C5-N7	-5.60	127.04	130.40
36	5	2176	U	C2-N3-C4	-5.60	123.64	127.00
36	5	2617	U	N3-C4-C5	-5.60	111.24	114.60
36	5	3182	G	O5'-P-OP2	5.60	117.42	110.70
1	2	402	C	C5-C6-N1	-5.60	118.20	121.00
1	2	571	G	N9-C4-C5	5.60	107.64	105.40
36	1	1077	U	C2-N3-C4	-5.60	123.64	127.00
1	6	748	U	N1-C2-O2	5.60	126.72	122.80
36	5	2937	G	N9-C4-C5	-5.60	103.16	105.40
1	2	428	A	O4'-C1'-N9	5.59	112.68	108.20
36	1	847	A	N1-C6-N6	5.59	121.96	118.60
1	6	1045	C	C6-N1-C2	-5.59	118.06	120.30
36	5	2819	A	C4-C5-N7	-5.59	107.90	110.70
39	12	3	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	2	499	U	P-O3'-C3'	5.59	126.41	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	13	A	C6-C5-N7	-5.59	128.38	132.30
1	6	978	A	N9-C4-C5	5.59	108.04	105.80
36	5	1103	A	C8-N9-C4	-5.59	103.56	105.80
36	5	1441	G	O5'-P-OP2	-5.59	100.67	105.70
36	5	1879	A	C6-C5-N7	-5.59	128.39	132.30
36	1	517	G	C6-C5-N7	-5.59	127.05	130.40
36	1	3081	C	N3-C2-O2	-5.59	117.99	121.90
1	6	1489	U	N3-C2-O2	-5.59	118.29	122.20
36	5	2699	G	C8-N9-C4	5.59	108.64	106.40
36	5	2949	U	N3-C2-O2	-5.59	118.29	122.20
1	6	555	A	P-O3'-C3'	5.59	126.40	119.70
36	5	3103	A	C6-N1-C2	-5.59	115.25	118.60
37	7	87	G	N3-C2-N2	-5.59	115.99	119.90
36	1	562	C	C6-N1-C2	-5.58	118.07	120.30
36	1	2144	A	C5-C6-N1	5.58	120.49	117.70
36	1	1292	C	C6-N1-C2	5.58	122.53	120.30
36	1	3308	C	N1-C2-O2	-5.58	115.55	118.90
36	5	640	U	N1-C2-O2	-5.58	118.89	122.80
36	5	2358	A	O5'-P-OP2	-5.58	100.67	105.70
1	2	734	A	P-O3'-C3'	5.58	126.40	119.70
36	1	92	G	N3-C4-N9	5.58	129.35	126.00
36	1	908	G	C8-N9-C1'	-5.58	119.75	127.00
36	1	3337	G	N1-C6-O6	-5.58	116.55	119.90
36	5	526	C	N3-C4-C5	5.58	124.13	121.90
36	5	2735	U	N3-C2-O2	-5.58	118.29	122.20
36	1	716	A	C4-C5-N7	5.58	113.49	110.70
1	6	396	G	N7-C8-N9	5.58	115.89	113.10
36	5	365	A	C4-C5-N7	5.58	113.49	110.70
36	1	650	C	C5-C6-N1	-5.58	118.21	121.00
36	1	1204	A	N1-C6-N6	5.58	121.95	118.60
36	5	1317	A	C5-C6-N6	-5.58	119.24	123.70
36	5	3197	G	N3-C2-N2	-5.58	116.00	119.90
37	7	1	G	C8-N9-C4	-5.58	104.17	106.40
36	1	965	A	OP1-P-O3'	5.58	117.47	105.20
36	1	2163	C	C2-N1-C1'	-5.58	112.67	118.80
36	1	2818	U	OP2-P-O3'	5.58	117.47	105.20
1	6	1310	U	N1-C2-O2	5.58	126.70	122.80
36	5	404	G	N1-C2-N3	5.58	127.25	123.90
36	5	3272	C	O5'-P-OP1	-5.58	100.68	105.70
36	1	2662	G	C4-C5-N7	5.57	113.03	110.80
1	6	297	U	N3-C4-O4	5.57	123.30	119.40
1	2	1759	C	N1-C2-O2	5.57	122.24	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	702	C	C6-N1-C2	-5.57	118.07	120.30
36	1	922	U	N3-C2-O2	-5.57	118.30	122.20
1	6	1631	A	N1-C6-N6	-5.57	115.26	118.60
36	5	2899	C	N1-C2-N3	5.57	123.10	119.20
36	1	2879	C	N3-C2-O2	5.57	125.80	121.90
36	1	922	U	C2-N1-C1'	5.57	124.38	117.70
1	2	863	A	N1-C6-N6	5.57	121.94	118.60
36	1	1128	U	C2-N3-C4	-5.57	123.66	127.00
36	1	1443	G	N7-C8-N9	5.57	115.88	113.10
36	1	2391	G	N3-C2-N2	-5.57	116.00	119.90
36	1	2984	C	N3-C2-O2	-5.57	118.00	121.90
36	5	938	C	N3-C4-C5	5.57	124.13	121.90
36	5	2704	A	C2-N3-C4	-5.56	107.82	110.60
36	5	2992	U	N1-C2-N3	-5.56	111.56	114.90
36	5	1449	A	C4-C5-C6	5.56	119.78	117.00
36	1	3112	G	C5-C6-O6	-5.56	125.26	128.60
1	2	553	G	C4-C5-N7	5.56	113.02	110.80
1	2	704	C	O4'-C1'-N1	5.56	112.65	108.20
1	2	1249	U	N3-C2-O2	-5.56	118.31	122.20
1	2	1654	G	N3-C4-N9	5.56	129.34	126.00
15	C3	22	ALA	C-N-CA	5.56	145.35	122.00
36	1	663	C	OP2-P-O3'	5.56	117.43	105.20
36	5	3313	U	N3-C2-O2	-5.56	118.31	122.20
38	8	36	G	N1-C6-O6	-5.56	116.56	119.90
36	1	1588	A	N1-C6-N6	-5.56	115.27	118.60
36	1	2434	U	C5-C4-O4	5.56	129.23	125.90
36	1	2935	U	N3-C4-C5	-5.56	111.27	114.60
36	5	940	G	C2-N3-C4	5.56	114.68	111.90
78	q2	93	LEU	CA-CB-CG	5.56	128.08	115.30
36	5	515	C	C4-C5-C6	5.56	120.18	117.40
36	5	2963	C	O5'-P-OP2	-5.56	100.70	105.70
36	5	3221	C	N3-C4-C5	-5.56	119.68	121.90
36	5	1389	G	N1-C6-O6	5.55	123.23	119.90
36	5	1847	A	OP2-P-O3'	5.55	117.42	105.20
1	6	973	A	C4-C5-C6	5.55	119.78	117.00
36	5	1056	U	C6-N1-C2	-5.55	117.67	121.00
36	5	2549	G	C6-C5-N7	-5.55	127.07	130.40
1	2	1473	U	N1-C2-O2	5.55	126.69	122.80
36	1	873	C	N1-C2-O2	-5.55	115.57	118.90
1	6	1072	C	C2-N1-C1'	5.55	124.91	118.80
36	1	357	A	O5'-P-OP2	-5.55	100.71	105.70
36	5	1484	U	C5-C6-N1	-5.55	119.92	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1541	G	N7-C8-N9	5.55	115.87	113.10
1	2	941	A	N1-C6-N6	5.55	121.93	118.60
36	1	2350	C	C4-C5-C6	5.54	120.17	117.40
36	5	620	U	C2-N1-C1'	5.54	124.35	117.70
36	1	587	U	C2-N3-C4	-5.54	123.67	127.00
36	1	3243	A	C8-N9-C4	5.54	108.02	105.80
1	6	625	C	N3-C2-O2	5.54	125.78	121.90
36	5	2145	A	N3-C4-C5	-5.54	122.92	126.80
36	5	3378	C	N3-C4-C5	5.54	124.12	121.90
38	8	42	G	C8-N9-C4	5.54	108.62	106.40
38	8	99	C	C6-N1-C2	5.54	122.52	120.30
1	2	1081	A	OP1-P-O3'	5.54	117.39	105.20
36	1	1846	C	C4-C5-C6	5.54	120.17	117.40
36	1	2257	C	O4'-C1'-N1	5.54	112.63	108.20
36	1	2975	U	N1-C2-O2	5.54	126.68	122.80
36	1	864	G	C4-C5-N7	-5.54	108.58	110.80
36	5	1127	G	O5'-P-OP2	-5.54	100.71	105.70
36	1	2404	A	N1-C2-N3	5.54	132.07	129.30
37	3	87	G	O5'-P-OP2	-5.54	100.72	105.70
36	5	3212	C	N1-C2-O2	-5.54	115.58	118.90
36	5	747	A	O5'-P-OP2	-5.54	100.72	105.70
36	5	2434	U	C5-C4-O4	5.54	129.22	125.90
1	2	1654	G	N3-C4-C5	-5.53	125.83	128.60
36	1	2884	C	C4-C5-C6	-5.53	114.63	117.40
36	1	3178	A	C5-C6-N1	-5.53	114.93	117.70
1	6	558	U	C5-C6-N1	5.53	125.47	122.70
1	6	1700	C	C6-N1-C1'	-5.53	114.16	120.80
36	5	61	A	C8-N9-C4	-5.53	103.59	105.80
1	2	720	G	P-O3'-C3'	5.53	126.34	119.70
36	1	189	G	C4-C5-N7	5.53	113.01	110.80
36	1	703	G	N3-C4-N9	-5.53	122.68	126.00
36	1	927	C	O5'-P-OP1	-5.53	100.72	105.70
36	1	2944	U	OP1-P-O3'	5.53	117.37	105.20
1	2	110	U	C5-C6-N1	5.53	125.46	122.70
36	1	362	U	C6-N1-C2	5.53	124.32	121.00
36	1	1133	A	C5-C6-N1	5.53	120.46	117.70
36	5	820	A	O5'-P-OP1	-5.53	100.72	105.70
36	5	1200	A	C4-C5-C6	5.53	119.76	117.00
36	1	942	U	OP1-P-OP2	-5.53	111.31	119.60
1	6	1200	G	C4-N9-C1'	-5.53	119.32	126.50
36	5	865	U	N1-C2-O2	-5.53	118.93	122.80
36	5	1155	C	C6-N1-C1'	-5.53	114.17	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2993	G	C5-C6-N1	5.52	114.26	111.50
1	2	453	U	C6-N1-C2	-5.52	117.69	121.00
36	1	711	A	N1-C6-N6	-5.52	115.29	118.60
36	5	421	G	N3-C4-C5	-5.52	125.84	128.60
36	5	751	A	O5'-P-OP2	-5.52	100.73	105.70
36	5	805	G	N1-C6-O6	-5.52	116.59	119.90
36	1	102	C	N3-C4-C5	-5.52	119.69	121.90
36	5	2242	A	N1-C6-N6	-5.52	115.29	118.60
1	6	1768	G	C5-C6-O6	5.52	131.91	128.60
36	5	2625	C	C2-N3-C4	-5.52	117.14	119.90
36	1	812	G	C4-C5-N7	-5.52	108.59	110.80
36	1	2297	U	N3-C2-O2	-5.52	118.34	122.20
36	5	87	U	C6-N1-C2	-5.52	117.69	121.00
36	5	2524	A	O4'-C1'-N9	5.52	112.61	108.20
1	6	696	C	O4'-C1'-N1	5.51	112.61	108.20
36	5	636	C	O5'-P-OP2	-5.51	100.74	105.70
36	5	646	A	C5-C6-N6	5.51	128.11	123.70
36	5	1158	A	C8-N9-C4	5.51	108.01	105.80
36	5	1795	U	C2-N1-C1'	5.51	124.32	117.70
36	5	2373	A	O5'-P-OP2	5.51	117.32	110.70
36	5	2653	C	C6-N1-C2	-5.51	118.09	120.30
36	5	2870	C	O4'-C1'-N1	5.51	112.61	108.20
36	5	3154	C	C5-C6-N1	5.51	123.76	121.00
36	5	2823	G	N9-C4-C5	5.51	107.61	105.40
36	5	1316	C	O5'-P-OP2	-5.51	100.74	105.70
36	5	3094	A	C8-N9-C4	5.51	108.00	105.80
36	1	279	U	N1-C2-O2	5.51	126.66	122.80
36	1	1581	C	N3-C2-O2	-5.51	118.04	121.90
36	5	2572	C	C6-N1-C1'	-5.51	114.19	120.80
24	D2	93	LEU	CA-CB-CG	5.51	127.97	115.30
36	1	2138	A	C5-C6-N1	-5.51	114.95	117.70
36	5	800	G	O4'-C1'-N9	-5.51	103.80	108.20
36	1	2640	A	C6-N1-C2	-5.50	115.30	118.60
36	5	2245	C	C6-N1-C2	-5.50	118.10	120.30
1	2	453	U	C5-C4-O4	5.50	129.20	125.90
1	2	1745	G	C6-N1-C2	-5.50	121.80	125.10
36	5	2849	C	N3-C2-O2	5.50	125.75	121.90
36	1	2388	U	C5-C4-O4	-5.50	122.60	125.90
36	5	2950	G	C5-N7-C8	-5.50	101.55	104.30
36	5	2971	A	C2-N3-C4	5.50	113.35	110.60
36	5	3215	A	C5-C6-N1	-5.50	114.95	117.70
37	7	33	U	C2-N1-C1'	5.50	124.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	402	C	N3-C4-N4	5.50	121.85	118.00
36	5	3382	U	N3-C2-O2	-5.50	118.35	122.20
36	1	885	U	C5-C6-N1	-5.50	119.95	122.70
1	6	787	G	N3-C4-N9	5.50	129.30	126.00
1	6	1640	C	C6-N1-C1'	-5.50	114.20	120.80
1	2	1190	C	C6-N1-C2	5.50	122.50	120.30
1	2	1595	U	C5-C6-N1	-5.50	119.95	122.70
1	2	1773	C	N3-C4-N4	5.50	121.85	118.00
38	4	16	G	N7-C8-N9	-5.50	110.35	113.10
36	5	639	G	N3-C2-N2	-5.50	116.05	119.90
36	5	2996	U	N1-C2-O2	5.50	126.65	122.80
1	2	402	C	N1-C2-O2	-5.49	115.60	118.90
36	1	287	G	C8-N9-C4	5.49	108.60	106.40
36	1	779	G	C8-N9-C4	5.49	108.60	106.40
62	N6	126	LEU	CA-CB-CG	5.49	127.93	115.30
36	1	931	C	N3-C4-C5	5.49	124.10	121.90
36	1	1152	G	C4-N9-C1'	5.49	133.64	126.50
1	6	363	G	C5-C6-O6	-5.49	125.31	128.60
36	5	198	A	C8-N9-C4	5.49	108.00	105.80
1	6	351	C	C2-N1-C1'	5.49	124.84	118.80
1	6	381	C	N3-C4-C5	5.49	124.10	121.90
36	1	1269	U	N3-C2-O2	-5.49	118.36	122.20
25	D3	33	LEU	CA-CB-CG	-5.49	102.68	115.30
36	5	2639	G	C6-N1-C2	-5.49	121.81	125.10
1	6	350	U	N1-C2-O2	-5.48	118.96	122.80
36	1	1477	A	C8-N9-C4	-5.48	103.61	105.80
38	4	14	C	N3-C4-C5	5.48	124.09	121.90
1	2	1202	A	C2-N3-C4	5.48	113.34	110.60
36	1	1532	C	N3-C4-C5	5.48	124.09	121.90
1	6	1628	U	N3-C2-O2	-5.48	118.36	122.20
36	5	868	C	C6-N1-C2	5.48	122.49	120.30
36	5	2392	C	C2-N3-C4	-5.48	117.16	119.90
1	6	1145	U	N3-C4-O4	5.48	123.24	119.40
1	6	1740	A	C8-N9-C4	5.48	107.99	105.80
1	6	1765	A	N7-C8-N9	-5.48	111.06	113.80
1	6	1768	G	C4-C5-N7	-5.48	108.61	110.80
36	5	372	A	N1-C6-N6	5.48	121.89	118.60
36	5	842	G	N1-C6-O6	5.48	123.19	119.90
36	5	2341	A	O5'-P-OP2	-5.48	100.77	105.70
36	5	2950	G	O4'-C1'-N9	5.48	112.58	108.20
36	1	895	A	C8-N9-C4	-5.47	103.61	105.80
36	1	1127	G	C5-C6-O6	-5.47	125.32	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	650	C	N1-C2-O2	-5.47	115.61	118.90
36	5	2189	U	C6-N1-C2	5.47	124.28	121.00
36	5	2699	G	N3-C2-N2	-5.47	116.07	119.90
1	2	1497	U	C2-N1-C1'	5.47	124.27	117.70
36	5	2917	G	C8-N9-C1'	-5.47	119.89	127.00
36	5	2673	A	C8-N9-C4	5.47	107.99	105.80
36	1	67	A	O5'-P-OP1	-5.47	100.78	105.70
36	1	343	U	OP2-P-O3'	5.47	117.23	105.20
36	1	709	A	O5'-P-OP1	5.47	117.26	110.70
36	1	2184	U	C5-C4-O4	-5.47	122.62	125.90
36	1	2632	G	C5-C6-N1	5.47	114.23	111.50
36	5	2216	G	C8-N9-C4	5.47	108.59	106.40
36	5	2278	C	C6-N1-C2	-5.47	118.11	120.30
36	1	3303	G	O4'-C1'-N9	5.47	112.58	108.20
36	5	2818	U	C5-C4-O4	-5.47	122.62	125.90
1	6	858	G	O4'-C1'-N9	5.47	112.57	108.20
36	5	125	C	N3-C4-N4	-5.47	114.17	118.00
36	5	2290	C	C5-C6-N1	-5.47	118.27	121.00
36	5	2388	U	N3-C2-O2	5.47	126.03	122.20
1	2	985	G	N3-C4-C5	-5.46	125.87	128.60
36	1	357	A	C8-N9-C4	5.46	107.99	105.80
73	O7	5	THR	C-N-CD	5.46	139.88	128.40
1	6	1414	U	N3-C2-O2	-5.46	118.38	122.20
36	5	2913	C	C6-N1-C2	-5.46	118.11	120.30
36	5	639	G	C5-C6-O6	-5.46	125.32	128.60
36	5	833	G	C8-N9-C4	5.46	108.58	106.40
1	6	957	G	N1-C6-O6	5.46	123.18	119.90
36	5	2593	A	P-O3'-C3'	5.46	126.25	119.70
36	1	283	G	O4'-C1'-N9	-5.46	103.83	108.20
1	2	1749	A	C8-N9-C4	5.46	107.98	105.80
36	5	399	A	O5'-P-OP1	-5.46	100.79	105.70
36	5	2800	G	N3-C2-N2	-5.46	116.08	119.90
36	5	2964	G	N1-C6-O6	-5.46	116.63	119.90
1	2	17	C	C6-N1-C2	-5.46	118.12	120.30
1	6	696	C	C6-N1-C1'	5.46	127.35	120.80
38	8	101	U	C6-N1-C2	-5.46	117.73	121.00
36	1	2726	C	N3-C4-N4	-5.45	114.18	118.00
36	1	3209	A	O5'-P-OP1	-5.45	100.79	105.70
38	4	30	C	N3-C4-C5	5.45	124.08	121.90
36	5	2884	C	C5-C4-N4	-5.45	116.38	120.20
36	5	3050	U	C4-C5-C6	5.45	122.97	119.70
36	5	1534	A	C5-N7-C8	5.45	106.63	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	978	G	N3-C4-C5	5.45	131.32	128.60
36	1	1550	C	N1-C2-O2	-5.45	115.63	118.90
36	1	2417	U	N1-C2-O2	-5.45	118.98	122.80
38	4	25	G	C4-C5-N7	-5.45	108.62	110.80
1	6	1475	A	C8-N9-C4	5.45	107.98	105.80
36	5	2806	U	C5-C6-N1	-5.45	119.97	122.70
1	2	829	A	P-O3'-C3'	5.45	126.24	119.70
36	1	3091	A	C5-N7-C8	-5.45	101.18	103.90
1	6	136	C	C6-N1-C1'	-5.45	114.26	120.80
36	5	1139	G	N1-C6-O6	-5.45	116.63	119.90
36	1	1587	A	N1-C6-N6	-5.45	115.33	118.60
36	5	1437	C	C5-C6-N1	5.45	123.72	121.00
36	5	3078	U	N3-C2-O2	-5.45	118.39	122.20
1	2	810	G	N9-C4-C5	-5.45	103.22	105.40
1	2	1324	G	N9-C4-C5	5.45	107.58	105.40
36	1	46	U	C5-C6-N1	-5.45	119.98	122.70
36	1	1329	U	N1-C1'-C2'	-5.45	106.01	112.00
36	1	2920	U	C6-N1-C2	5.45	124.27	121.00
36	1	3305	A	O5'-P-OP2	-5.45	100.80	105.70
1	6	433	C	C5-C4-N4	-5.45	116.39	120.20
36	5	864	G	N7-C8-N9	-5.45	110.38	113.10
36	5	1186	G	C4-C5-N7	5.45	112.98	110.80
36	5	2272	G	O4'-C1'-N9	5.45	112.56	108.20
36	5	2975	U	C4-C5-C6	-5.45	116.43	119.70
36	5	901	G	C4-N9-C1'	5.44	133.58	126.50
1	2	89	G	C8-N9-C4	5.44	108.58	106.40
1	2	380	U	N1-C2-O2	5.44	126.61	122.80
36	1	1683	A	C5-C6-N6	-5.44	119.35	123.70
36	5	1928	G	C4-C5-N7	5.44	112.98	110.80
36	5	3362	A	C4-C5-N7	5.44	113.42	110.70
36	1	730	C	C2-N3-C4	-5.44	117.18	119.90
36	1	1845	G	OP2-P-O3'	5.44	117.17	105.20
36	1	2121	G	C5-C6-N1	5.44	114.22	111.50
36	1	2950	G	O4'-C1'-N9	5.44	112.55	108.20
36	1	3207	U	C6-N1-C1'	5.44	128.82	121.20
1	6	1146	G	C6-C5-N7	-5.44	127.14	130.40
1	6	1768	G	C6-C5-N7	5.44	133.66	130.40
36	5	1850	A	C6-N1-C2	5.44	121.86	118.60
1	2	73	U	P-O3'-C3'	5.44	126.23	119.70
1	6	111	U	C2-N1-C1'	5.44	124.23	117.70
1	6	971	A	C8-N9-C4	-5.44	103.62	105.80
1	6	1535	U	C2-N1-C1'	5.44	124.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	953	G	N1-C6-O6	5.44	123.16	119.90
36	5	1367	G	C4-C5-C6	5.44	122.06	118.80
36	5	1404	G	C8-N9-C4	5.44	108.58	106.40
36	5	1440	G	C4-C5-N7	-5.44	108.62	110.80
36	5	3040	A	OP1-P-OP2	-5.44	111.44	119.60
36	1	2145	A	OP2-P-O3'	5.43	117.16	105.20
1	6	1652	C	C2-N3-C4	-5.43	117.18	119.90
36	5	2377	G	C5-N7-C8	5.43	107.02	104.30
36	1	1313	G	C6-C5-N7	-5.43	127.14	130.40
36	5	923	C	N1-C2-O2	5.43	122.16	118.90
36	5	2139	A	N1-C6-N6	-5.43	115.34	118.60
36	5	3057	U	C2-N1-C1'	5.43	124.22	117.70
36	1	364	G	C5-C6-O6	-5.43	125.34	128.60
36	1	1588	A	C6-C5-N7	5.43	136.10	132.30
36	1	2418	G	C2-N3-C4	5.43	114.61	111.90
38	4	113	U	C2-N1-C1'	-5.43	111.18	117.70
1	6	275	C	C2-N1-C1'	5.43	124.77	118.80
1	6	1749	A	C2-N3-C4	-5.43	107.89	110.60
36	5	226	C	N1-C2-O2	5.43	122.16	118.90
36	5	661	G	C4-C5-N7	5.43	112.97	110.80
36	5	1433	A	O4'-C1'-N9	-5.43	103.86	108.20
36	5	2333	C	C5-C4-N4	-5.43	116.40	120.20
36	1	2284	C	N3-C2-O2	-5.43	118.10	121.90
36	5	391	A	C8-N9-C4	5.43	107.97	105.80
1	2	1595	U	N1-C2-O2	-5.43	119.00	122.80
36	1	1094	U	C5-C6-N1	5.43	125.41	122.70
36	5	2687	G	N1-C6-O6	5.43	123.16	119.90
36	5	2957	G	C8-N9-C4	5.43	108.57	106.40
1	2	1462	G	N1-C6-O6	5.42	123.16	119.90
36	1	1695	U	C5-C6-N1	-5.42	119.99	122.70
1	6	558	U	N3-C2-O2	-5.42	118.40	122.20
36	5	87	U	C5-C6-N1	5.42	125.41	122.70
36	5	112	U	O4'-C1'-N1	5.42	112.54	108.20
36	5	365	A	N9-C4-C5	-5.42	103.63	105.80
36	5	411	U	N1-C2-N3	5.42	118.16	114.90
36	5	2531	C	C2-N1-C1'	5.42	124.77	118.80
36	5	2980	U	N3-C2-O2	-5.42	118.40	122.20
36	1	716	A	N1-C6-N6	5.42	121.85	118.60
36	1	1186	G	N3-C4-N9	5.42	129.25	126.00
36	1	2187	G	C6-C5-N7	-5.42	127.15	130.40
1	6	541	A	OP1-P-O3'	5.42	117.13	105.20
36	5	1369	A	N1-C6-N6	5.42	121.85	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1620	C	C6-N1-C2	-5.42	118.13	120.30
36	5	3146	G	N1-C2-N2	-5.42	111.32	116.20
1	2	320	U	C5-C6-N1	5.42	125.41	122.70
36	1	1834	U	N3-C4-C5	-5.42	111.35	114.60
1	6	1671	A	C8-N9-C4	5.42	107.97	105.80
36	5	559	A	C4-C5-C6	5.42	119.71	117.00
1	2	542	A	C4-N9-C1'	5.42	136.05	126.30
36	5	1336	U	O5'-P-OP1	5.42	117.20	110.70
36	5	2279	A	O4'-C1'-N9	5.42	112.53	108.20
36	5	2333	C	N1-C2-N3	-5.42	115.41	119.20
36	5	2706	G	C8-N9-C4	-5.42	104.23	106.40
1	6	1019	A	N7-C8-N9	-5.42	111.09	113.80
36	5	1879	A	C4-C5-N7	5.42	113.41	110.70
1	2	830	U	N1-C2-O2	5.41	126.59	122.80
36	5	271	C	N1-C2-O2	5.41	122.15	118.90
1	2	1456	C	N3-C2-O2	-5.41	118.11	121.90
38	4	16	G	C8-N9-C4	5.41	108.56	106.40
36	1	713	U	N1-C2-N3	5.41	118.15	114.90
37	3	83	U	N3-C4-C5	5.41	117.85	114.60
36	5	666	A	C8-N9-C4	5.41	107.96	105.80
36	1	343	U	C4-C5-C6	5.41	122.94	119.70
1	6	1218	G	C8-N9-C1'	5.41	134.03	127.00
36	5	2961	G	C8-N9-C4	-5.41	104.24	106.40
36	5	3049	A	N1-C6-N6	5.41	121.84	118.60
36	5	357	A	N1-C2-N3	5.41	132.00	129.30
37	7	37	G	N9-C4-C5	-5.41	103.24	105.40
36	1	1388	U	O5'-P-OP1	-5.41	100.83	105.70
36	1	3036	G	C8-N9-C4	-5.41	104.24	106.40
1	6	1129	U	C5-C4-O4	5.41	129.14	125.90
36	5	283	G	N9-C4-C5	-5.41	103.24	105.40
1	2	378	A	C4-C5-N7	5.40	113.40	110.70
36	1	2815	G	N9-C4-C5	-5.40	103.24	105.40
36	5	2139	A	N9-C4-C5	5.40	107.96	105.80
36	1	819	U	C6-N1-C2	5.40	124.24	121.00
36	1	1547	G	N1-C6-O6	-5.40	116.66	119.90
38	4	102	U	N1-C2-N3	5.40	118.14	114.90
36	5	2858	U	C6-N1-C2	-5.40	117.76	121.00
36	1	368	G	N1-C2-N2	-5.40	111.34	116.20
36	1	1113	G	C5-N7-C8	-5.40	101.60	104.30
36	1	1149	G	N3-C4-C5	5.40	131.30	128.60
73	O7	21	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	6	1399	C	C5-C6-N1	5.40	123.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2376	G	OP1-P-OP2	5.40	127.70	119.60
37	7	110	G	C8-N9-C4	5.40	108.56	106.40
36	5	2726	C	C4-C5-C6	5.40	120.10	117.40
36	5	659	G	C4-C5-N7	5.40	112.96	110.80
1	2	1486	G	N1-C6-O6	5.39	123.14	119.90
36	1	282	G	P-O3'-C3'	5.39	126.17	119.70
36	1	425	G	N1-C2-N2	-5.39	111.34	116.20
36	5	1620	U	N1-C2-O2	5.39	126.58	122.80
36	5	2129	U	N3-C2-O2	-5.39	118.42	122.20
36	5	2900	A	OP2-P-O3'	5.39	117.07	105.20
1	2	1041	G	C8-N9-C4	-5.39	104.24	106.40
1	6	306	U	C5-C6-N1	-5.39	120.00	122.70
1	6	364	G	N7-C8-N9	-5.39	110.40	113.10
36	5	2746	A	N1-C6-N6	-5.39	115.36	118.60
38	4	31	G	C8-N9-C4	5.39	108.56	106.40
1	6	956	C	C6-N1-C2	5.39	122.46	120.30
36	1	224	C	N3-C4-C5	-5.39	119.74	121.90
1	6	317	C	C5-C6-N1	-5.39	118.31	121.00
36	5	375	A	OP1-P-O3'	5.39	117.06	105.20
36	5	1496	C	N1-C2-O2	5.39	122.13	118.90
36	1	1186	G	N9-C4-C5	-5.39	103.25	105.40
36	1	1367	G	N9-C4-C5	-5.39	103.25	105.40
36	5	425	G	C8-N9-C4	5.39	108.56	106.40
1	2	139	C	P-O3'-C3'	5.39	126.16	119.70
36	5	2257	C	C5-C6-N1	5.39	123.69	121.00
36	1	785	G	C4-C5-N7	-5.38	108.65	110.80
1	6	114	C	C2-N1-C1'	5.38	124.72	118.80
36	5	3287	U	N1-C2-O2	5.38	126.57	122.80
37	7	6	C	N3-C2-O2	-5.38	118.13	121.90
1	2	1244	A	P-O3'-C3'	5.38	126.16	119.70
36	5	3339	A	N1-C6-N6	5.38	121.83	118.60
1	2	864	U	N1-C2-O2	5.38	126.57	122.80
36	1	2132	C	O5'-P-OP2	-5.38	100.86	105.70
36	1	2852	C	N3-C4-C5	5.38	124.05	121.90
36	5	929	A	O5'-P-OP1	5.38	117.16	110.70
36	5	1000	C	N3-C4-C5	5.38	124.05	121.90
36	5	1370	G	C5-C6-N1	5.38	114.19	111.50
38	4	64	U	N3-C2-O2	-5.38	118.43	122.20
36	1	718	G	C4-N9-C1'	5.38	133.49	126.50
1	6	144	U	N1-C2-O2	5.38	126.56	122.80
36	5	1774	C	N3-C4-C5	5.38	124.05	121.90
44	17	229	PHE	CB-CG-CD2	-5.38	117.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	266	A	C8-N9-C4	5.38	107.95	105.80
1	2	1291	G	C8-N9-C4	-5.38	104.25	106.40
36	1	2184	U	O5'-P-OP2	-5.38	100.86	105.70
36	1	2855	U	C2-N3-C4	-5.38	123.78	127.00
36	5	334	A	N7-C8-N9	-5.38	111.11	113.80
36	5	1924	U	C6-N1-C2	5.38	124.23	121.00
36	5	3066	U	C6-N1-C2	5.38	124.23	121.00
1	2	43	A	N1-C2-N3	5.37	131.99	129.30
1	2	554	C	C6-N1-C1'	-5.37	114.35	120.80
36	5	349	A	OP2-P-O3'	5.37	117.02	105.20
36	5	2403	G	N3-C4-C5	-5.37	125.91	128.60
36	5	3214	U	N3-C2-O2	-5.37	118.44	122.20
36	1	102	C	C6-N1-C2	-5.37	118.15	120.30
36	1	392	G	C8-N9-C4	5.37	108.55	106.40
36	1	743	C	C2-N1-C1'	-5.37	112.89	118.80
36	1	1100	U	C6-N1-C2	5.37	124.22	121.00
36	1	1475	A	N7-C8-N9	-5.37	111.11	113.80
36	1	2979	U	C2-N3-C4	-5.37	123.78	127.00
36	5	3057	U	N1-C2-N3	-5.37	111.68	114.90
36	1	641	C	O4'-C1'-N1	5.37	112.50	108.20
36	1	1365	G	C4-N9-C1'	5.37	133.48	126.50
36	5	1897	G	C6-C5-N7	-5.37	127.18	130.40
36	5	3309	G	C8-N9-C4	-5.37	104.25	106.40
36	1	2620	G	C8-N9-C4	5.37	108.55	106.40
36	5	519	A	N1-C6-N6	5.37	121.82	118.60
36	5	2417	U	OP2-P-O3'	5.37	117.01	105.20
36	5	3121	U	C2-N1-C1'	-5.37	111.26	117.70
38	8	84	C	C6-N1-C2	-5.37	118.15	120.30
36	5	2927	C	OP2-P-O3'	5.37	117.01	105.20
36	1	1815	U	P-O3'-C3'	5.37	126.14	119.70
36	5	304	G	N3-C2-N2	-5.37	116.14	119.90
36	5	1704	A	N3-C4-C5	5.37	130.56	126.80
36	5	2910	A	OP2-P-O3'	5.37	117.00	105.20
37	3	103	A	N1-C6-N6	5.36	121.82	118.60
36	5	916	G	OP1-P-O3'	5.36	117.00	105.20
36	5	1592	G	N7-C8-N9	5.36	115.78	113.10
36	1	402	A	C8-N9-C4	5.36	107.94	105.80
36	1	2875	U	O5'-P-OP1	-5.36	100.87	105.70
1	6	387	A	C2-N3-C4	5.36	113.28	110.60
36	5	834	U	C6-N1-C2	5.36	124.22	121.00
36	5	2906	C	N1-C2-O2	-5.36	115.68	118.90
36	5	1180	A	N9-C4-C5	5.36	107.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3181	C	C2-N1-C1'	5.36	124.70	118.80
36	1	1110	U	C5-C4-O4	-5.36	122.69	125.90
36	1	1604	G	C2-N3-C4	5.36	114.58	111.90
36	1	2293	C	N1-C2-O2	5.36	122.12	118.90
36	1	281	G	C5-C6-O6	-5.36	125.39	128.60
38	4	31	G	C5-C6-O6	-5.36	125.39	128.60
36	5	2704	A	N3-C4-C5	5.36	130.55	126.80
62	n6	35	LEU	CA-CB-CG	5.36	127.62	115.30
36	1	297	G	O4'-C1'-N9	5.36	112.48	108.20
9	s7	118	LEU	CA-CB-CG	5.36	127.62	115.30
36	5	1588	A	O5'-P-OP1	-5.36	100.88	105.70
36	5	2855	U	N3-C4-C5	5.36	117.81	114.60
36	1	2632	G	N3-C4-N9	5.35	129.21	126.00
36	5	2248	C	OP1-P-O3'	5.35	116.98	105.20
36	1	25	U	C4-C5-C6	5.35	122.91	119.70
36	1	1396	C	N3-C4-C5	5.35	124.04	121.90
38	4	142	C	C6-N1-C2	-5.35	118.16	120.30
36	5	1108	U	N1-C2-N3	5.35	118.11	114.90
36	5	3138	U	O5'-P-OP1	5.35	117.12	110.70
36	1	1001	G	C6-C5-N7	-5.35	127.19	130.40
1	6	194	U	N3-C2-O2	-5.35	118.45	122.20
36	5	55	G	OP2-P-O3'	5.35	116.97	105.20
36	5	3189	G	N3-C2-N2	-5.35	116.15	119.90
36	1	104	G	C5-C6-O6	-5.35	125.39	128.60
36	1	1445	U	C2-N1-C1'	-5.35	111.28	117.70
36	1	2357	A	C5-C6-N6	-5.35	119.42	123.70
1	6	363	G	N1-C6-O6	5.35	123.11	119.90
36	5	2906	C	N3-C2-O2	5.35	125.64	121.90
36	1	2607	G	N1-C6-O6	5.35	123.11	119.90
1	6	1583	A	C8-N9-C4	5.35	107.94	105.80
36	5	1150	A	C4-C5-N7	5.35	113.37	110.70
36	5	1749	A	N9-C4-C5	-5.35	103.66	105.80
36	5	1830	G	O5'-P-OP2	-5.35	100.89	105.70
36	5	1885	U	C5-C6-N1	-5.35	120.03	122.70
36	5	2778	G	C5-C6-O6	-5.35	125.39	128.60
36	1	1365	G	C4-C5-N7	5.35	112.94	110.80
38	4	113	U	N1-C2-N3	5.35	118.11	114.90
1	6	187	G	P-O3'-C3'	5.35	126.11	119.70
1	2	1761	U	P-O3'-C3'	5.34	126.11	119.70
36	1	2726	C	C5-C4-N4	5.34	123.94	120.20
36	1	2818	U	P-O3'-C3'	5.34	126.11	119.70
36	1	2869	U	N3-C2-O2	-5.34	118.46	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	c1	82	ARG	NE-CZ-NH1	-5.34	117.63	120.30
36	5	640	U	N3-C2-O2	5.34	125.94	122.20
36	5	2215	A	N1-C6-N6	5.34	121.81	118.60
36	5	994	G	N3-C4-N9	5.34	129.21	126.00
36	5	2733	A	N1-C6-N6	5.34	121.81	118.60
38	8	104	A	N3-C4-C5	5.34	130.54	126.80
36	5	994	G	N3-C2-N2	5.34	123.64	119.90
1	2	571	G	C6-C5-N7	5.34	133.60	130.40
36	1	682	U	N3-C4-O4	-5.34	115.66	119.40
36	1	3223	A	N1-C6-N6	-5.34	115.40	118.60
36	5	539	C	C6-N1-C2	-5.34	118.17	120.30
36	5	1476	G	C5-C6-O6	5.34	131.80	128.60
36	5	2305	G	N7-C8-N9	5.34	115.77	113.10
36	1	608	A	C4-C5-N7	5.34	113.37	110.70
36	1	1421	G	O5'-P-OP2	-5.34	100.90	105.70
1	6	1654	G	C5-C6-O6	-5.34	125.40	128.60
36	5	266	A	P-O3'-C3'	5.34	126.10	119.70
36	5	2549	G	C4-N9-C1'	5.34	133.44	126.50
36	5	2683	U	C6-N1-C2	-5.34	117.80	121.00
36	5	3343	G	C6-C5-N7	-5.34	127.20	130.40
36	1	972	A	C8-N9-C4	5.33	107.93	105.80
36	1	905	U	O5'-P-OP2	-5.33	100.90	105.70
36	1	960	U	N1-C2-N3	-5.33	111.70	114.90
36	1	1137	C	N1-C2-O2	-5.33	115.70	118.90
36	1	1192	C	C5-C6-N1	5.33	123.67	121.00
36	1	1837	U	C5-C4-O4	-5.33	122.70	125.90
1	6	1173	C	C6-N1-C2	-5.33	118.17	120.30
36	5	1152	G	N7-C8-N9	5.33	115.77	113.10
36	5	1747	G	C8-N9-C4	5.33	108.53	106.40
36	5	2433	U	C5-C6-N1	-5.33	120.03	122.70
36	1	1081	U	C5-C6-N1	5.33	125.37	122.70
36	1	2606	G	N3-C2-N2	5.33	123.63	119.90
36	1	3278	C	C6-N1-C2	-5.33	118.17	120.30
1	6	322	G	N1-C6-O6	5.33	123.10	119.90
1	6	978	A	N1-C6-N6	-5.33	115.40	118.60
1	6	1776	A	OP2-P-O3'	5.33	116.93	105.20
36	5	650	C	C6-N1-C2	5.33	122.43	120.30
1	6	542	A	C8-N9-C4	-5.33	103.67	105.80
36	5	721	G	C4-C5-N7	5.33	112.93	110.80
1	2	1611	A	O4'-C1'-N9	5.33	112.46	108.20
36	1	2315	G	C5-C6-N1	-5.33	108.83	111.50
36	5	1848	G	OP2-P-O3'	5.33	116.92	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2305	G	C6-C5-N7	-5.33	127.20	130.40
36	5	2728	G	N1-C6-O6	-5.33	116.70	119.90
36	5	2734	A	C8-N9-C4	5.33	107.93	105.80
36	1	384	A	C8-N9-C4	5.33	107.93	105.80
36	1	969	C	C5-C6-N1	-5.33	118.34	121.00
36	1	2388	U	C6-N1-C2	5.33	124.20	121.00
36	1	2427	U	N3-C4-O4	-5.33	115.67	119.40
36	1	3373	U	C6-N1-C2	5.33	124.19	121.00
36	5	1138	U	C2-N3-C4	-5.33	123.81	127.00
36	5	2761	G	C4-C5-N7	-5.33	108.67	110.80
36	5	2887	A	N3-C4-C5	-5.33	123.07	126.80
36	1	2870	C	C2-N1-C1'	-5.32	112.94	118.80
36	1	3149	G	C5-C6-N1	-5.32	108.84	111.50
1	6	90	C	N1-C2-O2	5.32	122.09	118.90
1	6	321	C	N3-C2-O2	-5.32	118.17	121.90
36	5	43	A	O5'-P-OP2	-5.32	100.91	105.70
36	5	1917	C	C4-C5-C6	5.32	120.06	117.40
1	2	329	G	N1-C2-N3	5.32	127.09	123.90
36	1	961	C	N1-C2-O2	-5.32	115.71	118.90
36	1	2946	A	C6-C5-N7	-5.32	128.57	132.30
51	M5	93	LYS	N-CA-C	5.32	125.37	111.00
36	5	951	A	C2-N3-C4	-5.32	107.94	110.60
36	5	1348	U	C6-N1-C2	-5.32	117.81	121.00
36	5	2291	A	OP1-P-O3'	5.32	116.91	105.20
38	8	100	U	C6-N1-C1'	-5.32	113.75	121.20
1	2	383	G	C8-N9-C4	-5.32	104.27	106.40
36	5	2615	G	C4-C5-N7	5.32	112.93	110.80
38	8	36	G	C5-C6-N1	5.32	114.16	111.50
1	2	1503	A	N1-C6-N6	5.32	121.79	118.60
36	1	2636	A	C8-N9-C4	-5.32	103.67	105.80
36	5	1420	C	C4-C5-C6	5.32	120.06	117.40
1	2	1108	G	O4'-C1'-N9	5.32	112.45	108.20
36	1	39	A	N9-C4-C5	-5.32	103.67	105.80
36	1	1124	U	C4-C5-C6	-5.32	116.51	119.70
36	1	2953	U	N3-C2-O2	5.32	125.92	122.20
36	1	3060	C	C6-N1-C2	5.32	122.43	120.30
14	c2	58	LEU	CA-CB-CG	5.32	127.53	115.30
36	5	354	U	C2-N1-C1'	5.32	124.08	117.70
36	5	3120	C	C5-C6-N1	5.32	123.66	121.00
36	1	659	G	N3-C4-N9	5.32	129.19	126.00
36	1	884	A	C5-C6-N6	-5.32	119.45	123.70
36	5	3040	A	N7-C8-N9	-5.32	111.14	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	M3	47	ALA	C-N-CD	5.31	139.56	128.40
1	2	428	A	C8-N9-C4	-5.31	103.67	105.80
12	C0	49	LEU	CA-CB-CG	5.31	127.52	115.30
36	1	609	G	C2-N3-C4	5.31	114.56	111.90
36	1	1480	G	C4-C5-N7	5.31	112.92	110.80
36	1	3269	U	P-O3'-C3'	5.31	126.08	119.70
36	5	658	G	C5-C6-O6	-5.31	125.41	128.60
36	5	2369	G	C5-C6-N1	5.31	114.16	111.50
36	1	1305	U	C2-N3-C4	5.31	130.19	127.00
1	6	1537	C	C5-C6-N1	5.31	123.66	121.00
1	2	934	C	C6-N1-C1'	-5.31	114.43	120.80
1	6	944	A	C2-N3-C4	-5.31	107.94	110.60
36	1	388	G	C8-N9-C4	-5.31	104.28	106.40
36	1	1655	G	O5'-P-OP1	-5.31	100.92	105.70
1	2	343	C	N3-C2-O2	-5.30	118.19	121.90
36	1	2323	G	C4-C5-N7	5.30	112.92	110.80
36	1	2852	C	C5-C4-N4	-5.30	116.49	120.20
1	6	542	A	N7-C8-N9	5.30	116.45	113.80
36	5	534	U	O5'-P-OP2	-5.30	100.93	105.70
36	5	1049	C	C5-C6-N1	5.30	123.65	121.00
36	5	3145	C	C6-N1-C2	5.30	122.42	120.30
37	7	105	C	C6-N1-C2	-5.30	118.18	120.30
1	2	599	A	N1-C6-N6	-5.30	115.42	118.60
37	7	110	G	O5'-P-OP2	-5.30	100.93	105.70
36	1	182	U	C2-N1-C1'	-5.30	111.34	117.70
36	5	1898	G	O4'-C1'-N9	5.30	112.44	108.20
1	2	1572	G	C4-C5-N7	5.30	112.92	110.80
36	1	2387	A	C8-N9-C4	5.30	107.92	105.80
36	1	2645	G	C8-N9-C4	5.30	108.52	106.40
36	1	2683	U	N3-C2-O2	5.30	125.91	122.20
36	1	3375	A	N9-C4-C5	5.30	107.92	105.80
36	5	2385	G	N9-C4-C5	-5.30	103.28	105.40
36	1	2715	A	O5'-P-OP1	-5.30	100.93	105.70
36	5	384	A	N7-C8-N9	-5.30	111.15	113.80
36	5	2730	G	N3-C2-N2	-5.30	116.19	119.90
36	1	2295	A	C8-N9-C4	-5.29	103.68	105.80
1	6	610	G	C4-N9-C1'	5.29	133.38	126.50
36	5	669	U	N1-C2-O2	-5.29	119.09	122.80
1	2	499	U	C2-N1-C1'	5.29	124.05	117.70
36	1	2811	A	C6-N1-C2	-5.29	115.42	118.60
36	5	283	G	C4-N9-C1'	5.29	133.38	126.50
36	5	2943	G	N3-C4-N9	5.29	129.18	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1193	A	C4-C5-N7	5.29	113.35	110.70
78	Q2	17	CYS	CA-CB-SG	5.29	123.52	114.00
1	6	136	C	N1-C2-O2	5.29	122.07	118.90
1	6	1085	G	N1-C6-O6	-5.29	116.72	119.90
1	6	1423	U	C5-C6-N1	-5.29	120.05	122.70
36	5	73	C	N3-C4-N4	5.29	121.70	118.00
36	5	901	G	N3-C4-N9	5.29	129.17	126.00
36	5	2193	U	N1-C2-O2	-5.29	119.10	122.80
36	1	780	A	N1-C2-N3	5.29	131.94	129.30
1	6	1128	C	N3-C4-C5	-5.29	119.78	121.90
36	1	584	G	C4-C5-N7	-5.29	108.68	110.80
36	1	1906	G	C6-C5-N7	-5.29	127.23	130.40
38	4	125	U	C5-C6-N1	5.29	125.34	122.70
36	5	1284	C	C5-C6-N1	5.29	123.64	121.00
1	2	1339	C	C3'-C2'-C1'	5.29	105.73	101.50
36	1	3057	U	N1-C2-N3	5.29	118.07	114.90
1	6	1060	U	N3-C2-O2	-5.29	118.50	122.20
1	6	1102	G	N1-C6-O6	5.29	123.07	119.90
36	5	1534	A	C2-N3-C4	5.29	113.24	110.60
1	2	428	A	N9-C4-C5	5.29	107.91	105.80
36	1	2662	G	N9-C4-C5	-5.29	103.29	105.40
1	6	160	C	N1-C2-O2	5.29	122.07	118.90
36	1	1307	G	C5'-C4'-C3'	-5.28	107.55	116.00
36	1	2165	G	C4-C5-N7	5.28	112.91	110.80
36	1	2395	G	C6-N1-C2	-5.28	121.93	125.10
36	1	3058	U	C2-N1-C1'	5.28	124.04	117.70
1	6	1768	G	N3-C4-N9	-5.28	122.83	126.00
36	5	1103	A	N7-C8-N9	5.28	116.44	113.80
37	7	34	C	C6-N1-C2	-5.28	118.19	120.30
1	2	1458	G	C8-N9-C1'	-5.28	120.13	127.00
36	5	2278	C	C4-C5-C6	-5.28	114.76	117.40
1	2	576	G	C5-C6-O6	-5.28	125.43	128.60
36	1	2855	U	N3-C4-O4	-5.28	115.70	119.40
36	1	3034	C	N1-C2-O2	5.28	122.07	118.90
36	1	1507	G	C6-C5-N7	-5.28	127.23	130.40
36	1	1881	A	N7-C8-N9	-5.28	111.16	113.80
1	6	1058	U	OP1-P-O3'	5.28	116.81	105.20
36	1	628	A	N1-C6-N6	5.28	121.77	118.60
36	1	637	C	C4-C5-C6	5.28	120.04	117.40
36	1	642	U	N3-C2-O2	-5.28	118.50	122.20
36	1	857	G	C5-C6-N1	-5.28	108.86	111.50
36	5	1149	G	C5-C6-O6	-5.28	125.43	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2273	G	C8-N9-C1'	5.28	133.86	127.00
36	5	346	C	C2-N1-C1'	5.28	124.60	118.80
36	5	2410	U	N1-C2-O2	-5.28	119.11	122.80
36	1	651	G	O5'-P-OP2	-5.27	100.95	105.70
36	1	3029	A	C8-N9-C4	-5.27	103.69	105.80
36	5	3173	G	N9-C4-C5	-5.27	103.29	105.40
36	1	1366	A	N1-C6-N6	-5.27	115.44	118.60
36	1	3004	C	N3-C2-O2	-5.27	118.21	121.90
36	5	2260	U	N3-C2-O2	-5.27	118.51	122.20
36	5	3228	C	P-O3'-C3'	5.27	126.03	119.70
36	1	2121	G	N3-C2-N2	5.27	123.59	119.90
1	6	353	A	N1-C6-N6	-5.27	115.44	118.60
1	6	858	G	N7-C8-N9	5.27	115.73	113.10
36	5	1520	G	C2-N3-C4	5.27	114.53	111.90
36	5	2159	U	C5-C4-O4	5.27	129.06	125.90
38	8	4	C	C6-N1-C2	-5.27	118.19	120.30
37	3	95	A	C6-C5-N7	-5.27	128.61	132.30
36	5	2133	U	C5-C6-N1	-5.27	120.07	122.70
36	5	2693	C	C2-N3-C4	-5.27	117.27	119.90
36	5	2890	A	N1-C6-N6	5.27	121.76	118.60
1	2	570	A	C5-C6-N6	-5.27	119.49	123.70
36	1	2335	G	C5-N7-C8	5.27	106.93	104.30
1	6	973	A	O5'-P-OP2	-5.27	100.96	105.70
36	5	1929	G	C8-N9-C4	5.27	108.51	106.40
36	5	2819	A	C5-C6-N6	5.27	127.91	123.70
36	1	784	A	O4'-C1'-N9	5.26	112.41	108.20
1	6	542	A	C4-N9-C1'	5.26	135.78	126.30
36	5	1391	C	N3-C2-O2	5.26	125.58	121.90
36	5	1407	A	C2-N3-C4	-5.26	107.97	110.60
36	5	2952	G	N3-C4-N9	5.26	129.16	126.00
36	5	2993	G	N9-C4-C5	-5.26	103.29	105.40
36	1	699	A	C2-N3-C4	-5.26	107.97	110.60
36	5	941	G	N1-C6-O6	-5.26	116.74	119.90
36	1	498	A	C5-C6-N6	5.26	127.91	123.70
36	1	1796	G	N3-C4-C5	-5.26	125.97	128.60
36	1	2916	U	N3-C4-O4	5.26	123.08	119.40
41	L4	182	LEU	CA-CB-CG	5.26	127.40	115.30
36	5	327	A	N7-C8-N9	-5.26	111.17	113.80
36	5	674	G	C8-N9-C4	-5.26	104.30	106.40
36	5	682	U	C6-N1-C1'	5.26	128.56	121.20
36	5	2639	G	N3-C4-N9	5.26	129.16	126.00
36	1	644	G	N1-C2-N3	5.26	127.06	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1532	C	C6-N1-C2	5.26	122.40	120.30
36	1	1794	G	N3-C2-N2	-5.26	116.22	119.90
36	1	2429	G	C4-C5-N7	-5.26	108.70	110.80
36	1	2823	G	N7-C8-N9	-5.26	110.47	113.10
36	1	908	G	N3-C2-N2	-5.26	116.22	119.90
36	1	2620	G	C5-C6-N1	5.26	114.13	111.50
36	1	1452	A	OP1-P-O3'	5.26	116.77	105.20
36	1	2390	A	N1-C6-N6	5.26	121.75	118.60
36	5	1858	A	N7-C8-N9	5.26	116.43	113.80
36	5	2345	A	N1-C2-N3	5.26	131.93	129.30
36	1	2887	A	C4-C5-N7	5.25	113.33	110.70
36	5	75	G	N3-C4-N9	5.25	129.15	126.00
36	5	2719	U	O5'-P-OP2	-5.25	100.97	105.70
42	15	51	LEU	CA-CB-CG	5.25	127.38	115.30
36	1	1103	A	N9-C4-C5	-5.25	103.70	105.80
36	1	1136	A	C6-C5-N7	-5.25	128.62	132.30
36	1	2175	U	N1-C2-O2	-5.25	119.12	122.80
36	1	2945	G	N9-C4-C5	-5.25	103.30	105.40
36	1	3091	A	N1-C6-N6	5.25	121.75	118.60
1	6	17	C	N3-C2-O2	-5.25	118.22	121.90
36	1	1440	G	C5-C6-O6	5.25	131.75	128.60
36	5	1725	C	C5-C6-N1	-5.25	118.38	121.00
36	1	341	G	C4-C5-N7	5.25	112.90	110.80
36	1	785	G	C2-N3-C4	5.25	114.53	111.90
36	1	1379	G	C5-C6-O6	5.25	131.75	128.60
36	5	315	C	N3-C4-C5	5.25	124.00	121.90
36	5	421	G	N1-C2-N3	5.25	127.05	123.90
36	5	421	G	C8-N9-C1'	-5.25	120.18	127.00
36	5	1440	G	N9-C4-C5	5.25	107.50	105.40
36	5	2176	U	O5'-P-OP2	5.25	117.00	110.70
36	1	42	C	C5-C6-N1	5.25	123.62	121.00
36	1	894	G	N3-C2-N2	-5.25	116.23	119.90
1	6	1537	C	C4-C5-C6	5.25	120.02	117.40
36	5	642	U	O5'-P-OP2	-5.25	100.98	105.70
36	1	2137	U	N3-C2-O2	-5.25	118.53	122.20
1	6	1200	G	C8-N9-C1'	5.25	133.82	127.00
1	2	1600	A	OP1-P-O3'	5.24	116.74	105.20
35	SM	134	ASP	CB-CG-OD2	5.24	123.02	118.30
36	1	2198	A	C6-N1-C2	-5.24	115.45	118.60
36	1	2945	G	C8-N9-C4	5.24	108.50	106.40
4	s2	229	LEU	CA-CB-CG	5.24	127.36	115.30
36	5	819	U	OP2-P-O3'	5.24	116.73	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	879	U	O5'-P-OP1	-5.24	100.98	105.70
36	5	919	U	O5'-P-OP2	-5.24	100.98	105.70
36	5	2663	G	C8-N9-C4	5.24	108.50	106.40
36	5	2808	A	N9-C4-C5	-5.24	103.70	105.80
36	5	2812	C	C2-N3-C4	-5.24	117.28	119.90
36	1	1399	A	C2-N3-C4	-5.24	107.98	110.60
1	6	1073	G	C8-N9-C4	5.24	108.50	106.40
36	5	1478	C	N1-C2-O2	-5.24	115.75	118.90
1	2	1414	U	N3-C2-O2	-5.24	118.53	122.20
36	1	936	A	OP2-P-O3'	5.24	116.73	105.20
36	1	1547	G	C5-C6-O6	5.24	131.74	128.60
36	1	2413	A	C8-N9-C4	5.24	107.90	105.80
36	1	2606	G	N3-C4-N9	5.24	129.14	126.00
36	5	954	U	C5-C6-N1	5.24	125.32	122.70
36	1	2815	G	C5-C6-N1	-5.24	108.88	111.50
76	Q0	103	LEU	CA-CB-CG	-5.24	103.25	115.30
36	1	2627	C	OP2-P-O3'	5.24	116.72	105.20
1	2	985	G	C2-N3-C4	5.24	114.52	111.90
36	5	355	A	N9-C4-C5	5.24	107.89	105.80
36	5	1847	A	N3-C4-N9	-5.24	123.21	127.40
36	5	2130	G	N3-C2-N2	5.24	123.56	119.90
36	5	2902	A	C5-C6-N6	-5.24	119.51	123.70
1	6	1593	A	N1-C6-N6	5.23	121.74	118.60
36	1	3207	U	O4'-C1'-N1	5.23	112.39	108.20
36	5	1452	A	C2-N3-C4	-5.23	107.98	110.60
1	2	1092	A	N9-C4-C5	-5.23	103.71	105.80
1	2	1559	A	O4'-C1'-N9	5.23	112.39	108.20
36	1	1150	A	C5-C6-N6	5.23	127.89	123.70
36	1	2198	A	C8-N9-C4	5.23	107.89	105.80
36	1	2323	G	N9-C4-C5	-5.23	103.31	105.40
36	5	1150	A	C5-C6-N6	-5.23	119.52	123.70
1	2	1462	G	N9-C4-C5	-5.23	103.31	105.40
36	1	1838	G	C5-C6-O6	-5.23	125.46	128.60
36	1	2424	A	C2-N3-C4	5.23	113.22	110.60
1	2	576	G	N1-C6-O6	5.23	123.04	119.90
1	2	1773	C	C5-C6-N1	5.23	123.61	121.00
36	1	869	G	C6-C5-N7	-5.23	127.26	130.40
36	1	2376	G	OP1-P-OP2	5.23	127.44	119.60
36	5	914	A	O5'-P-OP1	-5.23	100.99	105.70
36	5	938	C	C5-C4-N4	-5.23	116.54	120.20
36	1	2279	A	N9-C4-C5	-5.23	103.71	105.80
36	1	3024	A	N9-C4-C5	-5.23	103.71	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	335	G	C5-C6-O6	-5.22	125.47	128.60
36	1	2425	G	N3-C4-N9	5.22	129.13	126.00
36	1	2631	U	N3-C4-O4	-5.22	115.74	119.40
36	5	221	A	C2-N3-C4	-5.22	107.99	110.60
36	5	1355	A	P-O3'-C3'	5.22	125.97	119.70
36	5	2186	U	N1-C2-O2	5.22	126.46	122.80
36	1	2396	G	C6-C5-N7	-5.22	127.27	130.40
36	5	394	G	C5-C6-O6	5.22	131.73	128.60
36	5	2816	G	C2-N3-C4	-5.22	109.29	111.90
1	6	1697	G	N3-C4-C5	-5.22	125.99	128.60
36	1	156	G	N3-C4-N9	5.22	129.13	126.00
36	1	609	G	N3-C2-N2	-5.22	116.25	119.90
36	1	2360	C	C2-N3-C4	-5.22	117.29	119.90
36	5	894	G	C6-C5-N7	-5.22	127.27	130.40
36	5	2550	U	C6-N1-C2	-5.22	117.87	121.00
36	1	3369	G	N1-C6-O6	5.22	123.03	119.90
37	3	98	C	N1-C2-O2	-5.22	115.77	118.90
1	2	9	U	O5'-P-OP1	-5.22	101.00	105.70
36	1	304	G	C6-C5-N7	5.22	133.53	130.40
36	1	1168	U	O5'-P-OP1	5.22	116.96	110.70
36	1	1435	A	C5-N7-C8	-5.22	101.29	103.90
36	1	3001	C	N3-C4-C5	5.22	123.99	121.90
1	6	38	C	C6-N1-C2	5.22	122.39	120.30
36	5	708	G	C4-C5-N7	5.22	112.89	110.80
36	5	1151	U	O5'-P-OP1	-5.22	101.00	105.70
36	5	1841	A	C5-C6-N6	-5.22	119.53	123.70
36	5	2150	G	N3-C4-C5	-5.22	125.99	128.60
36	5	3180	A	C8-N9-C4	5.22	107.89	105.80
36	5	3310	A	N1-C2-N3	5.22	131.91	129.30
1	2	779	U	O4'-C1'-N1	5.21	112.37	108.20
36	1	684	G	C6-C5-N7	-5.21	127.27	130.40
41	L4	230	VAL	CB-CA-C	-5.21	101.49	111.40
1	6	401	A	O5'-P-OP1	-5.21	101.01	105.70
1	6	1041	G	C4-C5-N7	-5.21	108.71	110.80
1	6	1399	C	C6-N1-C2	-5.21	118.21	120.30
12	c0	88	PRO	N-CA-CB	5.21	109.56	103.30
36	5	1770	G	C4-N9-C1'	5.21	133.28	126.50
36	1	780	A	C4-C5-C6	5.21	119.61	117.00
36	1	2261	G	N3-C4-N9	5.21	129.13	126.00
36	1	2855	U	C6-N1-C2	5.21	124.13	121.00
36	5	2308	C	N1-C2-O2	-5.21	115.77	118.90
36	1	777	U	O5'-P-OP2	-5.21	101.01	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1191	U	O5'-P-OP1	-5.21	101.01	105.70
36	1	1431	G	N3-C2-N2	5.21	123.55	119.90
36	1	1885	U	N3-C2-O2	5.21	125.85	122.20
36	1	2356	A	N1-C6-N6	5.21	121.73	118.60
36	1	2723	U	N1-C2-O2	-5.21	119.15	122.80
36	1	2805	G	N9-C4-C5	-5.21	103.32	105.40
36	1	2893	C	C2-N3-C4	-5.21	117.29	119.90
36	5	1292	C	C2-N3-C4	-5.21	117.29	119.90
36	1	938	C	C2-N3-C4	-5.21	117.30	119.90
36	5	3351	U	C2-N1-C1'	5.21	123.95	117.70
36	1	1294	A	O4'-C1'-N9	5.21	112.37	108.20
36	1	2434	U	C5-C6-N1	-5.21	120.10	122.70
38	4	85	G	C8-N9-C4	-5.21	104.32	106.40
1	2	831	U	C2-N1-C1'	5.21	123.95	117.70
1	2	1241	G	C8-N9-C4	-5.21	104.32	106.40
36	1	2370	G	C2-N3-C4	-5.21	109.30	111.90
36	1	2958	A	C6-C5-N7	5.21	135.94	132.30
49	M3	85	LEU	CA-CB-CG	5.21	127.28	115.30
36	5	1440	G	C5-C6-O6	5.21	131.72	128.60
36	5	2136	C	OP2-P-O3'	5.21	116.66	105.20
36	5	2607	G	C5-N7-C8	-5.21	101.70	104.30
36	5	2818	U	O5'-P-OP1	-5.21	101.01	105.70
36	1	1149	G	C6-C5-N7	-5.21	127.28	130.40
36	1	3268	A	O4'-C1'-N9	-5.21	104.04	108.20
1	6	103	A	P-O3'-C3'	5.21	125.95	119.70
36	5	48	A	C8-N9-C4	-5.21	103.72	105.80
36	5	1339	C	O5'-P-OP1	-5.21	101.02	105.70
36	5	1370	G	N3-C4-N9	5.21	129.12	126.00
36	5	3308	C	OP2-P-O3'	5.21	116.65	105.20
36	1	395	A	O5'-P-OP2	-5.20	101.02	105.70
36	1	854	G	C8-N9-C4	5.20	108.48	106.40
36	1	2223	A	N1-C6-N6	5.20	121.72	118.60
36	5	760	G	N9-C4-C5	-5.20	103.32	105.40
36	5	881	C	C2-N3-C4	5.20	122.50	119.90
36	5	1152	G	N1-C2-N3	5.20	127.02	123.90
36	5	1197	A	C8-N9-C4	5.20	107.88	105.80
36	5	1500	G	N7-C8-N9	-5.20	110.50	113.10
37	7	37	G	N3-C4-N9	5.20	129.12	126.00
36	1	2307	G	N1-C6-O6	-5.20	116.78	119.90
36	5	35	A	N1-C6-N6	5.20	121.72	118.60
36	5	1889	G	N9-C4-C5	-5.20	103.32	105.40
73	o7	67	LEU	CA-CB-CG	5.20	127.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	42	G	N7-C8-N9	-5.20	110.50	113.10
1	2	605	A	N1-C6-N6	5.20	121.72	118.60
36	1	614	C	C6-N1-C2	5.20	122.38	120.30
1	2	321	C	N1-C2-O2	5.20	122.02	118.90
1	2	1560	U	N1-C2-N3	5.20	118.02	114.90
1	2	1745	G	N3-C4-N9	5.20	129.12	126.00
36	1	1431	G	N1-C6-O6	-5.20	116.78	119.90
36	1	2877	G	N1-C6-O6	-5.20	116.78	119.90
37	3	95	A	C4-C5-N7	5.20	113.30	110.70
36	5	1841	A	N9-C4-C5	-5.20	103.72	105.80
36	5	2967	A	C2-N3-C4	-5.20	108.00	110.60
1	6	371	G	N3-C4-N9	5.20	129.12	126.00
36	1	867	G	N1-C2-N3	5.20	127.02	123.90
36	1	1206	G	C5-C6-O6	5.20	131.72	128.60
36	1	1317	A	N1-C2-N3	-5.20	126.70	129.30
36	1	1388	U	OP1-P-OP2	5.20	127.39	119.60
1	6	1310	U	N3-C2-O2	-5.20	118.56	122.20
1	6	1573	A	P-O3'-C3'	5.20	125.94	119.70
36	1	1365	G	C5-N7-C8	-5.19	101.70	104.30
36	1	1434	G	C5-N7-C8	-5.19	101.70	104.30
36	1	3270	U	C2-N1-C1'	-5.19	111.47	117.70
36	1	78	U	N1-C2-N3	5.19	118.02	114.90
36	5	2187	G	N3-C2-N2	5.19	123.53	119.90
36	5	2887	A	N1-C6-N6	5.19	121.72	118.60
36	5	3206	C	OP1-P-OP2	5.19	127.39	119.60
37	7	84	A	OP1-P-O3'	5.19	116.63	105.20
38	8	92	A	N1-C6-N6	5.19	121.72	118.60
40	13	328	ILE	CG1-CB-CG2	-5.19	99.97	111.40
1	2	97	C	N3-C4-C5	5.19	123.98	121.90
1	2	696	C	C6-N1-C2	-5.19	118.22	120.30
36	1	10	C	C6-N1-C2	5.19	122.38	120.30
36	5	583	G	C5-C6-O6	5.19	131.71	128.60
36	5	1130	A	C2-N3-C4	5.19	113.19	110.60
1	2	1027	A	N1-C6-N6	5.19	121.71	118.60
1	2	1560	U	C6-N1-C2	-5.19	117.89	121.00
36	1	853	G	C8-N9-C4	5.19	108.47	106.40
36	1	3382	U	C5-C6-N1	5.19	125.29	122.70
36	5	514	G	C6-C5-N7	-5.19	127.29	130.40
36	5	1116	G	C4-N9-C1'	5.19	133.25	126.50
36	5	2632	G	C8-N9-C4	5.19	108.47	106.40
36	5	3207	U	C2-N1-C1'	-5.19	111.47	117.70
36	1	2301	U	N3-C2-O2	-5.19	118.57	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2144	A	C6-N1-C2	-5.18	115.49	118.60
36	5	2629	U	O5'-P-OP2	-5.18	101.03	105.70
36	5	3005	A	OP1-P-OP2	5.18	127.38	119.60
1	2	1556	A	O5'-P-OP1	-5.18	101.04	105.70
1	2	1792	G	C8-N9-C1'	-5.18	120.26	127.00
36	1	649	A	OP1-P-OP2	-5.18	111.83	119.60
1	6	382	C	N3-C4-C5	5.18	123.97	121.90
1	6	864	U	C5-C4-O4	5.18	129.01	125.90
36	5	2588	U	C6-N1-C2	-5.18	117.89	121.00
36	5	2767	U	C5-C4-O4	5.18	129.01	125.90
36	5	3120	C	N1-C2-O2	5.18	122.01	118.90
37	7	41	G	C8-N9-C4	5.18	108.47	106.40
38	8	114	G	O5'-P-OP1	-5.18	101.04	105.70
1	2	1199	G	C8-N9-C1'	-5.18	120.27	127.00
36	1	2809	C	N3-C2-O2	-5.18	118.27	121.90
1	6	565	C	C2-N3-C4	-5.18	117.31	119.90
36	1	1316	C	C6-N1-C2	-5.18	118.23	120.30
36	5	369	A	N7-C8-N9	5.18	116.39	113.80
36	5	2754	G	C8-N9-C4	5.18	108.47	106.40
1	2	734	A	OP1-P-O3'	5.18	116.59	105.20
36	1	363	G	C5-C6-O6	-5.18	125.49	128.60
36	1	2130	G	N1-C6-O6	-5.18	116.79	119.90
36	5	1359	C	C6-N1-C2	5.18	122.37	120.30
1	2	579	A	N1-C2-N3	5.17	131.89	129.30
36	1	785	G	N1-C6-O6	-5.17	116.80	119.90
36	1	1362	G	OP2-P-O3'	5.17	116.58	105.20
36	5	2584	G	OP2-P-O3'	5.17	116.59	105.20
36	1	496	C	O5'-P-OP1	-5.17	101.04	105.70
36	5	2158	A	C6-N1-C2	-5.17	115.50	118.60
36	5	3146	G	N3-C2-N2	5.17	123.52	119.90
36	1	1901	A	C5-C6-N1	5.17	120.29	117.70
36	1	1931	U	C6-N1-C2	5.17	124.10	121.00
36	1	2374	C	C4-C5-C6	5.17	119.99	117.40
1	6	339	C	N1-C2-O2	-5.17	115.80	118.90
36	5	2798	C	C6-N1-C2	5.17	122.37	120.30
36	5	276	U	OP1-P-O3'	5.17	116.57	105.20
1	6	364	G	C8-N9-C1'	-5.17	120.28	127.00
36	5	2362	C	C5-C4-N4	-5.17	116.58	120.20
36	5	2372	A	C4-C5-C6	5.17	119.58	117.00
36	1	3057	U	N3-C2-O2	-5.17	118.58	122.20
36	1	3266	G	C8-N9-C4	-5.17	104.33	106.40
36	5	838	G	N9-C4-C5	5.17	107.47	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1660	C	C6-N1-C2	-5.17	118.23	120.30
36	5	1834	U	N3-C4-C5	-5.17	111.50	114.60
36	5	2933	A	OP1-P-OP2	5.17	127.35	119.60
36	5	3008	A	N1-C2-N3	5.17	131.88	129.30
37	7	118	A	OP2-P-O3'	5.17	116.56	105.20
36	1	1481	A	N9-C4-C5	-5.17	103.73	105.80
36	1	3164	C	O4'-C1'-N1	5.17	112.33	108.20
36	5	820	A	C6-C5-N7	-5.17	128.69	132.30
36	5	895	A	C2-N3-C4	-5.17	108.02	110.60
36	5	938	C	OP1-P-O3'	5.17	116.56	105.20
1	2	749	U	C6-N1-C2	-5.16	117.90	121.00
36	1	364	G	N3-C4-C5	5.16	131.18	128.60
36	1	394	G	C5-C6-O6	5.16	131.70	128.60
36	1	1442	U	N3-C4-O4	5.16	123.02	119.40
36	1	3382	U	N3-C2-O2	-5.16	118.59	122.20
1	6	957	G	N3-C2-N2	-5.16	116.28	119.90
36	5	1524	A	C2-N3-C4	-5.16	108.02	110.60
36	5	2282	U	OP2-P-O3'	5.16	116.56	105.20
1	6	1663	G	O5'-P-OP1	5.16	116.89	110.70
1	2	75	U	C6-N1-C1'	-5.16	113.98	121.20
6	S4	193	GLY	N-CA-C	5.16	126.00	113.10
36	1	963	G	N1-C6-O6	5.16	123.00	119.90
36	1	1415	U	N1-C2-N3	5.16	118.00	114.90
36	1	2130	G	N3-C4-C5	-5.16	126.02	128.60
36	1	3024	A	N1-C6-N6	5.16	121.70	118.60
36	5	1115	G	C4-N9-C1'	5.16	133.21	126.50
36	5	1444	G	N3-C2-N2	-5.16	116.29	119.90
36	5	1847	A	C4-C5-C6	-5.16	114.42	117.00
38	8	96	A	C8-N9-C4	5.16	107.86	105.80
1	2	795	U	C4-C5-C6	5.16	122.80	119.70
36	1	394	G	N1-C6-O6	-5.16	116.81	119.90
36	1	1377	G	N3-C4-N9	5.16	129.09	126.00
36	5	968	G	O5'-P-OP1	-5.16	101.06	105.70
36	5	1452	A	C8-N9-C4	5.16	107.86	105.80
36	5	97	U	N3-C2-O2	5.16	125.81	122.20
36	5	2765	C	N3-C4-N4	5.16	121.61	118.00
36	5	3055	U	O5'-P-OP2	-5.16	101.06	105.70
36	1	948	C	N3-C4-C5	-5.16	119.84	121.90
36	1	1000	C	C2-N1-C1'	5.16	124.47	118.80
36	5	1794	G	C2-N3-C4	-5.16	109.32	111.90
36	5	83	U	N1-C2-O2	5.15	126.41	122.80
36	5	1284	C	C6-N1-C2	-5.15	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2134	G	C5-C6-N1	5.15	114.08	111.50
36	5	1749	A	N1-C6-N6	5.15	121.69	118.60
36	5	3058	U	C2-N1-C1'	5.15	123.88	117.70
36	1	376	G	C5-C6-N1	-5.15	108.92	111.50
36	1	1002	A	C8-N9-C4	5.15	107.86	105.80
36	1	2401	A	N9-C4-C5	-5.15	103.74	105.80
36	1	2812	C	C6-N1-C2	5.15	122.36	120.30
38	4	20	U	C2-N3-C4	-5.15	123.91	127.00
38	8	26	U	O5'-P-OP2	-5.15	101.06	105.70
1	2	1768	G	C4-C5-N7	-5.15	108.74	110.80
36	1	1521	G	C2-N3-C4	-5.15	109.33	111.90
1	6	794	U	N1-C2-O2	5.15	126.40	122.80
36	5	1083	G	OP1-P-OP2	5.15	127.32	119.60
36	5	403	C	OP1-P-OP2	5.15	127.32	119.60
36	5	996	A	C8-N9-C4	-5.15	103.74	105.80
36	5	2298	U	O5'-P-OP1	-5.15	101.07	105.70
36	5	3066	U	C5-C6-N1	-5.15	120.13	122.70
76	Q0	106	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	6	163	G	C5-N7-C8	-5.15	101.73	104.30
36	5	658	G	N1-C6-O6	5.15	122.99	119.90
36	5	1847	A	N1-C6-N6	-5.15	115.51	118.60
36	5	918	C	C5-C4-N4	-5.14	116.60	120.20
36	5	1186	G	C5-N7-C8	-5.14	101.73	104.30
1	2	1167	G	C5-C6-O6	-5.14	125.52	128.60
36	1	913	A	C8-N9-C4	-5.14	103.74	105.80
36	1	1352	A	P-O3'-C3'	5.14	125.87	119.70
36	1	1365	G	N1-C2-N3	5.14	126.99	123.90
36	1	2609	A	C8-N9-C4	5.14	107.86	105.80
1	6	1792	G	C4-C5-N7	5.14	112.86	110.80
36	5	197	G	C4-C5-N7	5.14	112.86	110.80
36	5	1126	G	C5-C6-N1	-5.14	108.93	111.50
36	5	1724	U	N1-C2-O2	-5.14	119.20	122.80
36	5	2953	U	N3-C4-O4	5.14	123.00	119.40
36	1	802	C	C6-N1-C2	-5.14	118.24	120.30
36	1	1377	G	C6-C5-N7	-5.14	127.31	130.40
36	5	840	C	C4-C5-C6	5.14	119.97	117.40
36	5	3134	A	C6-N1-C2	-5.14	115.52	118.60
1	2	1324	G	N3-C4-N9	-5.14	122.92	126.00
36	1	103	G	N3-C4-C5	-5.14	126.03	128.60
36	1	1891	A	N3-C4-C5	5.14	130.40	126.80
36	1	2374	C	N3-C2-O2	-5.14	118.30	121.90
36	1	2814	G	N1-C6-O6	5.14	122.98	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3302	U	C6-N1-C2	5.14	124.08	121.00
38	4	8	C	C6-N1-C2	5.14	122.36	120.30
1	6	1740	A	N1-C6-N6	-5.14	115.52	118.60
36	5	636	C	N1-C2-O2	5.14	121.98	118.90
36	5	716	A	N1-C6-N6	5.14	121.68	118.60
36	5	874	U	C5-C6-N1	-5.14	120.13	122.70
36	1	2554	A	P-O3'-C3'	5.14	125.87	119.70
36	5	1847	A	N3-C4-C5	5.14	130.40	126.80
36	5	2932	U	N1-C2-O2	5.14	126.40	122.80
38	8	14	C	O5'-P-OP2	-5.14	101.08	105.70
36	1	324	A	C8-N9-C4	-5.14	103.75	105.80
36	1	2414	G	C4-C5-C6	5.14	121.88	118.80
36	1	2869	U	C6-N1-C1'	-5.14	114.01	121.20
1	6	371	G	C6-C5-N7	-5.14	127.32	130.40
36	5	1495	U	C2-N1-C1'	5.14	123.86	117.70
36	5	1656	A	C8-N9-C4	5.14	107.85	105.80
36	5	3125	U	C5-C6-N1	-5.14	120.13	122.70
1	2	551	G	C5-N7-C8	-5.13	101.73	104.30
1	6	1634	C	N3-C2-O2	-5.13	118.31	121.90
36	5	939	U	C6-N1-C2	5.13	124.08	121.00
36	5	985	U	C5-C6-N1	-5.13	120.13	122.70
36	5	1440	G	C6-C5-N7	5.13	133.48	130.40
36	5	1552	G	C5-C6-O6	-5.13	125.52	128.60
36	5	2368	A	C5-C6-N1	5.13	120.27	117.70
36	1	1489	A	C4-C5-N7	5.13	113.27	110.70
36	1	2187	G	C4-C5-C6	5.13	121.88	118.80
1	6	1481	C	N1-C1'-C2'	-5.13	106.35	112.00
36	5	2257	C	P-O3'-C3'	5.13	125.86	119.70
36	1	1928	G	C5-C6-O6	-5.13	125.52	128.60
1	6	1077	C	O5'-P-OP1	-5.13	101.08	105.70
1	6	1575	G	N1-C6-O6	-5.13	116.82	119.90
36	5	3143	C	N3-C4-C5	5.13	123.95	121.90
38	8	25	G	O5'-P-OP2	-5.13	101.08	105.70
36	1	908	G	N1-C2-N2	5.13	120.82	116.20
36	1	2169	G	C2-N3-C4	5.13	114.47	111.90
36	5	57	A	N1-C6-N6	5.13	121.68	118.60
1	2	360	A	C8-N9-C4	5.13	107.85	105.80
36	1	2646	C	C2-N3-C4	-5.13	117.33	119.90
36	1	3183	A	C5-C6-N6	-5.13	119.60	123.70
41	L4	339	LEU	CA-CB-CG	5.13	127.10	115.30
36	5	2614	G	N1-C2-N3	5.13	126.98	123.90
38	8	44	A	N1-C6-N6	5.13	121.68	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	155	G	N3-C4-N9	5.13	129.08	126.00
36	1	1907	C	O5'-P-OP2	-5.13	101.08	105.70
36	1	3256	G	C5-C6-O6	-5.13	125.52	128.60
1	6	1171	A	C8-N9-C4	-5.13	103.75	105.80
36	5	45	A	O5'-P-OP2	-5.13	101.08	105.70
36	5	1868	G	C8-N9-C1'	-5.13	120.34	127.00
36	5	1297	C	C4-C5-C6	5.12	119.96	117.40
36	5	2709	C	C5-C4-N4	-5.12	116.61	120.20
1	2	95	G	C4-C5-N7	-5.12	108.75	110.80
1	2	687	G	N3-C2-N2	-5.12	116.31	119.90
36	1	1210	U	C5-C6-N1	-5.12	120.14	122.70
36	1	1655	G	C8-N9-C4	-5.12	104.35	106.40
1	2	1023	A	N1-C6-N6	5.12	121.67	118.60
36	1	2261	G	N3-C4-C5	-5.12	126.04	128.60
36	5	1177	G	OP1-P-OP2	-5.12	111.92	119.60
36	5	1367	G	C5-C6-N1	-5.12	108.94	111.50
36	5	2364	G	C4-C5-N7	-5.12	108.75	110.80
1	6	85	A	C8-N9-C4	-5.12	103.75	105.80
1	6	615	A	N1-C2-N3	5.12	131.86	129.30
36	5	267	G	O5'-P-OP1	-5.12	101.09	105.70
36	5	1151	U	N3-C4-C5	-5.12	111.53	114.60
36	1	1589	A	O4'-C1'-N9	-5.12	104.11	108.20
36	1	2404	A	N3-C4-C5	5.12	130.38	126.80
36	5	2656	A	C8-N9-C4	-5.12	103.75	105.80
36	5	3049	A	N9-C4-C5	-5.12	103.75	105.80
36	1	314	U	C6-N1-C2	-5.12	117.93	121.00
36	1	1122	U	C2-N3-C4	-5.12	123.93	127.00
36	1	2537	U	P-O3'-C3'	5.12	125.84	119.70
36	1	2977	G	O5'-P-OP1	-5.12	101.10	105.70
36	1	2991	A	C8-N9-C4	5.12	107.85	105.80
1	6	942	G	C4-C5-N7	5.12	112.85	110.80
36	5	24	G	N3-C4-C5	5.12	131.16	128.60
36	5	3091	A	N1-C2-N3	5.12	131.86	129.30
62	n6	76	LEU	CA-CB-CG	5.12	127.06	115.30
36	1	56	G	O5'-P-OP2	5.11	116.84	110.70
36	1	635	G	C8-N9-C4	5.11	108.44	106.40
36	1	1604	G	N3-C4-C5	-5.11	126.04	128.60
36	1	2165	G	C6-C5-N7	-5.11	127.33	130.40
36	1	3204	C	N3-C2-O2	-5.11	118.32	121.90
41	L4	84	ARG	NE-CZ-NH1	-5.11	117.74	120.30
36	5	414	U	C2-N3-C4	-5.11	123.93	127.00
36	1	1129	A	C5-C6-N6	-5.11	119.61	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1649	G	N1-C2-N2	-5.11	111.60	116.20
36	5	2191	U	C6-N1-C2	-5.11	117.93	121.00
36	5	1511	U	C5-C6-N1	-5.11	120.15	122.70
36	5	2118	C	N3-C2-O2	-5.11	118.32	121.90
36	5	3107	U	C5-C6-N1	-5.11	120.14	122.70
1	2	1370	U	P-O3'-C3'	5.11	125.83	119.70
1	2	1454	G	O5'-P-OP2	-5.11	101.10	105.70
36	1	285	A	N9-C4-C5	-5.11	103.76	105.80
36	1	1531	C	O5'-P-OP2	5.11	116.83	110.70
36	1	2834	G	N9-C4-C5	-5.11	103.36	105.40
36	1	3269	U	C6-N1-C2	-5.11	117.94	121.00
1	6	1784	C	N1-C2-O2	5.11	121.96	118.90
36	5	1375	G	C8-N9-C4	-5.11	104.36	106.40
36	5	3200	G	N1-C6-O6	5.11	122.96	119.90
39	12	208	ASP	CB-CG-OD2	-5.11	113.70	118.30
36	1	2756	C	N3-C4-N4	5.11	121.57	118.00
1	2	749	U	C2-N1-C1'	5.10	123.83	117.70
36	5	2433	U	C6-N1-C2	5.10	124.06	121.00
36	5	639	G	N1-C6-O6	5.10	122.96	119.90
36	5	867	G	O5'-P-OP2	5.10	116.82	110.70
36	5	2129	U	N3-C4-O4	-5.10	115.83	119.40
36	1	333	G	C8-N9-C4	5.10	108.44	106.40
38	4	47	C	C5-C6-N1	-5.10	118.45	121.00
36	5	3085	G	OP1-P-O3'	5.10	116.42	105.20
36	5	3207	U	C6-N1-C1'	5.10	128.34	121.20
38	4	21	C	N3-C2-O2	5.10	125.47	121.90
1	6	994	G	C8-N9-C4	-5.10	104.36	106.40
36	5	498	A	O5'-P-OP2	-5.10	101.11	105.70
36	5	1144	U	N3-C2-O2	-5.10	118.63	122.20
36	5	1781	C	O5'-P-OP2	-5.10	101.11	105.70
36	1	1409	G	C5-C6-N1	5.10	114.05	111.50
36	1	1520	G	N7-C8-N9	-5.10	110.55	113.10
36	1	2351	U	C6-N1-C2	-5.10	117.94	121.00
1	6	1024	U	O5'-P-OP1	-5.10	101.11	105.70
36	5	1910	A	C4-C5-N7	5.10	113.25	110.70
36	5	2884	C	N3-C2-O2	5.10	125.47	121.90
36	5	3092	C	C2-N3-C4	-5.10	117.35	119.90
1	2	501	U	OP1-P-O3'	5.10	116.41	105.20
36	1	787	G	C4-C5-N7	-5.10	108.76	110.80
36	1	972	A	N7-C8-N9	-5.10	111.25	113.80
16	c4	35	GLY	N-CA-C	5.10	125.84	113.10
36	1	640	U	N1-C2-O2	-5.09	119.23	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	893	C	C6-N1-C2	-5.09	118.26	120.30
36	1	1395	G	C8-N9-C4	5.09	108.44	106.40
36	1	1620	U	N1-C2-O2	5.09	126.37	122.80
36	1	3079	U	N3-C2-O2	5.09	125.77	122.20
38	4	125	U	C6-N1-C1'	-5.09	114.07	121.20
1	6	787	G	N3-C4-C5	-5.09	126.05	128.60
1	6	961	U	N3-C4-C5	-5.09	111.54	114.60
36	5	878	G	C6-C5-N7	-5.09	127.34	130.40
36	5	1452	A	O5'-P-OP1	-5.09	101.11	105.70
36	5	1620	U	C2-N1-C1'	5.09	123.81	117.70
36	5	2620	G	C2-N3-C4	5.09	114.45	111.90
36	5	3054	U	O5'-P-OP2	-5.09	101.11	105.70
36	5	220	G	OP1-P-O3'	5.09	116.40	105.20
36	5	822	G	O5'-P-OP1	-5.09	101.12	105.70
36	5	1928	G	C6-C5-N7	-5.09	127.34	130.40
36	5	2797	C	C6-N1-C2	-5.09	118.26	120.30
18	C6	28	LEU	CA-CB-CG	5.09	127.01	115.30
36	1	282	G	C8-N9-C4	-5.09	104.36	106.40
36	1	638	C	N1-C2-O2	5.09	121.95	118.90
36	1	1416	C	N3-C4-N4	-5.09	114.44	118.00
1	6	144	U	C2-N1-C1'	5.09	123.81	117.70
36	5	1181	U	C2-N3-C4	-5.09	123.95	127.00
36	5	2514	U	C5-C6-N1	5.09	125.25	122.70
36	1	217	U	OP1-P-O3'	5.09	116.39	105.20
36	1	903	U	N3-C2-O2	-5.09	118.64	122.20
1	6	453	U	C5-C4-O4	5.09	128.95	125.90
1	6	795	U	N3-C2-O2	-5.09	118.64	122.20
36	5	101	G	O4'-C1'-N9	5.09	112.27	108.20
1	2	159	U	C5-C6-N1	-5.09	120.16	122.70
1	2	1514	U	N3-C2-O2	-5.09	118.64	122.20
36	1	662	U	C6-N1-C2	-5.09	117.95	121.00
36	1	803	C	OP2-P-O3'	5.09	116.39	105.20
36	1	1825	G	N1-C6-O6	5.09	122.95	119.90
1	6	113	U	P-O3'-C3'	5.09	125.81	119.70
1	6	489	C	C2-N1-C1'	5.09	124.40	118.80
36	5	517	G	N3-C4-C5	-5.09	126.06	128.60
36	5	836	A	C8-N9-C4	5.09	107.83	105.80
36	1	635	G	O5'-P-OP1	-5.09	101.12	105.70
36	1	662	U	N3-C4-C5	-5.09	111.55	114.60
1	6	1478	G	C4-C5-C6	5.09	121.85	118.80
36	5	2599	U	C4-C5-C6	5.09	122.75	119.70
1	2	934	C	C5-C6-N1	5.08	123.54	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	187	A	C4-C5-C6	5.08	119.54	117.00
36	1	1046	A	N1-C6-N6	5.08	121.65	118.60
36	1	2297	U	P-O3'-C3'	5.08	125.80	119.70
36	5	110	G	N1-C6-O6	-5.08	116.85	119.90
36	5	1876	U	C5-C4-O4	-5.08	122.85	125.90
1	2	388	G	C5-C6-O6	-5.08	125.55	128.60
1	2	1341	A	C4-C5-C6	5.08	119.54	117.00
36	1	939	U	C5-C6-N1	-5.08	120.16	122.70
36	1	1592	G	C5-C6-O6	5.08	131.65	128.60
37	3	83	U	C6-N1-C2	5.08	124.05	121.00
1	6	383	G	C8-N9-C4	-5.08	104.37	106.40
36	5	780	A	C5-C6-N6	-5.08	119.63	123.70
36	5	1493	G	N3-C4-C5	5.08	131.14	128.60
36	5	2651	G	N3-C4-N9	-5.08	122.95	126.00
37	7	22	A	C4-N9-C1'	5.08	135.45	126.30
3	S1	70	LEU	CA-CB-CG	5.08	126.99	115.30
36	1	510	G	N3-C2-N2	-5.08	116.34	119.90
36	1	1342	C	N3-C4-C5	5.08	123.93	121.90
36	1	1927	G	C5-C6-O6	5.08	131.65	128.60
1	6	11	A	N1-C6-N6	-5.08	115.55	118.60
36	5	1193	A	C8-N9-C4	-5.08	103.77	105.80
36	1	2215	A	C8-N9-C4	5.08	107.83	105.80
36	1	3218	A	C3'-C2'-C1'	5.08	105.56	101.50
1	2	1503	A	O4'-C1'-N9	5.08	112.26	108.20
36	1	278	U	N1-C2-O2	-5.08	119.25	122.80
36	1	810	A	N7-C8-N9	5.08	116.34	113.80
36	1	2917	G	C5-C6-N1	5.08	114.04	111.50
36	5	2514	U	C6-N1-C2	-5.08	117.95	121.00
36	5	2940	A	N1-C6-N6	5.08	121.65	118.60
1	2	1200	G	N3-C2-N2	-5.08	116.35	119.90
36	1	1082	U	N3-C2-O2	-5.08	118.65	122.20
1	6	119	A	C5-C6-N1	-5.08	115.16	117.70
1	6	1614	A	O4'-C1'-N9	5.08	112.26	108.20
36	5	277	G	N9-C4-C5	5.08	107.43	105.40
36	5	1080	A	C8-N9-C4	5.08	107.83	105.80
36	5	3099	C	N1-C2-O2	-5.08	115.85	118.90
1	2	1572	G	N1-C6-O6	5.08	122.95	119.90
36	1	1410	U	O5'-P-OP1	-5.08	101.13	105.70
1	6	800	U	C5-C4-O4	5.08	128.94	125.90
1	6	911	U	N3-C2-O2	-5.08	118.65	122.20
1	6	1118	G	C2-N3-C4	-5.08	109.36	111.90
36	5	102	C	N3-C4-C5	-5.08	119.87	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	159	U	N3-C2-O2	5.07	125.75	122.20
36	1	907	G	O4'-C1'-N9	5.07	112.26	108.20
36	1	2868	U	N3-C2-O2	-5.07	118.65	122.20
36	1	3270	U	C5-C4-O4	5.07	128.94	125.90
36	5	98	G	C8-N9-C4	5.07	108.43	106.40
36	5	778	U	OP1-P-O3'	5.07	116.36	105.20
36	1	109	A	N1-C6-N6	-5.07	115.56	118.60
36	1	278	U	N3-C4-O4	5.07	122.95	119.40
36	1	576	C	N3-C4-C5	5.07	123.93	121.90
36	1	2354	C	C5-C4-N4	5.07	123.75	120.20
36	1	2651	G	C4-C5-N7	-5.07	108.77	110.80
36	1	3120	C	N1-C2-O2	5.07	121.94	118.90
1	6	858	G	C4-C5-N7	5.07	112.83	110.80
36	5	954	U	N3-C2-O2	-5.07	118.65	122.20
36	5	1149	G	N1-C2-N2	5.07	120.76	116.20
36	5	1910	A	C8-N9-C4	5.07	107.83	105.80
36	5	2966	G	C5-C6-O6	-5.07	125.56	128.60
36	1	648	C	N3-C2-O2	-5.07	118.35	121.90
36	1	651	G	C4-N9-C1'	5.07	133.09	126.50
36	1	859	G	C2-N3-C4	-5.07	109.37	111.90
36	1	2404	A	C6-C5-N7	-5.07	128.75	132.30
36	1	2405	C	O5'-P-OP1	-5.07	101.14	105.70
36	5	343	U	N1-C2-N3	5.07	117.94	114.90
36	5	800	G	C8-N9-C4	5.07	108.43	106.40
1	2	1762	A	N9-C4-C5	-5.07	103.77	105.80
36	5	526	C	C6-N1-C2	5.07	122.33	120.30
36	5	2393	G	C4-C5-N7	5.07	112.83	110.80
36	1	2728	G	C8-N9-C4	-5.06	104.37	106.40
1	2	571	G	C8-N9-C1'	5.06	133.58	127.00
36	1	851	C	C6-N1-C2	-5.06	118.28	120.30
36	1	924	G	C4-C5-N7	5.06	112.83	110.80
36	1	1112	A	C6-N1-C2	-5.06	115.56	118.60
36	1	1929	G	N9-C4-C5	-5.06	103.38	105.40
36	1	2805	G	C5-C6-O6	-5.06	125.56	128.60
1	6	603	U	N1-C2-O2	-5.06	119.26	122.80
36	5	901	G	C4-C5-C6	5.06	121.84	118.80
36	5	3057	U	C6-N1-C1'	-5.06	114.11	121.20
1	2	1269	U	C6-N1-C1'	-5.06	114.12	121.20
36	1	667	C	N1-C2-O2	5.06	121.94	118.90
36	1	2401	A	C4-C5-C6	-5.06	114.47	117.00
38	4	56	G	C8-N9-C4	5.06	108.42	106.40
1	6	1025	A	N1-C6-N6	5.06	121.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	93	C	N1-C2-O2	-5.06	115.86	118.90
36	5	805	G	N7-C8-N9	-5.06	110.57	113.10
36	5	885	U	N1-C2-O2	-5.06	119.26	122.80
36	5	1443	G	C5-C6-O6	5.06	131.64	128.60
36	5	1929	G	C5-C6-O6	-5.06	125.56	128.60
36	5	2335	G	OP2-P-O3'	5.06	116.33	105.20
1	2	571	G	C4-N9-C1'	-5.06	119.92	126.50
36	1	2104	A	C8-N9-C4	5.06	107.82	105.80
36	1	3190	C	N3-C4-C5	5.06	123.92	121.90
36	1	3270	U	N3-C4-O4	-5.06	115.86	119.40
1	6	45	U	O4'-C1'-N1	5.06	112.25	108.20
1	6	1103	U	N3-C4-O4	-5.06	115.86	119.40
36	5	1236	G	N1-C6-O6	5.06	122.93	119.90
36	1	2726	C	C2-N3-C4	-5.06	117.37	119.90
36	1	347	G	N7-C8-N9	5.05	115.63	113.10
36	1	743	C	N1-C2-O2	-5.05	115.87	118.90
36	1	2941	A	N1-C6-N6	5.05	121.63	118.60
38	4	100	U	C2-N1-C1'	5.05	123.77	117.70
1	6	1473	U	N1-C2-O2	5.05	126.34	122.80
36	5	1239	C	C2-N1-C1'	5.05	124.36	118.80
36	5	1775	G	N3-C4-N9	5.05	129.03	126.00
36	5	2852	C	C2-N3-C4	-5.05	117.37	119.90
36	5	3306	U	C6-N1-C2	5.05	124.03	121.00
1	2	1792	G	C4-N9-C1'	5.05	133.07	126.50
1	6	387	A	C5-N7-C8	5.05	106.43	103.90
36	5	224	C	N1-C2-O2	5.05	121.93	118.90
36	5	1493	G	O4'-C1'-N9	5.05	112.24	108.20
36	1	857	G	C6-C5-N7	-5.05	127.37	130.40
36	1	963	G	O5'-P-OP1	5.05	116.76	110.70
1	6	1361	U	C2-N1-C1'	5.05	123.76	117.70
36	5	719	U	N1-C2-O2	5.05	126.34	122.80
36	1	214	G	N1-C6-O6	5.05	122.93	119.90
36	1	2131	A	OP1-P-O3'	5.05	116.31	105.20
1	6	1568	C	P-O3'-C3'	5.05	125.76	119.70
36	5	810	A	C2-N3-C4	5.05	113.12	110.60
36	5	1303	A	OP1-P-OP2	5.05	127.17	119.60
36	5	2321	A	C4-C5-N7	5.05	113.22	110.70
36	1	1884	A	C2-N3-C4	-5.05	108.08	110.60
36	1	3143	C	C5-C6-N1	-5.05	118.48	121.00
1	6	1109	G	C5-C6-O6	-5.05	125.57	128.60
36	1	780	A	C6-N1-C2	-5.05	115.57	118.60
36	1	3050	U	C5-C4-O4	5.05	128.93	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3361	G	N3-C4-N9	5.05	129.03	126.00
36	5	2936	A	N1-C6-N6	5.05	121.63	118.60
1	2	1327	C	C5-C6-N1	5.04	123.52	121.00
36	1	968	G	C8-N9-C4	-5.04	104.38	106.40
36	1	1589	A	N1-C2-N3	5.04	131.82	129.30
1	6	114	C	N3-C2-O2	-5.04	118.37	121.90
1	2	1165	G	C4-C5-N7	5.04	112.82	110.80
36	1	1548	C	C2-N3-C4	-5.04	117.38	119.90
36	1	1901	A	N1-C6-N6	-5.04	115.57	118.60
36	1	2911	A	C2-N3-C4	-5.04	108.08	110.60
38	4	48	A	C6-N1-C2	-5.04	115.57	118.60
1	6	1046	G	C8-N9-C4	5.04	108.42	106.40
36	1	416	A	N7-C8-N9	-5.04	111.28	113.80
36	1	635	G	C6-N1-C2	-5.04	122.08	125.10
36	1	672	A	C8-N9-C4	5.04	107.82	105.80
1	6	359	A	C8-N9-C4	5.04	107.82	105.80
36	5	2944	U	N1-C2-O2	5.04	126.33	122.80
36	5	3057	U	N1-C2-O2	5.04	126.33	122.80
38	8	139	U	C5-C4-O4	5.04	128.93	125.90
36	1	1136	A	N7-C8-N9	5.04	116.32	113.80
36	1	2602	G	C4-C5-N7	-5.04	108.78	110.80
36	5	642	U	N1-C2-O2	5.04	126.33	122.80
36	5	652	G	C5-C6-N1	-5.04	108.98	111.50
36	5	1193	A	C5-C6-N6	-5.04	119.67	123.70
36	5	3195	U	OP1-P-O3'	5.04	116.29	105.20
36	1	114	A	O5'-P-OP1	-5.04	101.17	105.70
36	1	1340	G	C4-C5-N7	5.04	112.82	110.80
36	1	1435	A	O5'-P-OP2	5.04	116.75	110.70
36	1	1912	U	N3-C2-O2	-5.04	118.67	122.20
36	1	2376	G	C8-N9-C4	-5.04	104.39	106.40
36	1	2644	C	N1-C2-O2	5.04	121.92	118.90
36	5	48	A	N1-C6-N6	-5.04	115.58	118.60
36	5	659	G	N9-C4-C5	-5.04	103.39	105.40
36	5	2870	C	N3-C4-C5	5.04	123.92	121.90
36	5	3370	A	C2-N3-C4	5.04	113.12	110.60
36	1	763	G	P-O3'-C3'	5.04	125.75	119.70
36	5	3107	U	C2-N3-C4	-5.04	123.98	127.00
1	6	756	A	N7-C8-N9	5.04	116.32	113.80
1	6	1782	A	N9-C4-C5	5.04	107.81	105.80
36	5	1608	C	N1-C2-O2	5.04	121.92	118.90
36	5	3306	U	N1-C2-N3	-5.04	111.88	114.90
36	1	48	A	N1-C6-N6	-5.03	115.58	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1855	U	N3-C2-O2	-5.03	118.68	122.20
1	6	402	C	C5-C4-N4	-5.03	116.68	120.20
1	6	558	U	P-O3'-C3'	5.03	125.74	119.70
1	6	1025	A	O5'-P-OP1	-5.03	101.17	105.70
1	6	1113	A	N1-C2-N3	5.03	131.82	129.30
36	5	857	G	C2-N3-C4	-5.03	109.38	111.90
36	5	2339	C	C2-N1-C1'	5.03	124.34	118.80
1	2	803	A	N1-C6-N6	-5.03	115.58	118.60
36	1	215	G	N1-C6-O6	5.03	122.92	119.90
36	1	1837	U	N3-C4-O4	5.03	122.92	119.40
36	1	3362	A	C8-N9-C4	-5.03	103.79	105.80
1	2	901	G	C4-N9-C1'	5.03	133.04	126.50
36	1	808	A	C6-N1-C2	-5.03	115.58	118.60
36	1	2977	G	C5-C6-N1	5.03	114.02	111.50
36	1	3023	U	N3-C2-O2	-5.03	118.68	122.20
1	6	354	C	C4-C5-C6	-5.03	114.89	117.40
1	6	546	U	C5-C6-N1	-5.03	120.19	122.70
36	5	69	C	N3-C4-C5	-5.03	119.89	121.90
36	5	931	C	C2-N3-C4	-5.03	117.39	119.90
36	5	2366	C	C2-N3-C4	5.03	122.42	119.90
1	2	1131	A	C8-N9-C4	5.03	107.81	105.80
36	1	1370	G	C6-C5-N7	-5.03	127.38	130.40
36	5	1879	A	N9-C4-C5	-5.03	103.79	105.80
1	2	388	G	N1-C6-O6	5.03	122.92	119.90
36	1	201	A	N1-C2-N3	5.03	131.81	129.30
36	1	753	C	N3-C4-N4	5.03	121.52	118.00
36	1	1126	G	C5-C6-N1	-5.03	108.99	111.50
36	1	1141	C	N3-C4-C5	-5.03	119.89	121.90
1	6	18	C	N3-C4-C5	-5.03	119.89	121.90
36	5	2427	U	N1-C2-O2	-5.03	119.28	122.80
36	1	678	G	N3-C2-N2	-5.03	116.38	119.90
36	1	2611	U	N3-C4-C5	5.03	117.61	114.60
1	6	542	A	C6-C5-N7	-5.03	128.78	132.30
36	5	42	C	N1-C2-O2	5.03	121.92	118.90
36	5	330	G	O5'-P-OP2	-5.03	101.18	105.70
65	n9	20	GLY	N-CA-C	5.03	125.66	113.10
36	1	2794	G	O4'-C1'-N9	5.02	112.22	108.20
36	5	803	C	C5-C4-N4	-5.02	116.68	120.20
36	1	2412	G	N1-C6-O6	5.02	122.91	119.90
1	6	313	U	C2-N1-C1'	-5.02	111.67	117.70
1	6	787	G	C4-N9-C1'	5.02	133.03	126.50
1	6	1439	C	C5-C6-N1	5.02	123.51	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	755	A	C3'-C2'-C1'	5.02	105.52	101.50
1	2	497	G	P-O3'-C3'	5.02	125.72	119.70
1	2	542	A	C8-N9-C1'	-5.02	118.66	127.70
1	2	1600	A	P-O3'-C3'	5.02	125.72	119.70
12	C0	63	TYR	N-CA-C	5.02	124.56	111.00
36	1	637	C	C2-N3-C4	-5.02	117.39	119.90
36	1	1377	G	C5-N7-C8	-5.02	101.79	104.30
36	1	2513	U	P-O3'-C3'	5.02	125.72	119.70
37	3	53	U	N3-C2-O2	5.02	125.71	122.20
1	6	1333	C	N3-C4-C5	5.02	123.91	121.90
36	5	1155	C	N3-C4-C5	5.02	123.91	121.90
36	5	1156	C	N1-C2-N3	5.02	122.71	119.20
36	5	1850	A	C5-C6-N6	5.02	127.72	123.70
36	1	968	G	N3-C4-N9	5.02	129.01	126.00
1	6	417	A	C3'-C2'-C1'	5.02	105.52	101.50
36	5	984	G	C6-C5-N7	-5.02	127.39	130.40
36	5	2730	G	N3-C4-C5	5.02	131.11	128.60
36	5	3041	U	N1-C2-N3	-5.02	111.89	114.90
36	1	2765	C	N1-C2-O2	5.02	121.91	118.90
36	5	1101	G	C8-N9-C4	5.02	108.41	106.40
1	2	422	G	C6-C5-N7	-5.01	127.39	130.40
36	1	282	G	N3-C4-C5	-5.01	126.09	128.60
36	1	1851	G	C8-N9-C4	-5.01	104.39	106.40
36	5	2294	U	C2-N3-C4	-5.01	123.99	127.00
36	5	3066	U	N3-C4-C5	5.01	117.61	114.60
36	1	867	G	C5-C6-N1	-5.01	108.99	111.50
36	1	2130	G	N1-C2-N2	-5.01	111.69	116.20
36	1	645	A	C4-C5-N7	-5.01	108.19	110.70
36	1	815	G	N1-C6-O6	5.01	122.91	119.90
1	6	86	A	N1-C6-N6	5.01	121.61	118.60
36	5	106	A	N1-C6-N6	-5.01	115.59	118.60
36	5	1380	G	N9-C4-C5	-5.01	103.39	105.40
1	2	1012	U	O5'-P-OP1	-5.01	101.19	105.70
36	1	57	A	C2-N3-C4	-5.01	108.09	110.60
36	1	746	A	C5-C6-N6	-5.01	119.69	123.70
37	3	53	U	C2-N1-C1'	-5.01	111.69	117.70
36	5	2649	A	N1-C6-N6	-5.01	115.59	118.60
38	8	51	G	C4-N9-C1'	5.01	133.01	126.50
36	5	1870	C	C6-N1-C2	-5.01	118.30	120.30
36	1	1340	G	N3-C4-N9	5.01	129.00	126.00
36	1	2718	U	C2-N3-C4	-5.01	124.00	127.00
36	1	2852	C	C6-N1-C1'	-5.01	114.79	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	648	G	C4-N9-C1'	5.01	133.01	126.50
1	6	1280	C	N1-C2-O2	-5.01	115.90	118.90
36	5	376	G	C5-C6-N1	5.01	114.00	111.50
36	5	1333	C	C6-N1-C2	-5.01	118.30	120.30
36	5	2179	C	OP1-P-OP2	5.01	127.11	119.60
36	5	2411	U	C5-C6-N1	-5.01	120.20	122.70
1	2	735	C	OP1-P-OP2	-5.00	112.09	119.60
36	1	1537	A	N1-C6-N6	5.00	121.60	118.60
36	1	1838	G	N9-C4-C5	-5.00	103.40	105.40
36	1	859	G	C6-C5-N7	-5.00	127.40	130.40
36	1	3119	U	N3-C4-O4	-5.00	115.90	119.40
36	1	3217	C	C6-N1-C2	-5.00	118.30	120.30
38	4	70	G	N9-C4-C5	-5.00	103.40	105.40
41	L4	206	LEU	CA-CB-CG	5.00	126.81	115.30
1	6	1620	C	C5-C6-N1	5.00	123.50	121.00
36	5	1149	G	N9-C1'-C2'	-5.00	106.50	112.00
36	5	2849	C	C2-N3-C4	5.00	122.40	119.90
36	5	3011	A	C5-C6-N1	5.00	120.20	117.70
36	5	3172	A	N1-C2-N3	5.00	131.80	129.30
67	o1	90	PHE	CB-CG-CD1	-5.00	117.30	120.80
36	1	517	G	C4-C5-C6	5.00	121.80	118.80
36	1	1163	A	C2-N3-C4	-5.00	108.10	110.60
36	1	1646	G	C5-C6-O6	-5.00	125.60	128.60
36	1	1891	A	O5'-P-OP1	5.00	116.70	110.70
39	L2	96	LEU	CA-CB-CG	5.00	126.81	115.30
36	5	984	G	O5'-P-OP1	-5.00	101.20	105.70
36	5	2145	A	N3-C4-N9	5.00	131.40	127.40
36	5	2710	C	N3-C4-C5	-5.00	119.90	121.90
37	7	22	A	C4-C5-C6	5.00	119.50	117.00
38	8	104	A	N9-C4-C5	-5.00	103.80	105.80

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
17	C5	99	GLY	Peptide
19	C7	85	VAL	Peptide
27	D5	54	VAL	Peptide
27	D5	94	LYS	Peptide
27	D5	96	SER	Peptide

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Mol	Chain	Res	Type	Group
33	E1	105	TYR	Peptide
33	E1	146	SER	Peptide
39	L2	19	HIS	Peptide
42	L5	57	ASN	Peptide
43	L6	51	ARG	Peptide
43	L6	89	THR	Peptide
52	M6	110	PRO	Peptide
57	N1	16	GLN	Peptide
65	N9	19	ASN	Peptide
65	N9	20	GLY	Peptide
67	O1	5	LYS	Peptide
7	S5	99	MET	Peptide
9	S7	131	PHE	Peptide
16	c4	124	ASP	Peptide
17	c5	52	LYS	Peptide
20	c8	80	LYS	Peptide
22	d0	70	THR	Peptide
33	e1	146	SER	Peptide
39	l2	237	LEU	Peptide
42	l5	270	LYS	Peptide
43	l6	51	ARG	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
49	m3	74	GLY	Peptide
52	m6	110	PRO	Peptide
54	m8	14	GLY	Peptide
56	n0	133	ALA	Peptide
56	n0	170	THR	Peptide
63	n7	101	PHE	Peptide
64	n8	18	GLY	Peptide
64	n8	66	ALA	Peptide
65	n9	19	ASN	Peptide
65	n9	23	LYS	Peptide
67	o1	6	ASP	Peptide
67	o1	90	PHE	Peptide
68	o2	15	LYS	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	151 (74%)	32 (16%)	21 (10%)	0	3
2	s0	204/251 (81%)	152 (74%)	34 (17%)	18 (9%)	1	4
3	S1	212/254 (84%)	140 (66%)	34 (16%)	38 (18%)	0	0
3	s1	214/254 (84%)	168 (78%)	31 (14%)	15 (7%)	1	7
4	S2	215/253 (85%)	169 (79%)	31 (14%)	15 (7%)	1	7
4	s2	215/253 (85%)	173 (80%)	30 (14%)	12 (6%)	2	11
5	S3	221/239 (92%)	181 (82%)	25 (11%)	15 (7%)	1	7
5	s3	221/239 (92%)	178 (80%)	24 (11%)	19 (9%)	1	4
6	S4	258/260 (99%)	224 (87%)	23 (9%)	11 (4%)	2	16
6	s4	258/260 (99%)	220 (85%)	21 (8%)	17 (7%)	1	7
7	S5	204/224 (91%)	162 (79%)	25 (12%)	17 (8%)	1	5
7	s5	204/224 (91%)	152 (74%)	38 (19%)	14 (7%)	1	7
8	S6	224/236 (95%)	189 (84%)	23 (10%)	12 (5%)	2	12
8	s6	216/236 (92%)	179 (83%)	28 (13%)	9 (4%)	3	16
9	S7	182/189 (96%)	135 (74%)	30 (16%)	17 (9%)	0	3
9	s7	184/189 (97%)	148 (80%)	21 (11%)	15 (8%)	1	5
10	S8	184/200 (92%)	155 (84%)	19 (10%)	10 (5%)	2	12
10	s8	184/200 (92%)	155 (84%)	20 (11%)	9 (5%)	2	14
11	S9	183/196 (93%)	145 (79%)	28 (15%)	10 (6%)	2	11
11	s9	183/196 (93%)	142 (78%)	32 (18%)	9 (5%)	2	14
12	C0	94/105 (90%)	71 (76%)	16 (17%)	7 (7%)	1	6
12	c0	92/105 (88%)	63 (68%)	13 (14%)	16 (17%)	0	0
13	C1	153/155 (99%)	126 (82%)	18 (12%)	9 (6%)	1	10
13	c1	144/155 (93%)	122 (85%)	14 (10%)	8 (6%)	2	11
14	C2	122/142 (86%)	69 (57%)	34 (28%)	19 (16%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/142 (86%)	66 (54%)	34 (28%)	22 (18%)	0	0
15	C3	148/150 (99%)	122 (82%)	15 (10%)	11 (7%)	1	6
15	c3	148/150 (99%)	121 (82%)	17 (12%)	10 (7%)	1	7
16	C4	125/136 (92%)	86 (69%)	26 (21%)	13 (10%)	0	3
16	c4	126/136 (93%)	99 (79%)	18 (14%)	9 (7%)	1	6
17	C5	122/141 (86%)	88 (72%)	22 (18%)	12 (10%)	0	3
17	c5	133/141 (94%)	94 (71%)	23 (17%)	16 (12%)	0	1
18	C6	139/142 (98%)	115 (83%)	13 (9%)	11 (8%)	1	5
18	c6	140/142 (99%)	116 (83%)	16 (11%)	8 (6%)	1	10
19	C7	116/136 (85%)	89 (77%)	20 (17%)	7 (6%)	1	9
19	c7	113/136 (83%)	87 (77%)	16 (14%)	10 (9%)	1	4
20	C8	143/145 (99%)	117 (82%)	13 (9%)	13 (9%)	1	4
20	c8	143/145 (99%)	117 (82%)	17 (12%)	9 (6%)	1	8
21	C9	141/143 (99%)	116 (82%)	19 (14%)	6 (4%)	2	16
21	c9	141/143 (99%)	115 (82%)	19 (14%)	7 (5%)	2	13
22	D0	105/120 (88%)	83 (79%)	16 (15%)	6 (6%)	1	10
22	d0	108/120 (90%)	89 (82%)	11 (10%)	8 (7%)	1	6
23	D1	85/87 (98%)	60 (71%)	18 (21%)	7 (8%)	1	5
23	d1	85/87 (98%)	73 (86%)	7 (8%)	5 (6%)	1	10
24	D2	127/129 (98%)	109 (86%)	15 (12%)	3 (2%)	6	27
24	d2	127/129 (98%)	108 (85%)	15 (12%)	4 (3%)	4	23
25	D3	142/144 (99%)	109 (77%)	23 (16%)	10 (7%)	1	7
25	d3	142/144 (99%)	118 (83%)	17 (12%)	7 (5%)	2	14
26	D4	132/134 (98%)	107 (81%)	16 (12%)	9 (7%)	1	7
26	d4	132/134 (98%)	106 (80%)	14 (11%)	12 (9%)	1	4
27	D5	68/107 (64%)	46 (68%)	11 (16%)	11 (16%)	0	0
27	d5	67/107 (63%)	51 (76%)	12 (18%)	4 (6%)	1	9
28	D6	95/97 (98%)	65 (68%)	15 (16%)	15 (16%)	0	0
28	d6	95/97 (98%)	73 (77%)	16 (17%)	6 (6%)	1	8
29	D7	79/81 (98%)	62 (78%)	13 (16%)	4 (5%)	2	13
29	d7	79/81 (98%)	61 (77%)	9 (11%)	9 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	D8	61/66 (92%)	47 (77%)	11 (18%)	3 (5%)	2	14
30	d8	61/66 (92%)	42 (69%)	13 (21%)	6 (10%)	0	3
31	D9	51/55 (93%)	44 (86%)	7 (14%)	0	100	100
31	d9	51/55 (93%)	43 (84%)	3 (6%)	5 (10%)	0	3
32	E0	58/60 (97%)	47 (81%)	7 (12%)	4 (7%)	1	7
33	E1	69/76 (91%)	37 (54%)	17 (25%)	15 (22%)	0	0
33	e1	74/76 (97%)	38 (51%)	16 (22%)	20 (27%)	0	0
34	SR	316/318 (99%)	267 (84%)	42 (13%)	7 (2%)	6	29
34	sR	316/318 (99%)	264 (84%)	41 (13%)	11 (4%)	3	20
35	SM	155/273 (57%)	106 (68%)	21 (14%)	28 (18%)	0	0
35	sM	98/273 (36%)	60 (61%)	27 (28%)	11 (11%)	0	2
39	L2	250/253 (99%)	211 (84%)	26 (10%)	13 (5%)	2	12
39	l2	250/253 (99%)	210 (84%)	26 (10%)	14 (6%)	2	11
40	L3	384/386 (100%)	328 (85%)	41 (11%)	15 (4%)	3	18
40	l3	384/386 (100%)	338 (88%)	37 (10%)	9 (2%)	6	28
41	L4	359/361 (99%)	289 (80%)	49 (14%)	21 (6%)	1	10
41	l4	359/361 (99%)	298 (83%)	43 (12%)	18 (5%)	2	13
42	L5	294/296 (99%)	241 (82%)	35 (12%)	18 (6%)	1	9
42	l5	292/296 (99%)	257 (88%)	26 (9%)	9 (3%)	4	23
43	L6	152/175 (87%)	135 (89%)	10 (7%)	7 (5%)	2	15
43	l6	153/175 (87%)	133 (87%)	16 (10%)	4 (3%)	5	26
44	L7	220/243 (90%)	196 (89%)	17 (8%)	7 (3%)	4	22
44	l7	221/243 (91%)	194 (88%)	20 (9%)	7 (3%)	4	22
45	L8	231/255 (91%)	190 (82%)	33 (14%)	8 (4%)	3	20
45	l8	229/255 (90%)	179 (78%)	36 (16%)	14 (6%)	1	9
46	L9	189/191 (99%)	164 (87%)	20 (11%)	5 (3%)	5	26
46	l9	189/191 (99%)	164 (87%)	18 (10%)	7 (4%)	3	19
47	M0	207/220 (94%)	169 (82%)	32 (16%)	6 (3%)	4	24
47	m0	209/220 (95%)	164 (78%)	34 (16%)	11 (5%)	2	12
48	M1	167/173 (96%)	125 (75%)	19 (11%)	23 (14%)	0	1
48	m1	167/173 (96%)	137 (82%)	18 (11%)	12 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	155 (81%)	29 (15%)	7 (4%)	3	19
49	m3	192/198 (97%)	159 (83%)	22 (12%)	11 (6%)	1	10
50	M4	134/137 (98%)	114 (85%)	12 (9%)	8 (6%)	1	9
50	m4	135/137 (98%)	120 (89%)	12 (9%)	3 (2%)	6	29
51	M5	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	4	23
51	m5	201/203 (99%)	177 (88%)	15 (8%)	9 (4%)	2	15
52	M6	195/198 (98%)	172 (88%)	19 (10%)	4 (2%)	7	30
52	m6	195/198 (98%)	176 (90%)	15 (8%)	4 (2%)	7	30
53	M7	181/183 (99%)	154 (85%)	18 (10%)	9 (5%)	2	13
53	m7	153/183 (84%)	139 (91%)	11 (7%)	3 (2%)	7	31
54	M8	183/185 (99%)	158 (86%)	20 (11%)	5 (3%)	5	25
54	m8	183/185 (99%)	151 (82%)	24 (13%)	8 (4%)	2	15
55	M9	186/188 (99%)	165 (89%)	18 (10%)	3 (2%)	9	37
55	m9	186/188 (99%)	164 (88%)	17 (9%)	5 (3%)	5	25
56	N0	170/172 (99%)	155 (91%)	14 (8%)	1 (1%)	25	59
56	n0	170/172 (99%)	159 (94%)	9 (5%)	2 (1%)	13	44
57	N1	157/159 (99%)	135 (86%)	17 (11%)	5 (3%)	4	22
57	n1	157/159 (99%)	137 (87%)	16 (10%)	4 (2%)	5	27
58	N2	98/120 (82%)	77 (79%)	13 (13%)	8 (8%)	1	5
58	n2	96/120 (80%)	82 (85%)	11 (12%)	3 (3%)	4	23
59	N3	134/136 (98%)	121 (90%)	10 (8%)	3 (2%)	6	29
59	n3	134/136 (98%)	121 (90%)	12 (9%)	1 (1%)	22	57
60	N4	96/155 (62%)	75 (78%)	15 (16%)	6 (6%)	1	8
60	n4	133/155 (86%)	109 (82%)	15 (11%)	9 (7%)	1	7
61	N5	119/141 (84%)	107 (90%)	12 (10%)	0	100	100
61	n5	118/141 (84%)	96 (81%)	13 (11%)	9 (8%)	1	5
62	N6	124/126 (98%)	114 (92%)	6 (5%)	4 (3%)	4	22
62	n6	124/126 (98%)	105 (85%)	12 (10%)	7 (6%)	2	11
63	N7	133/135 (98%)	98 (74%)	24 (18%)	11 (8%)	1	5
63	n7	133/135 (98%)	98 (74%)	22 (16%)	13 (10%)	0	3
64	N8	146/148 (99%)	121 (83%)	14 (10%)	11 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	n8	146/148 (99%)	123 (84%)	18 (12%)	5 (3%)	3	21
65	N9	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	3	20
65	n9	56/58 (97%)	44 (79%)	9 (16%)	3 (5%)	2	12
66	O0	95/104 (91%)	81 (85%)	11 (12%)	3 (3%)	4	22
66	o0	98/104 (94%)	82 (84%)	14 (14%)	2 (2%)	7	31
67	O1	107/112 (96%)	94 (88%)	7 (6%)	6 (6%)	2	11
67	o1	107/112 (96%)	88 (82%)	12 (11%)	7 (6%)	1	8
68	O2	125/129 (97%)	109 (87%)	15 (12%)	1 (1%)	19	54
68	o2	125/129 (97%)	106 (85%)	11 (9%)	8 (6%)	1	8
69	O3	104/106 (98%)	96 (92%)	6 (6%)	2 (2%)	8	33
69	o3	104/106 (98%)	90 (86%)	10 (10%)	4 (4%)	3	19
70	O4	110/120 (92%)	100 (91%)	9 (8%)	1 (1%)	17	52
70	o4	110/120 (92%)	99 (90%)	9 (8%)	2 (2%)	8	34
71	O5	117/119 (98%)	100 (86%)	13 (11%)	4 (3%)	3	21
71	o5	117/119 (98%)	101 (86%)	14 (12%)	2 (2%)	9	36
72	O6	97/99 (98%)	74 (76%)	13 (13%)	10 (10%)	0	3
72	o6	97/99 (98%)	81 (84%)	10 (10%)	6 (6%)	1	9
73	O7	85/87 (98%)	74 (87%)	7 (8%)	4 (5%)	2	14
73	o7	85/87 (98%)	73 (86%)	10 (12%)	2 (2%)	6	27
74	O8	75/77 (97%)	66 (88%)	8 (11%)	1 (1%)	12	42
74	o8	75/77 (97%)	60 (80%)	11 (15%)	4 (5%)	2	12
75	O9	48/50 (96%)	40 (83%)	8 (17%)	0	100	100
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	7	30
76	Q0	50/52 (96%)	44 (88%)	4 (8%)	2 (4%)	3	17
76	q0	50/52 (96%)	45 (90%)	3 (6%)	2 (4%)	3	17
77	Q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	16
77	q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
78	Q2	103/105 (98%)	77 (75%)	18 (18%)	8 (8%)	1	5
78	q2	103/105 (98%)	93 (90%)	9 (9%)	1 (1%)	15	49
79	Q3	89/91 (98%)	76 (85%)	11 (12%)	2 (2%)	6	29
79	q3	89/91 (98%)	81 (91%)	6 (7%)	2 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	e0	60/62 (97%)	44 (73%)	9 (15%)	7 (12%)	0	1
81	p0	139/311 (45%)	114 (82%)	20 (14%)	5 (4%)	3	20
All	All	22333/24143 (92%)	18335 (82%)	2722 (12%)	1276 (6%)	1	10

All (1276) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	49	ASN
2	S0	66	ALA
2	S0	95	ALA
2	S0	139	VAL
2	S0	158	VAL
2	S0	187	ALA
2	S0	191	ARG
2	S0	192	THR
3	S1	37	THR
3	S1	49	ASN
3	S1	51	SER
3	S1	58	SER
3	S1	63	GLY
3	S1	79	HIS
3	S1	113	MET
3	S1	117	TRP
3	S1	148	ASN
3	S1	177	GLN
3	S1	206	PRO
3	S1	221	PRO
3	S1	223	PHE
4	S2	72	LEU
5	S3	62	ASN
5	S3	65	ARG
5	S3	93	ASP
5	S3	211	PRO
5	S3	220	PRO
6	S4	26	CYS
6	S4	104	ASP
6	S4	223	ASN
6	S4	242	LYS
7	S5	26	ALA

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Mol	Chain	Res	Type
7	S5	35	GLN
7	S5	39	GLU
7	S5	58	LEU
7	S5	153	GLY
8	S6	122	GLU
8	S6	149	LYS
8	S6	154	ARG
8	S6	173	PRO
8	S6	174	LYS
9	S7	5	GLN
9	S7	64	VAL
9	S7	111	LYS
9	S7	112	ARG
9	S7	116	ARG
9	S7	131	PHE
9	S7	134	GLU
10	S8	59	ARG
11	S9	121	SER
11	S9	134	ILE
12	C0	54	TYR
12	C0	60	SER
12	C0	81	ASN
12	C0	87	VAL
12	C0	88	PRO
13	C1	7	VAL
13	C1	96	LYS
14	C2	126	TRP
14	C2	127	GLY
15	C3	57	ALA
15	C3	138	ASN
16	C4	50	ALA
16	C4	92	LYS
16	C4	124	ASP
16	C4	125	SER
16	C4	126	THR
17	C5	39	ALA
17	C5	54	ALA
17	C5	125	PRO
17	C5	126	VAL
18	C6	41	PRO
18	C6	58	ASP
18	C6	114	ARG

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Mol	Chain	Res	Type
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	124	VAL
20	C8	14	ILE
20	C8	61	LEU
20	C8	82	PRO
20	C8	92	ILE
21	C9	53	TRP
22	D0	118	VAL
25	D3	70	LYS
25	D3	114	LYS
25	D3	131	SER
26	D4	33	ALA
27	D5	39	ALA
27	D5	44	GLN
27	D5	54	VAL
27	D5	97	LYS
28	D6	45	VAL
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
29	D7	38	PRO
29	D7	62	ILE
32	E0	47	VAL
33	E1	102	VAL
33	E1	103	LEU
33	E1	106	TYR
33	E1	127	GLY
33	E1	138	ARG
34	SR	98	GLU
35	SM	17	VAL
35	SM	18	VAL
35	SM	87	THR
35	SM	100	THR
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
39	L2	17	THR
39	L2	20	THR
39	L2	24	GLN

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Mol	Chain	Res	Type
39	L2	130	SER
39	L2	144	ASN
40	L3	3	HIS
40	L3	4	ARG
40	L3	5	LYS
40	L3	136	LYS
40	L3	140	ASP
40	L3	142	ALA
40	L3	187	SER
40	L3	188	ILE
41	L4	15	ALA
41	L4	130	ALA
41	L4	131	VAL
41	L4	146	PRO
41	L4	230	VAL
41	L4	270	SER
41	L4	311	HIS
41	L4	317	PRO
41	L4	318	LEU
41	L4	338	LYS
42	L5	7	ALA
42	L5	58	LYS
42	L5	178	ASN
42	L5	233	ALA
42	L5	234	ASP
42	L5	295	GLY
43	L6	6	ALA
43	L6	97	ASN
43	L6	98	VAL
44	L7	24	GLU
44	L7	26	VAL
45	L8	25	PRO
45	L8	36	ILE
47	M0	189	GLU
48	M1	8	PRO
48	M1	9	MET
48	M1	11	ASP
48	M1	12	LEU
48	M1	24	GLY
48	M1	74	PRO
48	M1	115	LYS
48	M1	151	SER

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Mol	Chain	Res	Type
48	M1	165	GLN
48	M1	173	ASP
49	M3	47	ALA
49	M3	50	PRO
49	M3	76	THR
49	M3	129	ASN
50	M4	8	LYS
50	M4	9	ALA
50	M4	10	SER
51	M5	74	PRO
51	M5	94	TYR
52	M6	111	PRO
53	M7	157	VAL
53	M7	182	ILE
54	M8	24	VAL
54	M8	99	THR
57	N1	124	VAL
57	N1	159	PHE
58	N2	51	GLY
60	N4	26	SER
60	N4	64	THR
60	N4	81	PRO
63	N7	7	ALA
63	N7	35	SER
63	N7	128	GLN
64	N8	29	PRO
64	N8	30	GLY
64	N8	66	ALA
66	O0	46	ALA
67	O1	6	ASP
67	O1	83	GLU
67	O1	84	ASP
71	O5	119	LYS
72	O6	33	ALA
72	O6	50	LEU
72	O6	64	SER
73	O7	12	HIS
73	O7	68	LYS
74	O8	33	LYS
76	Q0	78	ILE
77	Q1	23	ARG
78	Q2	15	LYS

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Mol	Chain	Res	Type
78	Q2	60	LYS
78	Q2	78	LYS
78	Q2	100	LYS
2	s0	4	PRO
2	s0	44	GLY
2	s0	95	ALA
2	s0	111	ILE
2	s0	158	VAL
2	s0	185	ARG
2	s0	186	GLY
2	s0	189	VAL
2	s0	203	PHE
2	s0	206	ASP
3	s1	82	ARG
3	s1	223	PHE
4	s2	92	ALA
4	s2	107	SER
4	s2	163	GLY
5	s3	59	LEU
5	s3	61	GLU
5	s3	90	ARG
5	s3	144	ALA
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
5	s3	221	SER
6	s4	24	SER
6	s4	104	ASP
6	s4	163	ASP
6	s4	196	VAL
7	s5	28	PRO
7	s5	29	ILE
7	s5	184	PHE
8	s6	25	ARG
8	s6	153	VAL
8	s6	154	ARG
8	s6	173	PRO
9	s7	30	SER
9	s7	64	VAL
9	s7	66	SER
9	s7	67	LEU
9	s7	74	GLN

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Mol	Chain	Res	Type
9	s7	131	PHE
9	s7	185	ILE
10	s8	101	ILE
11	s9	65	LYS
11	s9	91	LYS
11	s9	146	PHE
11	s9	147	MET
12	c0	2	LEU
12	c0	83	PRO
12	c0	88	PRO
12	c0	92	ILE
12	c0	97	PRO
13	c1	114	ALA
14	c2	22	VAL
14	c2	89	ILE
14	c2	109	GLU
14	c2	131	ASP
15	c3	66	ILE
15	c3	87	ASP
15	c3	137	PRO
16	c4	35	GLY
16	c4	50	ALA
16	c4	51	ASP
16	c4	76	ILE
17	c5	11	VAL
17	c5	51	SER
17	c5	71	GLU
17	c5	125	PRO
17	c5	126	VAL
17	c5	127	ARG
18	c6	42	GLU
18	c6	116	LEU
19	c7	88	VAL
19	c7	99	VAL
19	c7	103	ASP
19	c7	118	PRO
20	c8	91	ASP
20	c8	92	ILE
20	c8	145	ARG
21	c9	33	TYR
22	d0	49	ASN
22	d0	51	VAL

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Mol	Chain	Res	Type
22	d0	52	LYS
23	d1	4	ASP
26	d4	30	PRO
26	d4	33	ALA
26	d4	35	VAL
26	d4	49	LYS
27	d5	85	LYS
28	d6	82	ARG
29	d7	20	LYS
29	d7	57	GLU
29	d7	62	ILE
30	d8	32	PHE
30	d8	59	SER
30	d8	61	ARG
31	d9	6	VAL
80	e0	60	PRO
33	e1	79	LYS
33	e1	83	LYS
33	e1	84	VAL
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	102	VAL
33	e1	103	LEU
33	e1	106	TYR
34	sR	4	ASN
34	sR	163	ASP
34	sR	165	ASP
34	sR	250	TYR
35	sM	42	ALA
35	sM	50	ASN
35	sM	158	GLN
35	sM	172	VAL
39	l2	104	LEU
39	l2	194	ASN
40	l3	347	SER
41	l4	14	GLU
41	l4	90	PHE
41	l4	301	PRO
41	l4	304	GLN
41	l4	329	PRO
41	l4	349	THR

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Mol	Chain	Res	Type
41	l4	361	HIS
42	l5	116	ASP
42	l5	258	LYS
43	l6	98	VAL
45	l8	25	PRO
45	l8	26	LEU
45	l8	34	PHE
45	l8	36	ILE
45	l8	240	ASN
46	l9	62	ARG
47	m0	25	ALA
47	m0	194	GLY
47	m0	204	GLY
48	m1	8	PRO
48	m1	10	ARG
48	m1	39	GLN
48	m1	108	GLU
49	m3	47	ALA
49	m3	76	THR
49	m3	134	GLU
49	m3	141	ALA
51	m5	76	PRO
52	m6	110	PRO
55	m9	156	ASN
57	n1	135	PRO
57	n1	136	ARG
58	n2	50	LEU
59	n3	42	SER
60	n4	63	ILE
60	n4	76	VAL
60	n4	133	THR
61	n5	44	PRO
62	n6	77	LYS
62	n6	83	ASP
62	n6	84	LYS
62	n6	85	VAL
62	n6	92	GLY
62	n6	126	LEU
63	n7	36	HIS
63	n7	105	SER
63	n7	129	TRP
64	n8	47	LYS

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Mol	Chain	Res	Type
64	n8	76	ASP
65	n9	21	ILE
65	n9	23	LYS
65	n9	39	PHE
67	o1	64	VAL
67	o1	84	ASP
68	o2	4	LEU
68	o2	5	PRO
69	o3	90	PRO
71	o5	82	ALA
71	o5	119	LYS
72	o6	33	ALA
72	o6	63	ASN
72	o6	64	SER
72	o6	98	ARG
74	o8	18	ALA
81	p0	93	LEU
2	S0	140	ASN
2	S0	164	ASN
3	S1	36	SER
3	S1	60	ALA
3	S1	62	LYS
3	S1	93	GLY
3	S1	130	SER
3	S1	147	ALA
3	S1	202	LYS
4	S2	75	GLY
4	S2	79	GLU
4	S2	107	SER
4	S2	148	LEU
5	S3	216	PRO
6	S4	195	ILE
6	S4	245	LYS
7	S5	43	PHE
7	S5	51	VAL
7	S5	64	VAL
7	S5	81	ARG
7	S5	101	GLY
7	S5	150	GLY
8	S6	148	SER
8	S6	165	GLY
9	S7	32	PRO

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Mol	Chain	Res	Type
9	S7	73	VAL
9	S7	110	GLN
9	S7	133	THR
9	S7	155	ASP
10	S8	22	ARG
10	S8	50	GLY
10	S8	52	ASN
10	S8	149	SER
10	S8	186	GLY
11	S9	93	LEU
11	S9	117	GLY
11	S9	168	ARG
12	C0	64	TYR
13	C1	4	GLU
13	C1	29	LYS
13	C1	55	ASP
13	C1	95	PRO
13	C1	146	ALA
14	C2	82	PRO
14	C2	89	ILE
14	C2	91	VAL
14	C2	93	ASP
14	C2	130	THR
15	C3	22	ALA
15	C3	68	GLY
15	C3	106	ARG
16	C4	39	ILE
16	C4	42	VAL
16	C4	51	ASP
17	C5	51	SER
17	C5	60	LEU
18	C6	32	ASN
18	C6	97	VAL
18	C6	113	ASP
19	C7	84	TYR
20	C8	83	ALA
20	C8	144	ARG
21	C9	69	LYS
22	D0	49	ASN
23	D1	6	GLY
23	D1	12	TYR
25	D3	4	GLY

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Mol	Chain	Res	Type
25	D3	11	SER
25	D3	128	SER
26	D4	6	THR
26	D4	34	ASN
26	D4	36	SER
27	D5	43	ASP
28	D6	18	VAL
28	D6	36	ILE
28	D6	46	GLU
28	D6	75	VAL
29	D7	63	LEU
30	D8	36	THR
32	E0	51	ASN
33	E1	83	LYS
33	E1	84	VAL
33	E1	85	TYR
33	E1	98	VAL
34	SR	51	ASP
35	SM	42	ALA
35	SM	52	PRO
35	SM	139	GLU
35	SM	152	GLN
35	SM	172	VAL
35	SM	173	GLU
39	L2	234	LYS
40	L3	379	PHE
40	L3	385	LYS
41	L4	4	PRO
41	L4	190	GLY
41	L4	232	SER
41	L4	304	GLN
42	L5	59	ASP
42	L5	260	PHE
43	L6	100	LYS
44	L7	160	ARG
45	L8	39	ALA
45	L8	156	ASP
47	M0	117	GLY
47	M0	187	ALA
47	M0	194	GLY
48	M1	94	ARG
48	M1	167	TYR

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Mol	Chain	Res	Type
49	M3	141	ALA
50	M4	36	VAL
51	M5	75	VAL
51	M5	184	LYS
52	M6	110	PRO
56	N0	2	ALA
58	N2	11	ILE
58	N2	31	ALA
58	N2	50	LEU
58	N2	52	ASN
62	N6	52	ARG
62	N6	53	ASP
62	N6	84	LYS
63	N7	17	ARG
63	N7	102	GLU
64	N8	76	ASP
66	O0	100	ILE
70	O4	77	GLY
72	O6	28	TYR
72	O6	34	SER
72	O6	49	GLY
78	Q2	94	GLY
2	s0	30	GLN
2	s0	103	THR
3	s1	26	ARG
3	s1	81	PHE
3	s1	177	GLN
3	s1	194	ASN
4	s2	199	GLN
4	s2	238	SER
5	s3	160	SER
5	s3	179	GLN
6	s4	12	LEU
6	s4	95	THR
6	s4	164	LEU
6	s4	168	LYS
6	s4	195	ILE
6	s4	242	LYS
7	s5	35	GLN
7	s5	36	ALA
7	s5	43	PHE
7	s5	56	ALA

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Mol	Chain	Res	Type
7	s5	100	ASN
7	s5	151	GLY
7	s5	204	GLY
8	s6	174	LYS
9	s7	144	VAL
10	s8	62	THR
10	s8	94	ASN
10	s8	100	ALA
10	s8	148	ALA
11	s9	58	ASP
11	s9	134	ILE
11	s9	169	PRO
12	c0	23	ALA
12	c0	31	LYS
12	c0	32	HIS
13	c1	7	VAL
13	c1	55	ASP
13	c1	61	THR
13	c1	144	ALA
14	c2	26	ASP
14	c2	101	ALA
14	c2	119	SER
15	c3	19	SER
15	c3	60	VAL
16	c4	74	VAL
17	c5	9	LYS
17	c5	52	LYS
17	c5	131	ALA
18	c6	57	LEU
18	c6	113	ASP
20	c8	29	VAL
20	c8	60	GLU
20	c8	61	LEU
21	c9	28	LEU
21	c9	29	GLU
22	d0	15	GLN
22	d0	97	VAL
22	d0	118	VAL
24	d2	31	SER
25	d3	61	SER
25	d3	119	GLY
26	d4	42	GLU

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Mol	Chain	Res	Type
27	d5	103	ARG
28	d6	8	ASN
28	d6	13	LYS
29	d7	3	LEU
29	d7	38	PRO
29	d7	59	CYS
29	d7	60	SER
29	d7	75	GLU
31	d9	5	ASN
31	d9	7	TRP
80	e0	9	ALA
80	e0	47	VAL
33	e1	111	GLU
33	e1	124	PRO
33	e1	127	GLY
34	sR	149	ASP
34	sR	186	PHE
34	sR	218	GLY
34	sR	318	ALA
35	sM	47	ALA
35	sM	65	THR
35	sM	159	ALA
35	sM	167	PRO
39	l2	24	GLN
39	l2	142	ASP
39	l2	213	GLY
40	l3	143	GLY
40	l3	187	SER
41	l4	233	LEU
41	l4	302	ALA
41	l4	330	TYR
42	l5	85	ARG
42	l5	178	ASN
44	l7	191	VAL
45	l8	121	SER
45	l8	122	LYS
45	l8	133	LYS
46	l9	108	GLY
46	l9	144	ILE
47	m0	187	ALA
47	m0	196	PHE
47	m0	207	GLU

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Mol	Chain	Res	Type
48	m1	94	ARG
48	m1	115	LYS
49	m3	93	ILE
49	m3	135	ALA
49	m3	150	PRO
51	m5	183	THR
51	m5	184	LYS
52	m6	16	VAL
53	m7	67	ILE
53	m7	72	GLN
54	m8	91	ALA
55	m9	35	ALA
55	m9	155	LEU
56	n0	2	ALA
57	n1	16	GLN
57	n1	122	GLN
60	n4	71	ARG
60	n4	77	LYS
60	n4	83	THR
61	n5	25	LYS
61	n5	45	LYS
63	n7	130	PHE
64	n8	129	PHE
66	o0	99	ASP
68	o2	6	HIS
68	o2	110	ALA
68	o2	124	GLY
69	o3	88	ASN
69	o3	92	LYS
72	o6	4	LYS
74	o8	17	ARG
76	q0	101	ALA
81	p0	33	VAL
81	p0	198	PRO
2	S0	27	ARG
2	S0	65	ALA
2	S0	163	ASN
3	S1	26	ARG
3	S1	54	LEU
3	S1	78	ASP
3	S1	81	PHE
3	S1	82	ARG

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Mol	Chain	Res	Type
3	S1	112	SER
3	S1	114	VAL
3	S1	116	LYS
3	S1	179	SER
3	S1	207	LEU
3	S1	213	ARG
4	S2	91	ARG
4	S2	108	ASN
4	S2	146	THR
4	S2	236	PRO
5	S3	59	LEU
5	S3	81	PRO
5	S3	218	LEU
6	S4	3	ARG
6	S4	12	LEU
7	S5	63	GLN
7	S5	127	GLN
8	S6	25	ARG
8	S6	146	GLY
8	S6	152	ASP
9	S7	85	PHE
10	S8	120	THR
10	S8	153	GLU
11	S9	169	PRO
13	C1	145	ALA
14	C2	22	VAL
14	C2	106	ILE
14	C2	107	ASP
14	C2	108	ARG
14	C2	112	ALA
14	C2	128	ALA
15	C3	3	ARG
15	C3	27	LYS
17	C5	52	LYS
17	C5	130	ARG
18	C6	40	GLU
18	C6	138	PHE
20	C8	8	GLN
21	C9	31	PRO
21	C9	39	THR
22	D0	17	GLN
23	D1	10	GLU

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Mol	Chain	Res	Type
24	D2	79	PHE
24	D2	83	ILE
26	D4	4	ALA
26	D4	5	VAL
26	D4	54	ALA
27	D5	41	ILE
27	D5	42	LEU
27	D5	55	PRO
28	D6	63	ALA
29	D7	51	GLN
33	E1	128	ALA
33	E1	137	ASP
34	SR	15	GLY
34	SR	318	ALA
35	SM	97	THR
35	SM	101	ASP
35	SM	153	ASP
35	SM	174	LEU
39	L2	125	ALA
39	L2	127	ALA
39	L2	180	LEU
40	L3	378	ALA
41	L4	14	GLU
41	L4	268	ALA
41	L4	291	ASN
42	L5	15	ARG
42	L5	137	ASP
42	L5	258	LYS
42	L5	276	LYS
45	L8	37	GLY
45	L8	254	ASP
46	L9	50	ASN
46	L9	190	ASP
47	M0	211	ARG
48	M1	28	ASP
48	M1	64	LYS
48	M1	172	LEU
51	M5	81	TYR
51	M5	187	ARG
52	M6	182	ASN
54	M8	41	ASP
57	N1	18	ASP

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Mol	Chain	Res	Type
57	N1	123	GLY
58	N2	49	ASN
59	N3	46	LEU
59	N3	134	GLY
60	N4	97	LYS
62	N6	126	LEU
63	N7	18	TYR
64	N8	96	LYS
64	N8	97	GLU
66	O0	20	SER
67	O1	7	VAL
71	O5	97	ALA
72	O6	3	VAL
78	Q2	17	CYS
78	Q2	30	ALA
78	Q2	34	SER
2	s0	10	THR
2	s0	109	ASN
2	s0	114	SER
2	s0	183	ARG
3	s1	147	ALA
3	s1	206	PRO
4	s2	91	ARG
4	s2	182	PRO
5	s3	44	THR
5	s3	45	LYS
5	s3	93	ASP
5	s3	211	PRO
6	s4	38	LEU
8	s6	68	LEU
8	s6	149	LYS
8	s6	165	GLY
9	s7	10	SER
9	s7	34	LEU
9	s7	145	GLY
10	s8	147	ALA
12	c0	30	ALA
12	c0	94	GLU
14	c2	87	PRO
14	c2	90	LYS
14	c2	92	ALA
14	c2	118	ALA

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Mol	Chain	Res	Type
15	c3	18	TYR
15	c3	22	ALA
16	c4	90	ARG
17	c5	14	THR
17	c5	17	TYR
18	c6	13	LYS
18	c6	115	THR
19	c7	117	LEU
20	c8	14	ILE
20	c8	77	THR
22	d0	17	GLN
22	d0	96	PRO
23	d1	44	ARG
24	d2	6	VAL
24	d2	32	LYS
25	d3	27	ASN
25	d3	46	SER
26	d4	11	LYS
29	d7	53	ALA
30	d8	33	LEU
30	d8	64	ARG
80	e0	61	SER
33	e1	131	PHE
34	sR	141	LEU
35	sM	63	ASP
35	sM	83	LYS
39	l2	80	GLU
39	l2	130	SER
40	l3	385	LYS
40	l3	386	ASP
41	l4	132	ALA
41	l4	146	PRO
41	l4	272	VAL
41	l4	338	LYS
42	l5	215	ASP
42	l5	260	PHE
42	l5	279	LYS
43	l6	97	ASN
45	l8	203	VAL
46	l9	2	LYS
46	l9	38	LEU
46	l9	107	ASP

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Mol	Chain	Res	Type
47	m0	53	VAL
48	m1	114	ILE
48	m1	153	LYS
48	m1	167	TYR
49	m3	60	ALA
49	m3	130	GLY
50	m4	135	LEU
50	m4	136	ALA
51	m5	181	ASN
54	m8	41	ASP
54	m8	84	VAL
54	m8	99	THR
54	m8	171	LYS
61	n5	24	LEU
61	n5	38	LEU
61	n5	46	TYR
61	n5	47	ALA
61	n5	55	ASN
63	n7	134	LEU
64	n8	48	TYR
66	o0	98	SER
67	o1	47	ASP
67	o1	83	GLU
69	o3	59	VAL
73	o7	86	ALA
74	o8	49	SER
76	q0	78	ILE
79	q3	51	ALA
81	p0	102	SER
2	S0	5	ALA
2	S0	64	ILE
2	S0	195	TRP
3	S1	61	LEU
4	S2	150	GLN
4	S2	248	SER
5	S3	55	THR
5	S3	143	ARG
5	S3	217	ILE
6	S4	77	ARG
7	S5	21	THR
7	S5	65	ARG
9	S7	98	ILE

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Mol	Chain	Res	Type
10	S8	10	LYS
10	S8	152	ILE
11	S9	16	LYS
11	S9	98	ALA
11	S9	171	ARG
12	C0	35	ILE
13	C1	30	ARG
14	C2	21	GLU
14	C2	66	VAL
14	C2	119	SER
15	C3	13	SER
15	C3	31	GLU
16	C4	75	GLY
17	C5	29	SER
17	C5	69	GLU
18	C6	59	LYS
18	C6	142	TYR
19	C7	81	LYS
20	C8	7	GLU
20	C8	84	TRP
20	C8	91	ASP
21	C9	130	ARG
23	D1	2	GLU
23	D1	4	ASP
23	D1	11	LEU
23	D1	44	ARG
24	D2	57	ARG
25	D3	41	SER
25	D3	112	LYS
28	D6	59	TYR
28	D6	64	LEU
30	D8	51	ASN
33	E1	90	LYS
33	E1	111	GLU
33	E1	118	ARG
34	SR	226	ALA
35	SM	12	VAL
35	SM	15	ALA
35	SM	53	ARG
35	SM	72	ARG
35	SM	86	ASN
35	SM	154	TYR

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Mol	Chain	Res	Type
39	L2	251	LYS
40	L3	138	ALA
41	L4	140	HIS
41	L4	271	LYS
42	L5	6	ASP
42	L5	253	PHE
43	L6	36	PRO
43	L6	81	ALA
44	L7	25	GLN
44	L7	164	SER
45	L8	100	GLU
46	L9	96	HIS
48	M1	108	GLU
48	M1	114	ILE
48	M1	117	ASP
49	M3	176	GLU
50	M4	29	ALA
50	M4	71	ALA
50	M4	136	ALA
53	M7	108	ASP
53	M7	162	GLU
54	M8	4	ASP
54	M8	162	ALA
55	M9	5	ARG
63	N7	36	HIS
63	N7	103	GLN
64	N8	47	LYS
64	N8	78	LEU
64	N8	117	ARG
65	N9	25	LYS
68	O2	12	LYS
72	O6	21	THR
72	O6	78	GLY
73	O7	84	SER
76	Q0	79	GLU
79	Q3	75	ALA
79	Q3	76	ALA
3	s1	93	GLY
3	s1	106	THR
3	s1	224	ASP
3	s1	230	ALA
4	s2	106	ASP

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Mol	Chain	Res	Type
4	s2	150	GLN
4	s2	196	VAL
4	s2	235	LEU
6	s4	90	ILE
6	s4	166	SER
7	s5	98	MET
7	s5	223	SER
8	s6	70	PRO
10	s8	136	SER
10	s8	199	LYS
12	c0	35	ILE
12	c0	49	LEU
12	c0	82	LEU
12	c0	96	ASN
14	c2	58	LEU
14	c2	103	LEU
14	c2	106	ILE
14	c2	111	ASN
14	c2	127	GLY
16	c4	12	GLN
17	c5	7	ALA
17	c5	130	ARG
17	c5	132	GLY
18	c6	142	TYR
19	c7	67	ARG
19	c7	68	GLY
19	c7	98	GLY
19	c7	116	LYS
20	c8	4	VAL
21	c9	118	PRO
23	d1	6	GLY
23	d1	10	GLU
24	d2	68	ARG
25	d3	66	SER
25	d3	138	GLU
26	d4	68	LYS
26	d4	91	LEU
28	d6	59	TYR
31	d9	17	GLY
33	e1	86	THR
33	e1	105	TYR
33	e1	128	ALA

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Mol	Chain	Res	Type
33	e1	136	LYS
34	sR	281	TYR
35	sM	43	ASP
39	l2	56	ALA
39	l2	69	TYR
39	l2	180	LEU
39	l2	215	ASN
39	l2	249	SER
40	l3	40	PRO
40	l3	142	ALA
41	l4	339	LEU
42	l5	153	THR
44	l7	27	ALA
44	l7	158	LYS
45	l8	54	GLU
45	l8	77	GLN
45	l8	237	ILE
47	m0	145	LYS
47	m0	176	LEU
47	m0	220	GLN
48	m1	95	ASN
48	m1	168	ASP
51	m5	102	ALA
51	m5	187	ARG
52	m6	89	SER
54	m8	42	ALA
54	m8	113	LYS
54	m8	155	MET
56	n0	142	GLN
58	n2	23	THR
60	n4	72	SER
63	n7	5	LEU
67	o1	86	LYS
79	q3	4	ARG
2	S0	103	THR
2	S0	126	PRO
2	S0	189	VAL
3	S1	38	PHE
3	S1	158	SER
3	S1	176	VAL
4	S2	92	ALA
5	S3	212	LYS

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Mol	Chain	Res	Type
7	S5	54	LYS
8	S6	69	LEU
9	S7	74	GLN
14	C2	81	ASP
14	C2	87	PRO
14	C2	115	VAL
16	C4	18	ARG
16	C4	114	ARG
17	C5	101	ALA
20	C8	6	GLN
22	D0	59	PRO
22	D0	117	VAL
25	D3	96	VAL
25	D3	109	ARG
28	D6	62	TYR
30	D8	35	ASP
32	E0	60	PRO
33	E1	87	THR
34	SR	163	ASP
35	SM	63	ASP
35	SM	68	ARG
35	SM	88	ARG
39	L2	47	GLN
39	L2	229	ALA
40	L3	141	GLY
41	L4	82	THR
41	L4	233	LEU
42	L5	188	GLU
42	L5	252	ALA
42	L5	259	LYS
43	L6	5	LYS
45	L8	157	VAL
46	L9	42	ASP
47	M0	16	PRO
48	M1	34	SER
48	M1	78	GLU
48	M1	95	ASN
49	M3	136	GLU
52	M6	11	GLY
53	M7	75	GLU
53	M7	109	ALA
53	M7	160	ALA

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Mol	Chain	Res	Type
53	M7	169	THR
55	M9	53	LYS
55	M9	130	ASN
59	N3	16	GLY
60	N4	80	ARG
60	N4	86	SER
63	N7	16	GLY
63	N7	33	SER
64	N8	24	LYS
67	O1	5	LYS
69	O3	59	VAL
71	O5	75	TYR
73	O7	78	PHE
2	s0	139	VAL
4	s2	234	PRO
5	s3	43	PRO
5	s3	113	LEU
5	s3	161	GLY
5	s3	219	ALA
6	s4	3	ARG
6	s4	30	ARG
6	s4	245	LYS
9	s7	11	GLN
9	s7	133	THR
9	s7	186	PRO
10	s8	78	ILE
11	s9	167	ALA
12	c0	3	MET
14	c2	21	GLU
14	c2	63	VAL
15	c3	29	SER
16	c4	37	GLU
17	c5	6	ASN
18	c6	97	VAL
21	c9	119	LYS
26	d4	58	PHE
26	d4	77	ASN
26	d4	104	SER
28	d6	35	ALA
80	e0	51	ASN
80	e0	54	ARG
33	e1	97	LYS

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Mol	Chain	Res	Type
33	e1	148	TYR
34	sR	160	GLU
40	l3	221	THR
41	l4	311	HIS
41	l4	328	ASN
41	l4	342	LYS
43	l6	10	TYR
44	l7	228	SER
47	m0	47	PRO
51	m5	55	ALA
51	m5	170	LYS
52	m6	65	ASN
55	m9	154	ALA
60	n4	103	ALA
62	n6	125	LYS
63	n7	6	LYS
63	n7	17	ARG
63	n7	28	PRO
64	n8	56	VAL
67	o1	45	GLY
72	o6	34	SER
73	o7	85	LYS
75	o9	3	ALA
3	S1	23	PRO
3	S1	210	ILE
4	S2	39	THR
4	S2	62	PRO
5	S3	26	THR
5	S3	76	ARG
7	S5	45	LYS
9	S7	31	SER
9	S7	132	PRO
15	C3	28	LEU
15	C3	137	PRO
16	C4	40	ALA
18	C6	33	GLY
19	C7	87	GLU
20	C8	5	VAL
26	D4	95	GLY
27	D5	38	HIS
32	E0	50	VAL
34	SR	105	GLY

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Mol	Chain	Res	Type
35	SM	102	THR
40	L3	155	ALA
40	L3	317	ILE
44	L7	178	ILE
53	M7	84	PRO
64	N8	27	LYS
67	O1	82	GLU
71	O5	37	SER
72	O6	77	LEU
2	s0	85	ALA
3	s1	207	LEU
3	s1	233	GLY
7	s5	45	LYS
7	s5	55	ASP
12	c0	95	ARG
14	c2	107	ASP
14	c2	115	VAL
15	c3	78	ASN
21	c9	11	ALA
25	d3	101	GLU
26	d4	51	GLU
27	d5	44	GLN
27	d5	104	ALA
28	d6	63	ALA
31	d9	11	PRO
33	e1	81	LYS
39	l2	127	ALA
43	l6	107	ALA
44	l7	91	GLY
44	l7	178	ILE
45	l8	39	ALA
45	l8	69	LEU
46	l9	167	VAL
49	m3	101	ARG
50	m4	49	PRO
51	m5	81	TYR
61	n5	79	GLY
63	n7	16	GLY
63	n7	103	GLN
68	o2	122	PRO
70	o4	66	SER
78	q2	33	ALA

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Mol	Chain	Res	Type
27	D5	88	ILE
28	D6	9	GLY
50	M4	6	ILE
57	N1	36	VAL
58	N2	27	VAL
65	N9	21	ILE
6	s4	31	PRO
13	c1	113	PRO
13	c1	129	ARG
39	l2	172	GLY
48	m1	7	ASN
55	m9	15	VAL
58	n2	51	GLY
63	n7	104	PRO
6	S4	193	GLY
8	S6	9	VAL
16	C4	96	PRO
17	C5	68	PRO
20	C8	142	GLY
27	D5	71	ILE
39	L2	210	PRO
46	L9	98	PRO
3	s1	193	ILE
5	s3	115	ILE
13	c1	139	VAL
80	e0	45	VAL
40	l3	9	PRO
42	l5	125	VAL
68	o2	9	ILE
6	S4	111	VAL
11	S9	84	GLY
26	D4	35	VAL
28	D6	65	PRO
48	M1	23	VAL
48	M1	118	PRO
11	s9	162	SER
14	c2	40	GLY
19	c7	86	PRO
23	d1	77	GLY
53	m7	84	PRO
60	n4	98	PRO
63	n7	70	PRO

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Mol	Chain	Res	Type
81	p0	78	PRO
4	S2	74	PRO
21	C9	65	ILE
35	SM	20	LEU
42	L5	125	VAL
44	L7	91	GLY
63	N7	89	VAL
14	c2	66	VAL
15	c3	47	PRO
16	c4	88	GLY
21	c9	34	VAL
30	d8	20	GLY
44	l7	188	ILE
49	m3	133	PRO
67	o1	7	VAL
68	o2	68	PRO
74	o8	60	GLY
3	S1	35	PRO
22	D0	19	ILE
58	N2	60	GLY
9	s7	13	PRO
17	c5	117	GLY
70	o4	100	ILE
69	O3	104	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	134 (82%)	30 (18%)	1	7
2	s0	165/209 (79%)	135 (82%)	30 (18%)	1	7
3	S1	191/223 (86%)	156 (82%)	35 (18%)	1	7
3	s1	192/223 (86%)	154 (80%)	38 (20%)	1	5
4	S2	176/204 (86%)	132 (75%)	44 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	s2	176/204 (86%)	136 (77%)	40 (23%)	1	3
5	S3	182/194 (94%)	149 (82%)	33 (18%)	1	7
5	s3	182/194 (94%)	141 (78%)	41 (22%)	1	3
6	S4	221/221 (100%)	178 (80%)	43 (20%)	1	6
6	s4	221/221 (100%)	183 (83%)	38 (17%)	2	9
7	S5	173/190 (91%)	136 (79%)	37 (21%)	1	4
7	s5	173/190 (91%)	142 (82%)	31 (18%)	2	8
8	S6	188/201 (94%)	151 (80%)	37 (20%)	1	6
8	s6	187/201 (93%)	153 (82%)	34 (18%)	1	7
9	S7	165/169 (98%)	138 (84%)	27 (16%)	2	10
9	s7	165/169 (98%)	130 (79%)	35 (21%)	1	5
10	S8	150/161 (93%)	126 (84%)	24 (16%)	2	11
10	s8	150/161 (93%)	129 (86%)	21 (14%)	3	15
11	S9	158/165 (96%)	124 (78%)	34 (22%)	1	4
11	s9	158/165 (96%)	121 (77%)	37 (23%)	1	3
12	C0	77/98 (79%)	61 (79%)	16 (21%)	1	5
12	c0	73/98 (74%)	60 (82%)	13 (18%)	2	8
13	C1	129/136 (95%)	108 (84%)	21 (16%)	2	10
13	c1	129/136 (95%)	102 (79%)	27 (21%)	1	5
14	C2	88/118 (75%)	63 (72%)	25 (28%)	0	1
14	c2	88/118 (75%)	59 (67%)	29 (33%)	0	0
15	C3	127/127 (100%)	102 (80%)	25 (20%)	1	6
15	c3	127/127 (100%)	104 (82%)	23 (18%)	1	7
16	C4	81/104 (78%)	57 (70%)	24 (30%)	0	1
16	c4	97/104 (93%)	78 (80%)	19 (20%)	1	6
17	C5	101/117 (86%)	81 (80%)	20 (20%)	1	5
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	8
18	C6	117/118 (99%)	94 (80%)	23 (20%)	1	6
18	c6	118/118 (100%)	94 (80%)	24 (20%)	1	5
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	5
19	c7	92/124 (74%)	77 (84%)	15 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	C8	128/128 (100%)	96 (75%)	32 (25%)	0	2
20	c8	128/128 (100%)	99 (77%)	29 (23%)	1	3
21	C9	115/115 (100%)	91 (79%)	24 (21%)	1	5
21	c9	115/115 (100%)	94 (82%)	21 (18%)	1	7
22	D0	100/113 (88%)	76 (76%)	24 (24%)	0	2
22	d0	103/113 (91%)	78 (76%)	25 (24%)	0	2
23	D1	74/74 (100%)	54 (73%)	20 (27%)	0	1
23	d1	74/74 (100%)	52 (70%)	22 (30%)	0	1
24	D2	110/110 (100%)	89 (81%)	21 (19%)	1	6
24	d2	110/110 (100%)	94 (86%)	16 (14%)	3	13
25	D3	119/119 (100%)	91 (76%)	28 (24%)	1	3
25	d3	119/119 (100%)	103 (87%)	16 (13%)	4	16
26	D4	112/112 (100%)	102 (91%)	10 (9%)	9	34
26	d4	112/112 (100%)	98 (88%)	14 (12%)	4	18
27	D5	61/88 (69%)	51 (84%)	10 (16%)	2	10
27	d5	61/88 (69%)	51 (84%)	10 (16%)	2	10
28	D6	83/83 (100%)	62 (75%)	21 (25%)	0	1
28	d6	83/83 (100%)	71 (86%)	12 (14%)	3	13
29	D7	70/70 (100%)	56 (80%)	14 (20%)	1	5
29	d7	70/70 (100%)	52 (74%)	18 (26%)	0	1
30	D8	56/59 (95%)	46 (82%)	10 (18%)	2	8
30	d8	56/59 (95%)	43 (77%)	13 (23%)	1	3
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	9
31	d9	47/48 (98%)	40 (85%)	7 (15%)	3	13
32	E0	51/51 (100%)	39 (76%)	12 (24%)	1	3
33	E1	62/66 (94%)	42 (68%)	20 (32%)	0	0
33	e1	66/66 (100%)	47 (71%)	19 (29%)	0	1
34	SR	260/261 (100%)	219 (84%)	41 (16%)	2	11
34	sR	260/261 (100%)	231 (89%)	29 (11%)	6	24
35	SM	97/228 (42%)	78 (80%)	19 (20%)	1	6
35	sM	54/228 (24%)	44 (82%)	10 (18%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	L2	193/195 (99%)	156 (81%)	37 (19%)	1	6
39	l2	192/195 (98%)	145 (76%)	47 (24%)	0	2
40	L3	320/322 (99%)	250 (78%)	70 (22%)	1	4
40	l3	319/322 (99%)	248 (78%)	71 (22%)	1	3
41	L4	288/288 (100%)	224 (78%)	64 (22%)	1	4
41	l4	288/288 (100%)	231 (80%)	57 (20%)	1	5
42	L5	244/244 (100%)	197 (81%)	47 (19%)	1	6
42	l5	243/244 (100%)	191 (79%)	52 (21%)	1	4
43	L6	134/152 (88%)	106 (79%)	28 (21%)	1	5
43	l6	135/152 (89%)	113 (84%)	22 (16%)	2	10
44	L7	186/204 (91%)	162 (87%)	24 (13%)	4	18
44	l7	187/204 (92%)	161 (86%)	26 (14%)	3	15
45	L8	187/207 (90%)	152 (81%)	35 (19%)	1	7
45	l8	177/207 (86%)	148 (84%)	29 (16%)	2	10
46	L9	171/171 (100%)	132 (77%)	39 (23%)	1	3
46	l9	171/171 (100%)	134 (78%)	37 (22%)	1	4
47	M0	177/186 (95%)	139 (78%)	38 (22%)	1	4
47	m0	179/186 (96%)	144 (80%)	35 (20%)	1	6
48	M1	147/150 (98%)	119 (81%)	28 (19%)	1	6
48	m1	147/150 (98%)	112 (76%)	35 (24%)	0	2
49	M3	154/158 (98%)	127 (82%)	27 (18%)	2	8
49	m3	154/158 (98%)	123 (80%)	31 (20%)	1	5
50	M4	107/108 (99%)	89 (83%)	18 (17%)	2	9
50	m4	108/108 (100%)	91 (84%)	17 (16%)	2	11
51	M5	175/175 (100%)	146 (83%)	29 (17%)	2	9
51	m5	175/175 (100%)	139 (79%)	36 (21%)	1	5
52	M6	160/161 (99%)	142 (89%)	18 (11%)	6	23
52	m6	160/161 (99%)	131 (82%)	29 (18%)	1	7
53	M7	140/145 (97%)	115 (82%)	25 (18%)	2	8
53	m7	125/145 (86%)	106 (85%)	19 (15%)	3	12
54	M8	150/150 (100%)	119 (79%)	31 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	m8	150/150 (100%)	122 (81%)	28 (19%)	1	7
55	M9	153/153 (100%)	134 (88%)	19 (12%)	4	19
55	m9	153/153 (100%)	115 (75%)	38 (25%)	0	2
56	N0	156/156 (100%)	123 (79%)	33 (21%)	1	5
56	n0	156/156 (100%)	123 (79%)	33 (21%)	1	5
57	N1	136/136 (100%)	111 (82%)	25 (18%)	1	7
57	n1	136/136 (100%)	112 (82%)	24 (18%)	2	8
58	N2	87/106 (82%)	73 (84%)	14 (16%)	2	10
58	n2	85/106 (80%)	67 (79%)	18 (21%)	1	5
59	N3	104/104 (100%)	90 (86%)	14 (14%)	4	16
59	n3	104/104 (100%)	95 (91%)	9 (9%)	10	36
60	N4	57/129 (44%)	49 (86%)	8 (14%)	3	15
60	n4	100/129 (78%)	89 (89%)	11 (11%)	6	25
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	4
61	n5	104/117 (89%)	85 (82%)	19 (18%)	1	7
62	N6	109/109 (100%)	86 (79%)	23 (21%)	1	5
62	n6	109/109 (100%)	73 (67%)	36 (33%)	0	0
63	N7	115/115 (100%)	91 (79%)	24 (21%)	1	5
63	n7	115/115 (100%)	87 (76%)	28 (24%)	0	2
64	N8	118/118 (100%)	101 (86%)	17 (14%)	3	14
64	n8	118/118 (100%)	91 (77%)	27 (23%)	1	3
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1	6
65	n9	46/46 (100%)	34 (74%)	12 (26%)	0	1
66	O0	81/87 (93%)	65 (80%)	16 (20%)	1	5
66	o0	84/87 (97%)	65 (77%)	19 (23%)	1	3
67	O1	92/96 (96%)	71 (77%)	21 (23%)	1	3
67	o1	94/96 (98%)	67 (71%)	27 (29%)	0	1
68	O2	109/110 (99%)	91 (84%)	18 (16%)	2	10
68	o2	109/110 (99%)	88 (81%)	21 (19%)	1	6
69	O3	90/90 (100%)	82 (91%)	8 (9%)	9	34
69	o3	90/90 (100%)	71 (79%)	19 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	O4	95/102 (93%)	80 (84%)	15 (16%)	2	11
70	o4	95/102 (93%)	76 (80%)	19 (20%)	1	5
71	O5	104/104 (100%)	80 (77%)	24 (23%)	1	3
71	o5	103/104 (99%)	80 (78%)	23 (22%)	1	3
72	O6	81/81 (100%)	57 (70%)	24 (30%)	0	1
72	o6	80/81 (99%)	54 (68%)	26 (32%)	0	0
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	9
73	o7	70/70 (100%)	59 (84%)	11 (16%)	2	11
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0	1
74	o8	67/68 (98%)	48 (72%)	19 (28%)	0	1
75	O9	45/45 (100%)	39 (87%)	6 (13%)	4	16
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	8
76	Q0	47/47 (100%)	41 (87%)	6 (13%)	4	18
76	q0	47/47 (100%)	39 (83%)	8 (17%)	2	9
77	Q1	23/23 (100%)	16 (70%)	7 (30%)	0	0
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
78	Q2	90/90 (100%)	71 (79%)	19 (21%)	1	5
78	q2	90/90 (100%)	70 (78%)	20 (22%)	1	4
79	Q3	71/71 (100%)	61 (86%)	10 (14%)	3	15
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	5
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1	3
81	p0	105/253 (42%)	81 (77%)	24 (23%)	1	3
All	All	18727/20241 (92%)	15046 (80%)	3681 (20%)	1	6

All (3681) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	6	THR
2	S0	9	LEU
2	S0	30	GLN
2	S0	37	VAL
2	S0	49	ASN
2	S0	50	VAL
2	S0	78	SER

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Mol	Chain	Res	Type
2	S0	83	GLN
2	S0	84	ARG
2	S0	86	VAL
2	S0	87	LEU
2	S0	88	LYS
2	S0	101	ARG
2	S0	111	ILE
2	S0	117	GLU
2	S0	119	ARG
2	S0	131	GLN
2	S0	134	LYS
2	S0	140	ASN
2	S0	147	THR
2	S0	157	ASP
2	S0	164	ASN
2	S0	165	ARG
2	S0	172	LEU
2	S0	177	LEU
2	S0	184	LEU
2	S0	188	LEU
2	S0	196	SER
2	S0	200	ASP
2	S0	203	PHE
3	S1	21	VAL
3	S1	22	ASP
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	46	THR
3	S1	55	LYS
3	S1	61	LEU
3	S1	70	LEU
3	S1	76	SER
3	S1	77	GLU
3	S1	78	ASP
3	S1	81	PHE
3	S1	85	LYS
3	S1	96	LEU
3	S1	97	LEU
3	S1	105	PHE
3	S1	110	LEU
3	S1	111	ARG

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Mol	Chain	Res	Type
3	S1	140	ILE
3	S1	149	GLN
3	S1	154	SER
3	S1	166	LYS
3	S1	170	GLU
3	S1	180	THR
3	S1	181	LEU
3	S1	183	GLN
3	S1	184	LEU
3	S1	202	LYS
3	S1	211	HIS
3	S1	214	LYS
3	S1	215	VAL
3	S1	216	LYS
3	S1	218	LEU
3	S1	223	PHE
4	S2	41	LEU
4	S2	54	GLU
4	S2	58	LEU
4	S2	64	LYS
4	S2	69	ILE
4	S2	73	LEU
4	S2	76	LEU
4	S2	77	GLN
4	S2	87	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	113	LEU
4	S2	117	THR
4	S2	119	LYS
4	S2	134	LEU
4	S2	137	ILE
4	S2	139	ILE
4	S2	140	ARG
4	S2	141	ARG
4	S2	146	THR
4	S2	147	ASN
4	S2	148	LEU

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Mol	Chain	Res	Type
4	S2	156	THR
4	S2	166	THR
4	S2	174	ARG
4	S2	181	SER
4	S2	187	LEU
4	S2	194	GLU
4	S2	201	ASN
4	S2	207	LEU
4	S2	221	THR
4	S2	222	TYR
4	S2	224	PHE
4	S2	225	LEU
4	S2	226	THR
4	S2	229	LEU
4	S2	235	LEU
4	S2	237	VAL
4	S2	240	LEU
4	S2	245	ASP
5	S3	5	ILE
5	S3	6	SER
5	S3	9	ARG
5	S3	21	LEU
5	S3	23	GLU
5	S3	37	VAL
5	S3	62	ASN
5	S3	65	ARG
5	S3	69	LEU
5	S3	71	LEU
5	S3	84	ILE
5	S3	92	GLN
5	S3	93	ASP
5	S3	103	GLU
5	S3	117	ARG
5	S3	128	GLU
5	S3	137	VAL
5	S3	142	LEU
5	S3	157	LEU
5	S3	170	THR
5	S3	172	THR
5	S3	175	VAL
5	S3	176	LEU
5	S3	177	MET

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Mol	Chain	Res	Type
5	S3	178	ARG
5	S3	181	VAL
5	S3	189	MET
5	S3	195	SER
5	S3	207	THR
5	S3	209	ILE
5	S3	215	GLU
5	S3	222	VAL
5	S3	224	ASP
6	S4	6	LYS
6	S4	9	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	54	TYR
6	S4	62	LYS
6	S4	70	VAL
6	S4	77	ARG
6	S4	92	LEU
6	S4	102	VAL
6	S4	113	ARG
6	S4	115	THR
6	S4	117	GLU
6	S4	120	SER
6	S4	131	LEU
6	S4	142	HIS
6	S4	146	THR
6	S4	170	THR
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	197	HIS
6	S4	206	ASP
6	S4	211	LYS
6	S4	214	LEU
6	S4	215	ASP
6	S4	219	VAL
6	S4	221	ARG
6	S4	222	LEU

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Mol	Chain	Res	Type
6	S4	226	PHE
6	S4	227	VAL
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU
6	S4	247	SER
6	S4	248	ILE
6	S4	256	ARG
6	S4	258	GLN
6	S4	259	GLN
7	S5	23	VAL
7	S5	25	LEU
7	S5	32	GLU
7	S5	34	GLN
7	S5	38	THR
7	S5	39	GLU
7	S5	41	LYS
7	S5	43	PHE
7	S5	45	LYS
7	S5	48	PHE
7	S5	49	GLU
7	S5	65	ARG
7	S5	70	VAL
7	S5	76	ARG
7	S5	83	ARG
7	S5	89	ILE
7	S5	90	ILE
7	S5	93	LEU
7	S5	94	THR
7	S5	99	MET
7	S5	117	THR
7	S5	119	ASP
7	S5	126	ASP
7	S5	130	ILE
7	S5	139	ASN
7	S5	147	THR
7	S5	148	ARG
7	S5	149	VAL
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	162	VAL

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Mol	Chain	Res	Type
7	S5	166	ARG
7	S5	194	LEU
7	S5	213	LYS
7	S5	216	GLU
7	S5	225	ARG
8	S6	6	SER
8	S6	13	GLN
8	S6	21	GLU
8	S6	25	ARG
8	S6	32	ILE
8	S6	44	GLU
8	S6	45	PHE
8	S6	58	LYS
8	S6	68	LEU
8	S6	71	THR
8	S6	76	LEU
8	S6	77	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	94	ARG
8	S6	98	ARG
8	S6	109	LEU
8	S6	119	GLN
8	S6	120	GLU
8	S6	125	THR
8	S6	126	ASP
8	S6	127	THR
8	S6	129	VAL
8	S6	132	ARG
8	S6	137	ARG
8	S6	143	LYS
8	S6	154	ARG
8	S6	155	ASP
8	S6	158	ILE
8	S6	169	TYR
8	S6	170	THR
8	S6	175	ILE
8	S6	201	GLN
8	S6	211	LEU
8	S6	212	LEU
8	S6	217	SER
8	S6	223	LYS

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Mol	Chain	Res	Type
9	S7	16	LEU
9	S7	28	GLU
9	S7	34	LEU
9	S7	37	GLU
9	S7	38	LEU
9	S7	42	GLN
9	S7	50	ASP
9	S7	60	ILE
9	S7	67	LEU
9	S7	70	PHE
9	S7	75	THR
9	S7	77	LEU
9	S7	85	PHE
9	S7	87	ASP
9	S7	97	ARG
9	S7	99	LEU
9	S7	104	ARG
9	S7	109	VAL
9	S7	114	ARG
9	S7	122	HIS
9	S7	126	LEU
9	S7	144	VAL
9	S7	161	GLN
9	S7	164	TYR
9	S7	167	GLU
9	S7	174	ASN
9	S7	185	ILE
10	S8	4	SER
10	S8	5	ARG
10	S8	21	PHE
10	S8	25	ARG
10	S8	29	LEU
10	S8	36	THR
10	S8	46	VAL
10	S8	61	GLU
10	S8	70	GLU
10	S8	74	LYS
10	S8	76	THR
10	S8	82	VAL
10	S8	95	THR
10	S8	137	LYS
10	S8	138	ASN

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Mol	Chain	Res	Type
10	S8	151	LYS
10	S8	152	ILE
10	S8	155	SER
10	S8	161	SER
10	S8	164	ARG
10	S8	176	SER
10	S8	185	GLU
10	S8	193	LEU
10	S8	196	LEU
11	S9	3	ARG
11	S9	6	ARG
11	S9	7	THR
11	S9	17	ARG
11	S9	28	LEU
11	S9	40	LYS
11	S9	69	ARG
11	S9	70	LEU
11	S9	78	ARG
11	S9	82	ARG
11	S9	83	VAL
11	S9	88	GLU
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	97	LEU
11	S9	99	LEU
11	S9	101	VAL
11	S9	103	ASP
11	S9	105	LEU
11	S9	109	LEU
11	S9	110	GLN
11	S9	115	LYS
11	S9	130	THR
11	S9	134	ILE
11	S9	138	LYS
11	S9	145	SER
11	S9	149	ARG
11	S9	151	ASP
11	S9	162	SER
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG

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Mol	Chain	Res	Type
11	S9	182	GLU
12	C0	1	MET
12	C0	6	GLU
12	C0	8	ARG
12	C0	20	VAL
12	C0	27	PHE
12	C0	28	ASN
12	C0	29	GLN
12	C0	46	LEU
12	C0	47	GLN
12	C0	55	VAL
12	C0	56	LYS
12	C0	60	SER
12	C0	71	GLU
12	C0	76	LEU
12	C0	78	GLU
12	C0	82	LEU
13	C1	8	GLN
13	C1	16	GLN
13	C1	21	ASN
13	C1	27	THR
13	C1	29	LYS
13	C1	40	LEU
13	C1	44	THR
13	C1	54	ILE
13	C1	67	ARG
13	C1	69	LYS
13	C1	74	THR
13	C1	80	MET
13	C1	83	THR
13	C1	99	ARG
13	C1	109	VAL
13	C1	118	GLN
13	C1	125	VAL
13	C1	131	ILE
13	C1	136	ARG
13	C1	138	ASN
13	C1	143	SER
14	C2	28	LEU
14	C2	33	ARG
14	C2	36	LEU
14	C2	37	VAL

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Mol	Chain	Res	Type
14	C2	41	LEU
14	C2	43	ARG
14	C2	45	LEU
14	C2	46	ARG
14	C2	50	LYS
14	C2	52	LEU
14	C2	58	LEU
14	C2	59	LEU
14	C2	61	VAL
14	C2	62	LEU
14	C2	66	VAL
14	C2	71	ILE
14	C2	86	VAL
14	C2	89	ILE
14	C2	103	LEU
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	133	LEU
14	C2	139	HIS
14	C2	140	PHE
15	C3	3	ARG
15	C3	9	LYS
15	C3	11	ILE
15	C3	16	ILE
15	C3	21	ASN
15	C3	27	LYS
15	C3	39	LYS
15	C3	42	ARG
15	C3	45	LEU
15	C3	58	HIS
15	C3	61	THR
15	C3	64	ARG
15	C3	66	ILE
15	C3	75	LEU
15	C3	76	LYS
15	C3	88	LEU
15	C3	102	LEU
15	C3	103	GLU
15	C3	110	ASP
15	C3	114	ARG
15	C3	115	LEU

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Mol	Chain	Res	Type
15	C3	117	LEU
15	C3	125	LEU
15	C3	142	GLU
15	C3	149	LEU
16	C4	14	PHE
16	C4	16	VAL
16	C4	24	ASN
16	C4	29	HIS
16	C4	30	VAL
16	C4	31	THR
16	C4	39	ILE
16	C4	42	VAL
16	C4	51	ASP
16	C4	55	SER
16	C4	56	SER
16	C4	89	THR
16	C4	92	LYS
16	C4	93	THR
16	C4	99	GLN
16	C4	102	LEU
16	C4	103	ARG
16	C4	108	SER
16	C4	123	SER
16	C4	124	ASP
16	C4	125	SER
16	C4	127	ARG
16	C4	136	ARG
16	C4	137	LEU
17	C5	11	VAL
17	C5	13	LYS
17	C5	20	VAL
17	C5	21	ASP
17	C5	22	LEU
17	C5	26	LEU
17	C5	28	MET
17	C5	29	SER
17	C5	34	VAL
17	C5	35	LYS
17	C5	40	ARG
17	C5	44	ARG
17	C5	47	ARG
17	C5	52	LYS

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Mol	Chain	Res	Type
17	C5	60	LEU
17	C5	94	VAL
17	C5	108	ARG
17	C5	110	GLU
17	C5	116	LEU
17	C5	121	ILE
18	C6	4	VAL
18	C6	8	GLN
18	C6	17	THR
18	C6	26	LYS
18	C6	28	LEU
18	C6	43	ILE
18	C6	47	LYS
18	C6	53	LEU
18	C6	54	LEU
18	C6	55	VAL
18	C6	57	LEU
18	C6	66	ARG
18	C6	69	VAL
18	C6	94	GLN
18	C6	98	ASP
18	C6	101	SER
18	C6	106	LYS
18	C6	118	ILE
18	C6	123	ARG
18	C6	127	LYS
18	C6	128	LYS
18	C6	137	ARG
18	C6	138	PHE
19	C7	3	ARG
19	C7	5	ARG
19	C7	25	THR
19	C7	34	LEU
19	C7	48	ASN
19	C7	49	LYS
19	C7	54	THR
19	C7	58	MET
19	C7	69	ILE
19	C7	71	PHE
19	C7	72	LYS
19	C7	73	LEU
19	C7	83	GLN

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Mol	Chain	Res	Type
19	C7	84	TYR
19	C7	86	PRO
19	C7	105	GLN
19	C7	107	SER
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	8	GLN
20	C8	11	PHE
20	C8	13	HIS
20	C8	14	ILE
20	C8	15	LEU
20	C8	17	LEU
20	C8	25	ASN
20	C8	26	ILE
20	C8	28	ILE
20	C8	40	ARG
20	C8	54	LEU
20	C8	57	ARG
20	C8	60	GLU
20	C8	61	LEU
20	C8	71	GLN
20	C8	72	ILE
20	C8	77	THR
20	C8	80	LYS
20	C8	92	ILE
20	C8	93	THR
20	C8	108	LYS
20	C8	110	ARG
20	C8	114	GLU
20	C8	115	ARG
20	C8	116	LEU
20	C8	132	ARG
20	C8	136	GLN
20	C8	140	THR
20	C8	141	THR
20	C8	143	ARG
21	C9	4	VAL
21	C9	6	VAL
21	C9	18	TYR
21	C9	22	LEU

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Mol	Chain	Res	Type
21	C9	24	ARG
21	C9	28	LEU
21	C9	33	TYR
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	41	SER
21	C9	57	ARG
21	C9	63	ARG
21	C9	65	ILE
21	C9	67	MET
21	C9	70	GLN
21	C9	71	VAL
21	C9	84	LYS
21	C9	94	ILE
21	C9	123	ARG
21	C9	125	SER
21	C9	130	ARG
21	C9	131	ASP
21	C9	144	GLU
22	D0	15	GLN
22	D0	18	GLN
22	D0	19	ILE
22	D0	27	THR
22	D0	31	VAL
22	D0	34	LEU
22	D0	39	SER
22	D0	41	ILE
22	D0	47	GLN
22	D0	51	VAL
22	D0	52	LYS
22	D0	57	ARG
22	D0	60	THR
22	D0	65	ILE
22	D0	66	SER
22	D0	74	GLU
22	D0	76	SER
22	D0	81	THR
22	D0	85	ARG
22	D0	89	ARG
22	D0	99	ILE
22	D0	103	ILE

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Mol	Chain	Res	Type
22	D0	105	GLN
22	D0	114	VAL
23	D1	1	MET
23	D1	2	GLU
23	D1	3	ASN
23	D1	5	LYS
23	D1	7	GLN
23	D1	9	VAL
23	D1	11	LEU
23	D1	18	SER
23	D1	25	LYS
23	D1	32	VAL
23	D1	41	GLU
23	D1	49	GLU
23	D1	50	TYR
23	D1	52	THR
23	D1	68	SER
23	D1	69	LEU
23	D1	75	ASN
23	D1	78	LEU
23	D1	80	LYS
23	D1	84	SER
24	D2	12	ASN
24	D2	23	ARG
24	D2	24	GLN
24	D2	25	VAL
24	D2	27	ILE
24	D2	29	PRO
24	D2	49	GLU
24	D2	53	ILE
24	D2	56	HIS
24	D2	65	LEU
24	D2	68	ARG
24	D2	74	VAL
24	D2	76	SER
24	D2	81	VAL
24	D2	83	ILE
24	D2	93	LEU
24	D2	98	GLN
24	D2	103	ILE
24	D2	105	THR
24	D2	117	ARG

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Mol	Chain	Res	Type
24	D2	126	LEU
25	D3	7	ARG
25	D3	9	LEU
25	D3	14	LYS
25	D3	18	HIS
25	D3	19	ARG
25	D3	31	LYS
25	D3	40	SER
25	D3	41	SER
25	D3	47	SER
25	D3	73	ARG
25	D3	74	VAL
25	D3	79	ASN
25	D3	82	LYS
25	D3	83	VAL
25	D3	84	THR
25	D3	96	VAL
25	D3	100	ASP
25	D3	101	GLU
25	D3	103	LEU
25	D3	107	PHE
25	D3	109	ARG
25	D3	110	LYS
25	D3	114	LYS
25	D3	131	SER
25	D3	132	LEU
25	D3	136	TRP
25	D3	140	LYS
25	D3	144	ARG
26	D4	28	LEU
26	D4	32	ARG
26	D4	34	ASN
26	D4	51	GLU
26	D4	57	VAL
26	D4	61	ARG
26	D4	102	LYS
26	D4	105	ARG
26	D4	124	ARG
26	D4	127	LYS
27	D5	58	ARG
27	D5	59	TYR
27	D5	62	VAL

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Mol	Chain	Res	Type
27	D5	68	ARG
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	95	HIS
27	D5	96	SER
27	D5	100	ILE
28	D6	4	LYS
28	D6	5	ARG
28	D6	12	LYS
28	D6	30	ILE
28	D6	34	LYS
28	D6	36	ILE
28	D6	38	ARG
28	D6	41	ILE
28	D6	45	VAL
28	D6	46	GLU
28	D6	50	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	68	TYR
28	D6	69	ASN
28	D6	76	SER
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
28	D6	90	GLU
29	D7	3	LEU
29	D7	4	VAL
29	D7	14	SER
29	D7	17	ARG
29	D7	23	THR
29	D7	33	LEU
29	D7	36	LYS
29	D7	42	ASN
29	D7	48	SER
29	D7	55	THR
29	D7	57	GLU
29	D7	61	THR
29	D7	67	THR
29	D7	81	ARG

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Mol	Chain	Res	Type
30	D8	13	ILE
30	D8	15	VAL
30	D8	19	THR
30	D8	33	LEU
30	D8	51	ASN
30	D8	52	ASP
30	D8	57	MET
30	D8	58	GLU
30	D8	62	GLU
30	D8	64	ARG
31	D9	7	TRP
31	D9	9	SER
31	D9	12	ARG
31	D9	19	ARG
31	D9	22	ARG
31	D9	30	LEU
31	D9	32	ARG
31	D9	36	LEU
32	E0	3	LYS
32	E0	15	LYS
32	E0	16	SER
32	E0	20	LYS
32	E0	25	GLU
32	E0	28	LYS
32	E0	31	LYS
32	E0	42	ARG
32	E0	47	VAL
32	E0	49	LEU
32	E0	50	VAL
32	E0	56	MET
33	E1	84	VAL
33	E1	85	TYR
33	E1	86	THR
33	E1	89	LYS
33	E1	90	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	97	LYS
33	E1	102	VAL
33	E1	108	VAL
33	E1	109	ASP
33	E1	111	GLU

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Mol	Chain	Res	Type
33	E1	113	LYS
33	E1	120	GLU
33	E1	130	VAL
33	E1	135	HIS
33	E1	137	ASP
33	E1	139	LEU
33	E1	150	VAL
33	E1	151	ASN
34	SR	6	VAL
34	SR	10	ARG
34	SR	16	HIS
34	SR	17	ASN
34	SR	29	GLN
34	SR	39	ASP
34	SR	50	ASP
34	SR	52	GLN
34	SR	59	ARG
34	SR	60	SER
34	SR	66	HIS
34	SR	71	CYS
34	SR	74	THR
34	SR	76	ASP
34	SR	87	LYS
34	SR	96	THR
34	SR	106	HIS
34	SR	112	SER
34	SR	117	LYS
34	SR	134	TRP
34	SR	136	ILE
34	SR	137	LYS
34	SR	141	LEU
34	SR	144	LEU
34	SR	165	ASP
34	SR	191	ASP
34	SR	202	LEU
34	SR	207	ASP
34	SR	211	ILE
34	SR	222	LEU
34	SR	229	LYS
34	SR	232	TYR
34	SR	238	ASP
34	SR	248	ASN

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Mol	Chain	Res	Type
34	SR	265	LEU
34	SR	266	ASP
34	SR	268	GLN
34	SR	277	GLU
34	SR	299	GLN
34	SR	308	ASN
34	SR	317	THR
35	SM	23	LYS
35	SM	37	VAL
35	SM	43	ASP
35	SM	61	ILE
35	SM	62	ARG
35	SM	68	ARG
35	SM	69	ARG
35	SM	72	ARG
35	SM	77	THR
35	SM	84	LYS
35	SM	89	ARG
35	SM	91	THR
35	SM	94	HIS
35	SM	96	ARG
35	SM	100	THR
35	SM	103	LYS
35	SM	105	LYS
35	SM	113	ASP
35	SM	139	GLU
39	L2	18	SER
39	L2	19	HIS
39	L2	32	LEU
39	L2	41	ILE
39	L2	44	ILE
39	L2	45	VAL
39	L2	49	VAL
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

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Mol	Chain	Res	Type
39	L2	98	VAL
39	L2	101	VAL
39	L2	104	LEU
39	L2	118	GLU
39	L2	134	VAL
39	L2	142	ASP
39	L2	143	GLU
39	L2	158	ILE
39	L2	179	LEU
39	L2	180	LEU
39	L2	181	LYS
39	L2	190	ARG
39	L2	193	ARG
39	L2	202	VAL
39	L2	204	MET
39	L2	207	VAL
39	L2	227	ARG
39	L2	230	VAL
39	L2	231	SER
39	L2	242	ARG
39	L2	252	THR
40	L3	2	SER
40	L3	7	GLU
40	L3	10	ARG
40	L3	17	LEU
40	L3	19	ARG
40	L3	20	LYS
40	L3	21	ARG
40	L3	25	ILE
40	L3	30	LYS
40	L3	37	ARG
40	L3	47	LEU
40	L3	56	ILE
40	L3	67	PHE
40	L3	71	GLU
40	L3	79	VAL
40	L3	84	VAL
40	L3	85	VAL
40	L3	86	VAL
40	L3	100	ARG
40	L3	103	THR
40	L3	104	THR

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Mol	Chain	Res	Type
40	L3	114	VAL
40	L3	116	ARG
40	L3	120	LYS
40	L3	121	ASN
40	L3	134	SER
40	L3	139	GLN
40	L3	145	GLU
40	L3	146	ARG
40	L3	148	LEU
40	L3	157	VAL
40	L3	160	VAL
40	L3	187	SER
40	L3	188	ILE
40	L3	189	SER
40	L3	192	VAL
40	L3	196	ARG
40	L3	202	THR
40	L3	206	ASP
40	L3	210	GLU
40	L3	212	ASN
40	L3	218	ILE
40	L3	232	ARG
40	L3	235	THR
40	L3	237	LYS
40	L3	238	LEU
40	L3	244	ARG
40	L3	252	ILE
40	L3	264	VAL
40	L3	274	SER
40	L3	284	ARG
40	L3	289	ASP
40	L3	300	ARG
40	L3	304	THR
40	L3	305	ILE
40	L3	317	ILE
40	L3	320	ASP
40	L3	324	VAL
40	L3	325	LYS
40	L3	328	ILE
40	L3	332	ARG
40	L3	338	LEU
40	L3	347	SER

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Mol	Chain	Res	Type
40	L3	354	VAL
40	L3	355	SER
40	L3	357	LYS
40	L3	375	GLU
40	L3	380	MET
40	L3	383	LEU
40	L3	387	LEU
41	L4	4	PRO
41	L4	16	THR
41	L4	20	LEU
41	L4	22	LEU
41	L4	25	VAL
41	L4	40	THR
41	L4	46	LYS
41	L4	53	SER
41	L4	55	LYS
41	L4	71	VAL
41	L4	74	ILE
41	L4	93	MET
41	L4	118	LYS
41	L4	120	TYR
41	L4	124	SER
41	L4	133	SER
41	L4	135	VAL
41	L4	136	LEU
41	L4	138	ARG
41	L4	144	LYS
41	L4	145	ILE
41	L4	150	LEU
41	L4	152	VAL
41	L4	156	LEU
41	L4	169	LEU
41	L4	176	SER
41	L4	177	ASP
41	L4	179	LEU
41	L4	182	LEU
41	L4	186	LYS
41	L4	187	LEU
41	L4	193	LYS
41	L4	194	TYR
41	L4	195	ARG
41	L4	203	ARG

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Mol	Chain	Res	Type
41	L4	206	LEU
41	L4	211	GLU
41	L4	220	ARG
41	L4	223	PRO
41	L4	230	VAL
41	L4	246	ARG
41	L4	256	THR
41	L4	258	LEU
41	L4	266	THR
41	L4	270	SER
41	L4	275	THR
41	L4	284	SER
41	L4	286	VAL
41	L4	287	THR
41	L4	288	ARG
41	L4	289	ILE
41	L4	292	SER
41	L4	295	ILE
41	L4	297	SER
41	L4	306	THR
41	L4	307	GLN
41	L4	308	LYS
41	L4	323	VAL
41	L4	333	VAL
41	L4	338	LYS
41	L4	339	LEU
41	L4	343	LYS
41	L4	347	THR
41	L4	349	THR
42	L5	4	GLN
42	L5	5	LYS
42	L5	8	LYS
42	L5	9	SER
42	L5	10	SER
42	L5	22	ARG
42	L5	23	ARG
42	L5	32	GLN
42	L5	36	LEU
42	L5	41	LYS
42	L5	58	LYS
42	L5	63	GLN
42	L5	64	ILE

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Mol	Chain	Res	Type
42	L5	65	ILE
42	L5	66	SER
42	L5	69	ILE
42	L5	70	THR
42	L5	93	THR
42	L5	110	LEU
42	L5	112	LYS
42	L5	115	LEU
42	L5	131	LEU
42	L5	140	ARG
42	L5	146	LEU
42	L5	148	ILE
42	L5	152	ARG
42	L5	154	THR
42	L5	155	THR
42	L5	164	LYS
42	L5	173	VAL
42	L5	177	GLU
42	L5	185	PHE
42	L5	187	THR
42	L5	188	GLU
42	L5	190	ILE
42	L5	196	ARG
42	L5	208	MET
42	L5	222	LEU
42	L5	234	ASP
42	L5	241	THR
42	L5	257	GLU
42	L5	259	LYS
42	L5	263	GLU
42	L5	273	ARG
42	L5	279	LYS
42	L5	290	ILE
42	L5	293	LEU
43	L6	2	SER
43	L6	4	GLN
43	L6	9	TRP
43	L6	15	VAL
43	L6	21	THR
43	L6	31	ARG
43	L6	35	VAL
43	L6	41	ILE

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Mol	Chain	Res	Type
43	L6	46	ARG
43	L6	48	ARG
43	L6	50	LYS
43	L6	52	VAL
43	L6	64	LEU
43	L6	65	ILE
43	L6	78	ARG
43	L6	84	VAL
43	L6	89	THR
43	L6	108	LYS
43	L6	109	GLU
43	L6	129	GLU
43	L6	134	ARG
43	L6	136	GLU
43	L6	150	LYS
43	L6	152	THR
43	L6	155	LEU
43	L6	160	SER
43	L6	170	LYS
43	L6	173	MET
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	78	GLU
44	L7	82	LYS
44	L7	83	LEU
44	L7	89	ILE
44	L7	93	ASN
44	L7	98	LYS
44	L7	110	ARG
44	L7	121	LYS
44	L7	124	LEU
44	L7	143	THR
44	L7	164	SER
44	L7	178	ILE
44	L7	179	LEU
44	L7	180	SER
44	L7	182	ASP
44	L7	184	LEU
44	L7	185	ILE
44	L7	228	SER
44	L7	229	PHE

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Mol	Chain	Res	Type
44	L7	239	LEU
44	L7	244	ASN
45	L8	26	LEU
45	L8	61	GLN
45	L8	63	LYS
45	L8	65	LEU
45	L8	66	SER
45	L8	69	LEU
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	84	ARG
45	L8	92	LYS
45	L8	95	ASN
45	L8	101	THR
45	L8	106	LYS
45	L8	107	GLU
45	L8	118	GLU
45	L8	132	VAL
45	L8	136	LEU
45	L8	145	ASN
45	L8	149	LYS
45	L8	152	LEU
45	L8	156	ASP
45	L8	163	VAL
45	L8	169	LEU
45	L8	181	LYS
45	L8	183	LYS
45	L8	185	ARG
45	L8	194	THR
45	L8	203	VAL
45	L8	204	ARG
45	L8	206	GLU
45	L8	241	LYS
45	L8	246	MET
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

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Mol	Chain	Res	Type
46	L9	19	SER
46	L9	20	ILE
46	L9	31	ARG
46	L9	33	THR
46	L9	34	LEU
46	L9	36	LYS
46	L9	41	ILE
46	L9	48	VAL
46	L9	49	ASN
46	L9	52	LEU
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	76	ASP
46	L9	77	ASN
46	L9	82	VAL
46	L9	129	ARG
46	L9	132	VAL
46	L9	133	THR
46	L9	138	THR
46	L9	139	ASN
46	L9	140	VAL
46	L9	147	SER
46	L9	151	VAL
46	L9	152	GLU
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	164	ILE
46	L9	168	ARG
46	L9	172	ILE
46	L9	173	ARG
46	L9	189	GLU
46	L9	190	ASP
47	M0	3	ARG
47	M0	21	ARG
47	M0	23	ASN
47	M0	24	ARG
47	M0	26	VAL
47	M0	29	SER
47	M0	30	LYS
47	M0	32	ARG

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Mol	Chain	Res	Type
47	M0	33	ILE
47	M0	36	LEU
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	58	GLU
47	M0	62	SER
47	M0	63	GLU
47	M0	74	LYS
47	M0	87	LEU
47	M0	90	ARG
47	M0	91	VAL
47	M0	129	VAL
47	M0	139	ARG
47	M0	141	LYS
47	M0	143	SER
47	M0	145	LYS
47	M0	146	ASP
47	M0	156	ARG
47	M0	163	GLN
47	M0	165	ILE
47	M0	169	LYS
47	M0	174	THR
47	M0	177	ASP
47	M0	178	ARG
47	M0	184	LYS
47	M0	203	LYS
48	M1	9	MET
48	M1	10	ARG
48	M1	11	ASP
48	M1	12	LEU
48	M1	13	LYS
48	M1	16	LYS
48	M1	23	VAL
48	M1	26	SER
48	M1	28	ASP
48	M1	29	ARG
48	M1	40	LEU
48	M1	44	THR

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Mol	Chain	Res	Type
48	M1	46	VAL
48	M1	70	THR
48	M1	80	LEU
48	M1	94	ARG
48	M1	99	THR
48	M1	101	ASN
48	M1	107	ASP
48	M1	111	ASP
48	M1	112	LEU
48	M1	130	VAL
48	M1	137	ARG
48	M1	140	ARG
48	M1	147	THR
48	M1	157	GLU
48	M1	158	ASP
48	M1	166	LYS
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	58	VAL
49	M3	59	ARG
49	M3	63	VAL
49	M3	67	ARG
49	M3	69	VAL
49	M3	70	ARG
49	M3	85	LEU
49	M3	107	GLU
49	M3	115	ARG
49	M3	121	SER
49	M3	123	ILE
49	M3	124	ILE
49	M3	131	LYS
49	M3	136	GLU
49	M3	144	THR
49	M3	164	GLU
49	M3	168	ARG
49	M3	175	SER
49	M3	190	LYS

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Mol	Chain	Res	Type
49	M3	194	GLU
50	M4	4	ASP
50	M4	5	SER
50	M4	15	VAL
50	M4	20	VAL
50	M4	41	GLN
50	M4	45	LEU
50	M4	53	VAL
50	M4	58	ILE
50	M4	63	VAL
50	M4	74	ARG
50	M4	82	SER
50	M4	90	VAL
50	M4	91	CYS
50	M4	92	GLU
50	M4	106	ARG
50	M4	113	THR
50	M4	133	LYS
50	M4	135	LEU
51	M5	10	LEU
51	M5	18	VAL
51	M5	22	LEU
51	M5	36	ILE
51	M5	49	ARG
51	M5	80	THR
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	113	LEU
51	M5	117	ASN
51	M5	124	ASP
51	M5	133	ILE
51	M5	138	GLN
51	M5	142	ILE
51	M5	151	ILE
51	M5	153	ASP
51	M5	155	VAL
51	M5	159	ARG
51	M5	170	LYS

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Mol	Chain	Res	Type
51	M5	182	ASN
51	M5	184	LYS
51	M5	190	THR
51	M5	194	GLN
51	M5	198	SER
51	M5	201	ARG
52	M6	33	ILE
52	M6	34	VAL
52	M6	58	LEU
52	M6	67	THR
52	M6	78	ARG
52	M6	82	LYS
52	M6	85	ARG
52	M6	106	GLU
52	M6	110	PRO
52	M6	113	ASP
52	M6	116	LYS
52	M6	117	ARG
52	M6	122	GLN
52	M6	124	LEU
52	M6	128	ARG
52	M6	143	THR
52	M6	182	ASN
52	M6	190	VAL
53	M7	9	THR
53	M7	24	VAL
53	M7	29	THR
53	M7	32	THR
53	M7	36	ILE
53	M7	43	LYS
53	M7	49	GLU
53	M7	51	VAL
53	M7	52	LEU
53	M7	53	ASP
53	M7	56	ARG
53	M7	69	ARG
53	M7	78	VAL
53	M7	79	THR
53	M7	103	GLU
53	M7	112	LEU
53	M7	114	VAL
53	M7	119	VAL

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Mol	Chain	Res	Type
53	M7	120	ASN
53	M7	126	ARG
53	M7	127	ARG
53	M7	138	LYS
53	M7	142	SER
53	M7	171	ARG
53	M7	181	ARG
54	M8	7	SER
54	M8	12	ARG
54	M8	17	THR
54	M8	20	LYS
54	M8	24	VAL
54	M8	26	LEU
54	M8	32	LEU
54	M8	34	THR
54	M8	39	ARG
54	M8	40	THR
54	M8	49	LEU
54	M8	57	ILE
54	M8	63	SER
54	M8	64	VAL
54	M8	66	ARG
54	M8	74	GLU
54	M8	80	THR
54	M8	81	VAL
54	M8	86	THR
54	M8	99	THR
54	M8	101	VAL
54	M8	111	ARG
54	M8	127	LEU
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	147	ARG
54	M8	150	VAL
54	M8	168	THR
54	M8	171	LYS
54	M8	180	ARG
55	M9	5	ARG
55	M9	8	LYS
55	M9	22	VAL
55	M9	41	ILE

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Mol	Chain	Res	Type
55	M9	44	LEU
55	M9	46	LYS
55	M9	74	ARG
55	M9	86	GLU
55	M9	89	LEU
55	M9	99	LEU
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	115	ILE
55	M9	134	HIS
55	M9	138	LEU
55	M9	153	LYS
55	M9	175	GLN
55	M9	177	VAL
56	N0	1	MET
56	N0	8	GLN
56	N0	16	THR
56	N0	23	LYS
56	N0	45	LEU
56	N0	51	VAL
56	N0	61	ILE
56	N0	63	GLN
56	N0	71	LYS
56	N0	80	ARG
56	N0	81	TYR
56	N0	85	SER
56	N0	87	THR
56	N0	92	LYS
56	N0	97	VAL
56	N0	100	VAL
56	N0	104	GLU
56	N0	115	ARG
56	N0	117	ARG
56	N0	122	HIS
56	N0	131	LYS
56	N0	132	THR
56	N0	137	ARG
56	N0	138	GLN
56	N0	139	TYR
56	N0	145	THR
56	N0	149	LYS

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Mol	Chain	Res	Type
56	N0	155	ARG
56	N0	156	VAL
56	N0	157	GLN
56	N0	160	THR
56	N0	167	ARG
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	68	THR
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	83	ARG
57	N1	87	LYS
57	N1	88	ARG
57	N1	89	LEU
57	N1	102	ARG
57	N1	104	GLU
57	N1	106	LEU
57	N1	110	LYS
57	N1	124	VAL
57	N1	126	VAL
57	N1	127	GLN
57	N1	139	ARG
57	N1	141	VAL
57	N1	143	THR
57	N1	146	ASN
57	N1	158	THR
58	N2	10	LYS
58	N2	14	THR
58	N2	16	THR
58	N2	27	VAL
58	N2	38	ILE
58	N2	43	VAL
58	N2	52	ASN
58	N2	66	VAL
58	N2	75	TYR
58	N2	81	LYS
58	N2	88	GLN

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Mol	Chain	Res	Type
58	N2	93	ILE
58	N2	100	THR
58	N2	105	LEU
59	N3	13	ILE
59	N3	45	ARG
59	N3	48	ARG
59	N3	63	LYS
59	N3	64	LYS
59	N3	69	LEU
59	N3	72	LYS
59	N3	73	VAL
59	N3	74	MET
59	N3	91	VAL
59	N3	102	ILE
59	N3	104	ASN
59	N3	115	THR
59	N3	135	VAL
60	N4	4	GLU
60	N4	5	ILE
60	N4	7	SER
60	N4	25	ASP
60	N4	39	LEU
60	N4	52	THR
60	N4	54	LEU
60	N4	64	THR
61	N5	26	VAL
61	N5	27	ARG
61	N5	36	LYS
61	N5	37	THR
61	N5	38	LEU
61	N5	63	ILE
61	N5	70	GLU
61	N5	71	THR
61	N5	73	MET
61	N5	74	LYS
61	N5	75	LYS
61	N5	81	ILE
61	N5	92	LYS
61	N5	108	LEU
61	N5	109	LYS
61	N5	113	LEU
61	N5	115	ARG

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Mol	Chain	Res	Type
61	N5	125	ARG
61	N5	133	LEU
61	N5	134	ASP
61	N5	135	ILE
61	N5	139	ILE
61	N5	142	ILE
62	N6	6	LEU
62	N6	13	ARG
62	N6	26	GLN
62	N6	36	SER
62	N6	37	LYS
62	N6	38	GLU
62	N6	39	LEU
62	N6	42	GLN
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	60	ARG
62	N6	72	SER
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	83	ASP
62	N6	112	ASP
62	N6	115	ARG
62	N6	127	GLU
63	N7	17	ARG
63	N7	21	LYS
63	N7	24	VAL
63	N7	27	LYS
63	N7	34	LYS
63	N7	46	ILE
63	N7	51	LEU
63	N7	60	LYS
63	N7	72	ILE
63	N7	73	LYS
63	N7	74	VAL
63	N7	75	VAL
63	N7	83	THR

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Mol	Chain	Res	Type
63	N7	86	THR
63	N7	87	LEU
63	N7	99	GLU
63	N7	102	GLU
63	N7	103	GLN
63	N7	106	GLN
63	N7	107	ARG
63	N7	109	GLU
63	N7	121	ARG
63	N7	123	GLN
63	N7	134	LEU
64	N8	4	ARG
64	N8	6	THR
64	N8	8	THR
64	N8	10	LYS
64	N8	16	SER
64	N8	26	ARG
64	N8	42	ARG
64	N8	60	TYR
64	N8	76	ASP
64	N8	78	LEU
64	N8	91	LEU
64	N8	93	SER
64	N8	95	SER
64	N8	115	LYS
64	N8	120	ASN
64	N8	125	VAL
64	N8	133	LEU
65	N9	13	THR
65	N9	22	LYS
65	N9	24	PRO
65	N9	25	LYS
65	N9	28	LYS
65	N9	40	ARG
65	N9	42	ASN
65	N9	50	THR
65	N9	59	LYS
66	O0	10	ILE
66	O0	14	LEU
66	O0	16	LEU
66	O0	30	THR
66	O0	32	LYS

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Mol	Chain	Res	Type
66	O0	34	LEU
66	O0	36	GLN
66	O0	40	LYS
66	O0	61	MET
66	O0	76	GLU
66	O0	77	LEU
66	O0	83	LYS
66	O0	87	VAL
66	O0	100	ILE
66	O0	101	LEU
66	O0	103	THR
67	O1	7	VAL
67	O1	8	VAL
67	O1	12	TYR
67	O1	16	LEU
67	O1	28	ARG
67	O1	35	GLU
67	O1	36	ILE
67	O1	44	MET
67	O1	64	VAL
67	O1	68	GLU
67	O1	73	LEU
67	O1	79	ARG
67	O1	82	GLU
67	O1	84	ASP
67	O1	86	LYS
67	O1	96	VAL
67	O1	102	LYS
67	O1	104	LEU
67	O1	106	THR
67	O1	107	VAL
67	O1	110	GLU
68	O2	14	THR
68	O2	19	ARG
68	O2	24	ARG
68	O2	28	VAL
68	O2	33	ARG
68	O2	38	ILE
68	O2	51	SER
68	O2	54	LYS
68	O2	59	SER
68	O2	67	SER

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Mol	Chain	Res	Type
68	O2	73	THR
68	O2	75	LEU
68	O2	82	LEU
68	O2	106	VAL
68	O2	109	LEU
68	O2	111	ARG
68	O2	125	ARG
68	O2	128	LEU
69	O3	4	SER
69	O3	45	LEU
69	O3	47	LYS
69	O3	59	VAL
69	O3	80	VAL
69	O3	90	PRO
69	O3	98	VAL
69	O3	105	SER
70	O4	5	VAL
70	O4	8	ARG
70	O4	20	ILE
70	O4	24	LYS
70	O4	29	ILE
70	O4	52	GLN
70	O4	56	THR
70	O4	57	LEU
70	O4	58	ARG
70	O4	60	ARG
70	O4	71	THR
70	O4	79	SER
70	O4	86	LYS
70	O4	87	GLU
70	O4	104	VAL
71	O5	4	VAL
71	O5	13	SER
71	O5	15	GLU
71	O5	21	LEU
71	O5	27	GLU
71	O5	30	GLU
71	O5	36	LEU
71	O5	38	ARG
71	O5	44	ILE
71	O5	46	THR
71	O5	48	ARG

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Mol	Chain	Res	Type
71	O5	49	LYS
71	O5	62	GLN
71	O5	68	GLN
71	O5	71	LYS
71	O5	85	THR
71	O5	86	ARG
71	O5	89	ARG
71	O5	90	ARG
71	O5	100	VAL
71	O5	102	GLU
71	O5	105	ARG
71	O5	107	LYS
71	O5	119	LYS
72	O6	11	LEU
72	O6	18	THR
72	O6	20	MET
72	O6	21	THR
72	O6	25	LYS
72	O6	26	ILE
72	O6	28	TYR
72	O6	36	ARG
72	O6	42	SER
72	O6	45	ARG
72	O6	50	LEU
72	O6	52	PRO
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	64	SER
72	O6	68	ARG
72	O6	71	LYS
72	O6	72	VAL
72	O6	76	ARG
72	O6	81	THR
72	O6	88	GLU
72	O6	98	ARG
72	O6	99	ARG
73	O7	3	LYS
73	O7	7	SER
73	O7	24	ARG
73	O7	25	ARG
73	O7	26	SER

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Mol	Chain	Res	Type
73	O7	33	THR
73	O7	36	SER
73	O7	45	ARG
73	O7	55	ARG
73	O7	58	THR
73	O7	59	THR
73	O7	67	LEU
74	O8	5	ILE
74	O8	6	THR
74	O8	8	ILE
74	O8	12	LEU
74	O8	22	THR
74	O8	25	VAL
74	O8	28	ASN
74	O8	31	LEU
74	O8	32	ASN
74	O8	41	THR
74	O8	46	ARG
74	O8	53	THR
74	O8	54	LEU
74	O8	61	LYS
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	23	LEU
75	O9	28	ARG
75	O9	29	LEU
75	O9	51	ILE
76	Q0	77	ILE
76	Q0	78	ILE
76	Q0	85	LEU
76	Q0	93	LYS
76	Q0	113	ARG
76	Q0	127	LEU
77	Q1	9	ARG
77	Q1	11	ARG
77	Q1	13	LEU
77	Q1	16	LYS
77	Q1	19	LYS

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Mol	Chain	Res	Type
77	Q1	24	SER
77	Q1	25	LYS
78	Q2	3	ASN
78	Q2	4	VAL
78	Q2	8	ARG
78	Q2	20	HIS
78	Q2	21	THR
78	Q2	26	THR
78	Q2	35	LEU
78	Q2	45	ARG
78	Q2	47	GLN
78	Q2	55	LYS
78	Q2	60	LYS
78	Q2	71	ARG
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	88	CYS
78	Q2	92	GLU
78	Q2	100	LYS
78	Q2	104	LEU
79	Q3	5	THR
79	Q3	11	THR
79	Q3	16	VAL
79	Q3	25	GLN
79	Q3	45	LYS
79	Q3	58	SER
79	Q3	60	CYS
79	Q3	70	THR
79	Q3	73	THR
79	Q3	91	GLU
2	s0	10	THR
2	s0	12	GLU
2	s0	21	ASN
2	s0	30	GLN
2	s0	41	ARG
2	s0	43	ASP
2	s0	45	VAL
2	s0	48	ILE
2	s0	57	LEU
2	s0	59	LEU
2	s0	80	THR

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Mol	Chain	Res	Type
2	s0	87	LEU
2	s0	88	LYS
2	s0	93	THR
2	s0	108	THR
2	s0	110	TYR
2	s0	119	ARG
2	s0	124	THR
2	s0	127	ARG
2	s0	131	GLN
2	s0	144	ILE
2	s0	154	GLU
2	s0	172	LEU
2	s0	179	ARG
2	s0	183	ARG
2	s0	184	LEU
2	s0	185	ARG
2	s0	189	VAL
2	s0	191	ARG
2	s0	202	TYR
3	s1	21	VAL
3	s1	25	THR
3	s1	47	LEU
3	s1	51	SER
3	s1	62	LYS
3	s1	65	VAL
3	s1	70	LEU
3	s1	74	GLN
3	s1	78	ASP
3	s1	81	PHE
3	s1	82	ARG
3	s1	84	ILE
3	s1	89	ASP
3	s1	105	PHE
3	s1	107	THR
3	s1	110	LEU
3	s1	120	LEU
3	s1	122	GLU
3	s1	125	VAL
3	s1	126	THR
3	s1	127	VAL
3	s1	130	SER
3	s1	152	ARG

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Mol	Chain	Res	Type
3	s1	154	SER
3	s1	173	THR
3	s1	175	GLU
3	s1	181	LEU
3	s1	184	LEU
3	s1	202	LYS
3	s1	204	ILE
3	s1	206	PRO
3	s1	212	VAL
3	s1	215	VAL
3	s1	219	LYS
3	s1	222	LYS
3	s1	223	PHE
3	s1	228	LEU
3	s1	232	HIS
4	s2	41	LEU
4	s2	53	ILE
4	s2	55	GLU
4	s2	58	LEU
4	s2	61	LEU
4	s2	69	ILE
4	s2	72	LEU
4	s2	73	LEU
4	s2	77	GLN
4	s2	80	VAL
4	s2	81	MET
4	s2	83	ILE
4	s2	84	LYS
4	s2	87	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	97	ARG
4	s2	102	VAL
4	s2	106	ASP
4	s2	111	VAL
4	s2	113	LEU
4	s2	117	THR
4	s2	141	ARG
4	s2	146	THR
4	s2	148	LEU
4	s2	158	THR
4	s2	164	SER

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Mol	Chain	Res	Type
4	s2	182	PRO
4	s2	185	LYS
4	s2	199	GLN
4	s2	205	ARG
4	s2	207	LEU
4	s2	209	ASN
4	s2	218	ILE
4	s2	221	THR
4	s2	222	TYR
4	s2	225	LEU
4	s2	229	LEU
4	s2	240	LEU
4	s2	245	ASP
5	s3	4	LEU
5	s3	7	LYS
5	s3	9	ARG
5	s3	10	LYS
5	s3	21	LEU
5	s3	34	TYR
5	s3	37	VAL
5	s3	40	ARG
5	s3	44	THR
5	s3	53	THR
5	s3	59	LEU
5	s3	61	GLU
5	s3	67	ASN
5	s3	69	LEU
5	s3	84	ILE
5	s3	89	GLU
5	s3	90	ARG
5	s3	93	ASP
5	s3	94	ARG
5	s3	111	ASN
5	s3	115	ILE
5	s3	116	ARG
5	s3	120	TYR
5	s3	125	TYR
5	s3	127	MET
5	s3	129	SER
5	s3	132	LYS
5	s3	134	CYS
5	s3	141	LYS

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Mol	Chain	Res	Type
5	s3	142	LEU
5	s3	158	ILE
5	s3	168	ILE
5	s3	169	ASP
5	s3	172	THR
5	s3	176	LEU
5	s3	202	LEU
5	s3	210	GLU
5	s3	212	LYS
5	s3	213	GLU
5	s3	223	LYS
5	s3	225	TYR
6	s4	6	LYS
6	s4	9	LEU
6	s4	11	ARG
6	s4	23	LEU
6	s4	24	SER
6	s4	38	LEU
6	s4	42	LEU
6	s4	48	LEU
6	s4	49	ARG
6	s4	50	ASN
6	s4	51	ARG
6	s4	52	LEU
6	s4	67	GLN
6	s4	70	VAL
6	s4	78	THR
6	s4	95	THR
6	s4	98	ASN
6	s4	104	ASP
6	s4	113	ARG
6	s4	115	THR
6	s4	116	ASP
6	s4	123	LEU
6	s4	127	LYS
6	s4	131	LEU
6	s4	146	THR
6	s4	148	ARG
6	s4	160	VAL
6	s4	175	PHE
6	s4	176	ASP
6	s4	180	LEU

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Mol	Chain	Res	Type
6	s4	182	TYR
6	s4	184	THR
6	s4	219	VAL
6	s4	221	ARG
6	s4	222	LEU
6	s4	223	ASN
6	s4	245	LYS
6	s4	246	LEU
7	s5	23	VAL
7	s5	24	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	31	GLU
7	s5	33	VAL
7	s5	38	THR
7	s5	45	LYS
7	s5	59	VAL
7	s5	63	GLN
7	s5	68	ILE
7	s5	76	ARG
7	s5	93	LEU
7	s5	94	THR
7	s5	96	SER
7	s5	102	ARG
7	s5	112	ARG
7	s5	119	ASP
7	s5	125	THR
7	s5	134	VAL
7	s5	147	THR
7	s5	148	ARG
7	s5	157	ARG
7	s5	170	GLN
7	s5	175	LEU
7	s5	186	ASN
7	s5	190	ILE
7	s5	192	GLU
7	s5	194	LEU
7	s5	216	GLU
7	s5	219	ARG
8	s6	15	THR
8	s6	25	ARG
8	s6	30	LYS

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Mol	Chain	Res	Type
8	s6	31	ARG
8	s6	43	ASP
8	s6	57	ASP
8	s6	67	VAL
8	s6	69	LEU
8	s6	71	THR
8	s6	73	ILE
8	s6	76	LEU
8	s6	81	VAL
8	s6	93	LYS
8	s6	97	VAL
8	s6	108	VAL
8	s6	109	LEU
8	s6	115	LYS
8	s6	121	LEU
8	s6	126	ASP
8	s6	127	THR
8	s6	129	VAL
8	s6	143	LYS
8	s6	148	SER
8	s6	151	ASP
8	s6	153	VAL
8	s6	154	ARG
8	s6	155	ASP
8	s6	157	VAL
8	s6	170	THR
8	s6	179	VAL
8	s6	180	THR
8	s6	193	LEU
8	s6	207	GLU
8	s6	215	ARG
9	s7	9	LEU
9	s7	10	SER
9	s7	14	THR
9	s7	15	GLU
9	s7	24	PHE
9	s7	33	GLU
9	s7	35	LYS
9	s7	50	ASP
9	s7	67	LEU
9	s7	73	VAL
9	s7	77	LEU

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Mol	Chain	Res	Type
9	s7	79	ARG
9	s7	80	GLU
9	s7	86	GLN
9	s7	97	ARG
9	s7	108	GLN
9	s7	112	ARG
9	s7	114	ARG
9	s7	115	SER
9	s7	116	ARG
9	s7	117	THR
9	s7	118	LEU
9	s7	123	ASP
9	s7	130	VAL
9	s7	143	LEU
9	s7	144	VAL
9	s7	148	LYS
9	s7	149	ILE
9	s7	150	GLN
9	s7	163	ASP
9	s7	166	LEU
9	s7	177	THR
9	s7	180	GLN
9	s7	181	ILE
9	s7	185	ILE
10	s8	8	ARG
10	s8	18	ARG
10	s8	25	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	43	ILE
10	s8	46	VAL
10	s8	60	ILE
10	s8	61	GLU
10	s8	62	THR
10	s8	66	SER
10	s8	74	LYS
10	s8	92	ARG
10	s8	120	THR
10	s8	123	LYS
10	s8	151	LYS
10	s8	152	ILE
10	s8	155	SER

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Mol	Chain	Res	Type
10	s8	183	ILE
10	s8	184	LEU
10	s8	185	GLU
11	s9	3	ARG
11	s9	6	ARG
11	s9	7	THR
11	s9	9	SER
11	s9	16	LYS
11	s9	28	LEU
11	s9	37	LYS
11	s9	41	GLU
11	s9	49	LEU
11	s9	53	ARG
11	s9	54	ARG
11	s9	58	ASP
11	s9	78	ARG
11	s9	82	ARG
11	s9	89	ASP
11	s9	96	VAL
11	s9	105	LEU
11	s9	108	ARG
11	s9	109	LEU
11	s9	110	GLN
11	s9	111	THR
11	s9	118	LEU
11	s9	120	LYS
11	s9	126	ARG
11	s9	130	THR
11	s9	133	HIS
11	s9	134	ILE
11	s9	140	ILE
11	s9	142	ASN
11	s9	149	ARG
11	s9	150	LEU
11	s9	151	ASP
11	s9	162	SER
11	s9	172	VAL
11	s9	179	ARG
11	s9	180	LYS
11	s9	182	GLU
12	c0	2	LEU
12	c0	5	LYS

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Mol	Chain	Res	Type
12	c0	15	LEU
12	c0	21	VAL
12	c0	27	PHE
12	c0	33	GLU
12	c0	47	GLN
12	c0	48	SER
12	c0	55	VAL
12	c0	57	THR
12	c0	60	SER
12	c0	67	THR
12	c0	71	GLU
13	c1	3	THR
13	c1	5	LEU
13	c1	6	THR
13	c1	10	GLU
13	c1	21	ASN
13	c1	26	LYS
13	c1	27	THR
13	c1	30	ARG
13	c1	31	THR
13	c1	32	LYS
13	c1	33	ARG
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	77	SER
13	c1	78	THR
13	c1	80	MET
13	c1	86	ILE
13	c1	87	ARG
13	c1	109	VAL
13	c1	117	VAL
13	c1	123	VAL
13	c1	129	ARG
13	c1	138	ASN
14	c2	30	VAL
14	c2	36	LEU
14	c2	37	VAL
14	c2	38	HIS

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Mol	Chain	Res	Type
14	c2	39	ASP
14	c2	43	ARG
14	c2	45	LEU
14	c2	50	LYS
14	c2	52	LEU
14	c2	53	THR
14	c2	54	ARG
14	c2	58	LEU
14	c2	59	LEU
14	c2	61	VAL
14	c2	62	LEU
14	c2	65	SER
14	c2	71	ILE
14	c2	74	LEU
14	c2	83	GLU
14	c2	85	LYS
14	c2	89	ILE
14	c2	93	ASP
14	c2	103	LEU
14	c2	116	VAL
14	c2	120	VAL
14	c2	121	VAL
14	c2	132	GLU
14	c2	136	ILE
14	c2	140	PHE
15	c3	14	SER
15	c3	20	ARG
15	c3	21	ASN
15	c3	27	LYS
15	c3	35	GLU
15	c3	39	LYS
15	c3	53	LEU
15	c3	66	ILE
15	c3	67	THR
15	c3	80	LEU
15	c3	84	ILE
15	c3	87	ASP
15	c3	93	LYS
15	c3	102	LEU
15	c3	103	GLU
15	c3	107	LYS
15	c3	115	LEU

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Mol	Chain	Res	Type
15	c3	116	ILE
15	c3	125	LEU
15	c3	127	ARG
15	c3	131	THR
15	c3	138	ASN
15	c3	139	TRP
16	c4	13	VAL
16	c4	16	VAL
16	c4	18	ARG
16	c4	33	LEU
16	c4	51	ASP
16	c4	52	ARG
16	c4	65	GLN
16	c4	81	VAL
16	c4	82	LYS
16	c4	92	LYS
16	c4	102	LEU
16	c4	107	ARG
16	c4	110	LEU
16	c4	114	ARG
16	c4	119	THR
16	c4	123	SER
16	c4	124	ASP
16	c4	133	ARG
16	c4	136	ARG
17	c5	12	PHE
17	c5	24	LYS
17	c5	27	GLU
17	c5	29	SER
17	c5	36	LEU
17	c5	40	ARG
17	c5	44	ARG
17	c5	51	SER
17	c5	69	GLU
17	c5	71	GLU
17	c5	72	LYS
17	c5	92	SER
17	c5	107	ILE
17	c5	110	GLU
17	c5	112	LEU
17	c5	122	THR
17	c5	125	PRO

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Mol	Chain	Res	Type
17	c5	127	ARG
18	c6	6	SER
18	c6	23	LYS
18	c6	28	LEU
18	c6	37	THR
18	c6	38	LEU
18	c6	40	GLU
18	c6	43	ILE
18	c6	47	LYS
18	c6	50	GLU
18	c6	53	LEU
18	c6	55	VAL
18	c6	57	LEU
18	c6	66	ARG
18	c6	68	ARG
18	c6	69	VAL
18	c6	83	GLN
18	c6	90	VAL
18	c6	94	GLN
18	c6	110	THR
18	c6	114	ARG
18	c6	115	THR
18	c6	137	ARG
18	c6	140	LYS
18	c6	143	ARG
19	c7	3	ARG
19	c7	8	THR
19	c7	29	GLN
19	c7	34	LEU
19	c7	40	THR
19	c7	46	LEU
19	c7	69	ILE
19	c7	72	LYS
19	c7	75	GLU
19	c7	83	GLN
19	c7	85	VAL
19	c7	88	VAL
19	c7	104	ASN
19	c7	106	THR
19	c7	107	SER
20	c8	2	SER
20	c8	3	LEU

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Mol	Chain	Res	Type
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	15	LEU
20	c8	16	ARG
20	c8	25	ASN
20	c8	26	ILE
20	c8	33	THR
20	c8	34	THR
20	c8	36	LYS
20	c8	40	ARG
20	c8	63	GLN
20	c8	74	GLN
20	c8	85	PHE
20	c8	89	GLN
20	c8	94	ASP
20	c8	100	THR
20	c8	105	VAL
20	c8	116	LEU
20	c8	119	ILE
20	c8	133	VAL
20	c8	134	ARG
20	c8	136	GLN
20	c8	138	THR
20	c8	143	ARG
20	c8	144	ARG
20	c8	145	ARG
21	c9	27	LYS
21	c9	28	LEU
21	c9	29	GLU
21	c9	30	VAL
21	c9	34	VAL
21	c9	37	VAL
21	c9	41	SER
21	c9	57	ARG
21	c9	68	ARG
21	c9	70	GLN
21	c9	71	VAL
21	c9	75	LYS
21	c9	86	ARG
21	c9	88	VAL
21	c9	116	ILE

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Mol	Chain	Res	Type
21	c9	117	SER
21	c9	123	ARG
21	c9	129	GLN
21	c9	139	THR
21	c9	140	LEU
21	c9	142	GLU
22	d0	13	GLU
22	d0	22	ILE
22	d0	25	THR
22	d0	27	THR
22	d0	31	VAL
22	d0	34	LEU
22	d0	44	ASN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	61	LYS
22	d0	70	THR
22	d0	74	GLU
22	d0	77	LYS
22	d0	81	THR
22	d0	85	ARG
22	d0	88	LYS
22	d0	89	ARG
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	105	GLN
22	d0	107	THR
22	d0	108	ILE
22	d0	115	GLU
23	d1	2	GLU
23	d1	5	LYS
23	d1	10	GLU
23	d1	11	LEU
23	d1	12	TYR
23	d1	32	VAL
23	d1	33	GLN
23	d1	38	LYS
23	d1	41	GLU
23	d1	44	ARG
23	d1	49	GLU

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Mol	Chain	Res	Type
23	d1	52	THR
23	d1	66	ASP
23	d1	69	LEU
23	d1	74	GLN
23	d1	75	ASN
23	d1	78	LEU
23	d1	79	LEU
23	d1	81	ASN
23	d1	85	TYR
23	d1	86	SER
23	d1	87	ARG
24	d2	6	VAL
24	d2	7	LEU
24	d2	23	ARG
24	d2	24	GLN
24	d2	25	VAL
24	d2	26	LEU
24	d2	37	PHE
24	d2	43	LYS
24	d2	65	LEU
24	d2	74	VAL
24	d2	83	ILE
24	d2	88	LYS
24	d2	93	LEU
24	d2	103	ILE
24	d2	105	THR
24	d2	107	SER
25	d3	9	LEU
25	d3	14	LYS
25	d3	16	ARG
25	d3	17	VAL
25	d3	19	ARG
25	d3	28	ASN
25	d3	40	SER
25	d3	73	ARG
25	d3	84	THR
25	d3	96	VAL
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	109	ARG
25	d3	121	ARG

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Mol	Chain	Res	Type
25	d3	123	LYS
26	d4	6	THR
26	d4	8	ARG
26	d4	13	ILE
26	d4	22	GLN
26	d4	26	ASP
26	d4	36	SER
26	d4	38	ASP
26	d4	42	GLU
26	d4	43	LYS
26	d4	49	LYS
26	d4	51	GLU
26	d4	88	THR
26	d4	125	LEU
26	d4	132	ARG
27	d5	53	GLU
27	d5	57	TYR
27	d5	63	SER
27	d5	71	ILE
27	d5	78	ILE
27	d5	81	ARG
27	d5	88	ILE
27	d5	92	ILE
27	d5	93	SER
27	d5	97	LYS
28	d6	3	LYS
28	d6	10	ARG
28	d6	11	ASN
28	d6	30	ILE
28	d6	41	ILE
28	d6	44	ILE
28	d6	66	LYS
28	d6	67	THR
28	d6	82	ARG
28	d6	87	ARG
28	d6	89	ARG
28	d6	90	GLU
29	d7	3	LEU
29	d7	4	VAL
29	d7	11	THR
29	d7	19	HIS
29	d7	25	VAL

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Mol	Chain	Res	Type
29	d7	26	GLN
29	d7	37	CYS
29	d7	40	CYS
29	d7	41	LEU
29	d7	43	ILE
29	d7	44	THR
29	d7	49	HIS
29	d7	52	THR
29	d7	61	THR
29	d7	62	ILE
29	d7	72	LYS
29	d7	74	SER
29	d7	78	SER
30	d8	5	THR
30	d8	16	LEU
30	d8	19	THR
30	d8	22	ARG
30	d8	30	VAL
30	d8	33	LEU
30	d8	36	THR
30	d8	40	ILE
30	d8	52	ASP
30	d8	54	LEU
30	d8	58	GLU
30	d8	64	ARG
30	d8	66	LEU
31	d9	21	CYS
31	d9	23	VAL
31	d9	25	SER
31	d9	30	LEU
31	d9	32	ARG
31	d9	36	LEU
31	d9	54	LYS
80	e0	14	VAL
80	e0	15	LYS
80	e0	21	VAL
80	e0	24	THR
80	e0	26	LYS
80	e0	29	LYS
80	e0	38	LEU
80	e0	39	LEU
80	e0	44	PHE

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Mol	Chain	Res	Type
80	e0	49	LEU
80	e0	54	ARG
80	e0	56	MET
33	e1	82	LYS
33	e1	84	VAL
33	e1	87	THR
33	e1	90	LYS
33	e1	96	LYS
33	e1	97	LYS
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	108	VAL
33	e1	109	ASP
33	e1	113	LYS
33	e1	116	LYS
33	e1	120	GLU
33	e1	121	CYS
33	e1	130	VAL
33	e1	135	HIS
33	e1	147	VAL
33	e1	148	TYR
34	sR	10	ARG
34	sR	23	LEU
34	sR	25	THR
34	sR	29	GLN
34	sR	50	ASP
34	sR	58	VAL
34	sR	59	ARG
34	sR	64	HIS
34	sR	65	SER
34	sR	66	HIS
34	sR	74	THR
34	sR	76	ASP
34	sR	96	THR
34	sR	108	SER
34	sR	114	ASP
34	sR	123	ILE
34	sR	145	LEU
34	sR	159	ASN
34	sR	176	LYS
34	sR	202	LEU

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Mol	Chain	Res	Type
34	sR	228	LYS
34	sR	232	TYR
34	sR	234	LEU
34	sR	245	PHE
34	sR	260	ILE
34	sR	295	SER
34	sR	297	ASP
34	sR	309	VAL
34	sR	312	VAL
35	sM	23	LYS
35	sM	34	LYS
35	sM	43	ASP
35	sM	45	SER
35	sM	49	LYS
35	sM	61	ILE
35	sM	74	LYS
35	sM	75	ASP
35	sM	76	VAL
35	sM	77	THR
39	l2	7	ASN
39	l2	10	LYS
39	l2	15	ILE
39	l2	30	ARG
39	l2	32	LEU
39	l2	41	ILE
39	l2	44	ILE
39	l2	46	LYS
39	l2	48	ILE
39	l2	49	VAL
39	l2	52	SER
39	l2	61	VAL
39	l2	70	ARG
39	l2	74	GLU
39	l2	82	VAL
39	l2	84	THR
39	l2	95	SER
39	l2	96	LEU
39	l2	101	VAL
39	l2	112	ILE
39	l2	114	SER
39	l2	119	LYS
39	l2	134	VAL

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Mol	Chain	Res	Type
39	12	137	ILE
39	12	142	ASP
39	12	147	ARG
39	12	152	SER
39	12	155	LYS
39	12	168	VAL
39	12	169	ILE
39	12	179	LEU
39	12	188	LYS
39	12	191	LEU
39	12	193	ARG
39	12	200	ARG
39	12	202	VAL
39	12	204	MET
39	12	205	ASN
39	12	215	ASN
39	12	224	THR
39	12	227	ARG
39	12	230	VAL
39	12	233	GLN
39	12	241	ARG
39	12	243	THR
39	12	246	LEU
39	12	247	ARG
40	13	4	ARG
40	13	5	LYS
40	13	10	ARG
40	13	17	LEU
40	13	19	ARG
40	13	21	ARG
40	13	24	SER
40	13	37	ARG
40	13	38	SER
40	13	39	LYS
40	13	44	THR
40	13	47	LEU
40	13	56	ILE
40	13	65	SER
40	13	69	LYS
40	13	70	ARG
40	13	73	VAL
40	13	74	GLU

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Mol	Chain	Res	Type
40	l3	77	THR
40	l3	85	VAL
40	l3	102	LEU
40	l3	103	THR
40	l3	104	THR
40	l3	114	VAL
40	l3	125	SER
40	l3	132	LYS
40	l3	148	LEU
40	l3	150	ARG
40	l3	160	VAL
40	l3	169	THR
40	l3	183	LEU
40	l3	187	SER
40	l3	188	ILE
40	l3	192	VAL
40	l3	196	ARG
40	l3	197	GLU
40	l3	202	THR
40	l3	205	VAL
40	l3	208	VAL
40	l3	211	GLN
40	l3	213	GLU
40	l3	222	LYS
40	l3	232	ARG
40	l3	235	THR
40	l3	237	LYS
40	l3	238	LEU
40	l3	244	ARG
40	l3	246	LEU
40	l3	248	LYS
40	l3	249	VAL
40	l3	252	ILE
40	l3	261	MET
40	l3	266	ARG
40	l3	274	SER
40	l3	282	ILE
40	l3	284	ARG
40	l3	296	THR
40	l3	302	LYS
40	l3	308	MET
40	l3	316	GLU

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Mol	Chain	Res	Type
40	l3	320	ASP
40	l3	322	ILE
40	l3	328	ILE
40	l3	332	ARG
40	l3	338	LEU
40	l3	340	LYS
40	l3	341	SER
40	l3	347	SER
40	l3	348	ARG
40	l3	376	LYS
40	l3	382	THR
41	l4	2	SER
41	l4	3	ARG
41	l4	14	GLU
41	l4	16	THR
41	l4	18	ASN
41	l4	41	SER
41	l4	47	ARG
41	l4	48	GLN
41	l4	55	LYS
41	l4	64	SER
41	l4	73	ARG
41	l4	90	PHE
41	l4	92	ASN
41	l4	93	MET
41	l4	98	ARG
41	l4	99	MET
41	l4	118	LYS
41	l4	120	TYR
41	l4	136	LEU
41	l4	144	LYS
41	l4	150	LEU
41	l4	156	LEU
41	l4	170	LYS
41	l4	172	VAL
41	l4	176	SER
41	l4	177	ASP
41	l4	179	LEU
41	l4	186	LYS
41	l4	187	LEU
41	l4	200	THR
41	l4	202	ARG

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Mol	Chain	Res	Type
41	14	203	ARG
41	14	206	LEU
41	14	215	ILE
41	14	220	ARG
41	14	222	VAL
41	14	230	VAL
41	14	233	LEU
41	14	246	ARG
41	14	258	LEU
41	14	265	GLU
41	14	276	LEU
41	14	291	ASN
41	14	300	ARG
41	14	306	THR
41	14	307	GLN
41	14	313	LEU
41	14	319	LYS
41	14	321	LYS
41	14	323	VAL
41	14	327	LEU
41	14	339	LEU
41	14	347	THR
41	14	356	THR
41	14	357	GLU
41	14	358	THR
41	14	359	LEU
42	15	15	ARG
42	15	23	ARG
42	15	25	GLU
42	15	34	LYS
42	15	35	ARG
42	15	41	LYS
42	15	51	LEU
42	15	58	LYS
42	15	61	ILE
42	15	66	SER
42	15	68	THR
42	15	70	THR
42	15	73	VAL
42	15	74	VAL
42	15	89	THR
42	15	107	ARG

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Mol	Chain	Res	Type
42	15	110	LEU
42	15	112	LYS
42	15	113	LEU
42	15	118	THR
42	15	132	THR
42	15	135	VAL
42	15	140	ARG
42	15	144	VAL
42	15	146	LEU
42	15	148	ILE
42	15	151	GLN
42	15	152	ARG
42	15	155	THR
42	15	158	ARG
42	15	164	LYS
42	15	177	GLU
42	15	183	TRP
42	15	185	PHE
42	15	187	THR
42	15	190	ILE
42	15	194	LEU
42	15	206	GLN
42	15	210	GLU
42	15	211	LEU
42	15	218	ARG
42	15	221	GLU
42	15	226	TYR
42	15	227	LEU
42	15	236	LEU
42	15	241	THR
42	15	242	SER
42	15	258	LYS
42	15	259	LYS
42	15	261	THR
42	15	268	GLU
42	15	279	LYS
43	16	12	SER
43	16	18	LEU
43	16	19	LYS
43	16	21	THR
43	16	36	PRO
43	16	50	LYS

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Mol	Chain	Res	Type
43	16	65	ILE
43	16	76	LEU
43	16	78	ARG
43	16	80	ASN
43	16	82	ARG
43	16	84	VAL
43	16	89	THR
43	16	91	VAL
43	16	93	VAL
43	16	98	VAL
43	16	108	LYS
43	16	131	LYS
43	16	152	THR
43	16	155	LEU
43	16	160	SER
43	16	162	SER
44	17	26	VAL
44	17	41	ARG
44	17	54	GLU
44	17	60	ARG
44	17	78	GLU
44	17	82	LYS
44	17	83	LEU
44	17	88	ARG
44	17	98	LYS
44	17	100	ARG
44	17	101	LYS
44	17	110	ARG
44	17	124	LEU
44	17	129	LEU
44	17	130	ILE
44	17	156	ILE
44	17	158	LYS
44	17	173	LEU
44	17	175	LYS
44	17	178	ILE
44	17	179	LEU
44	17	184	LEU
44	17	208	SER
44	17	229	PHE
44	17	239	LEU
44	17	244	ASN

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Mol	Chain	Res	Type
45	18	41	GLN
45	18	50	VAL
45	18	65	LEU
45	18	67	ILE
45	18	68	ARG
45	18	71	VAL
45	18	74	THR
45	18	79	GLN
45	18	81	THR
45	18	89	GLU
45	18	90	THR
45	18	109	LEU
45	18	111	LYS
45	18	136	LEU
45	18	147	LYS
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	185	ARG
45	18	200	LEU
45	18	211	LEU
45	18	217	THR
45	18	224	ASP
45	18	230	LYS
45	18	231	LYS
45	18	248	LYS
46	19	5	GLN
46	19	6	THR
46	19	17	THR
46	19	18	VAL
46	19	19	SER
46	19	24	ILE
46	19	31	ARG
46	19	33	THR
46	19	39	LYS
46	19	43	VAL
46	19	52	LEU
46	19	55	VAL
46	19	62	ARG

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Mol	Chain	Res	Type
46	19	63	LYS
46	19	68	LEU
46	19	69	ARG
46	19	70	THR
46	19	89	LYS
46	19	92	TYR
46	19	107	ASP
46	19	118	LEU
46	19	121	LYS
46	19	129	ARG
46	19	130	ASP
46	19	132	VAL
46	19	133	THR
46	19	138	THR
46	19	143	GLU
46	19	144	ILE
46	19	146	LEU
46	19	151	VAL
46	19	152	GLU
46	19	157	ASN
46	19	161	LEU
46	19	162	GLN
46	19	177	ASP
46	19	191	LEU
47	m0	4	ARG
47	m0	24	ARG
47	m0	30	LYS
47	m0	36	LEU
47	m0	38	LYS
47	m0	39	LYS
47	m0	48	LEU
47	m0	52	LEU
47	m0	53	VAL
47	m0	57	LEU
47	m0	59	GLN
47	m0	60	LEU
47	m0	63	GLU
47	m0	71	CYS
47	m0	76	MET
47	m0	77	THR
47	m0	87	LEU
47	m0	99	ILE

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Mol	Chain	Res	Type
47	m0	103	LEU
47	m0	128	ARG
47	m0	130	ASP
47	m0	139	ARG
47	m0	144	ASN
47	m0	156	ARG
47	m0	163	GLN
47	m0	167	LEU
47	m0	168	SER
47	m0	169	LYS
47	m0	177	ASP
47	m0	178	ARG
47	m0	197	VAL
47	m0	201	SER
47	m0	208	ASN
47	m0	211	ARG
47	m0	217	PHE
48	m1	6	GLN
48	m1	9	MET
48	m1	10	ARG
48	m1	11	ASP
48	m1	12	LEU
48	m1	13	LYS
48	m1	16	LYS
48	m1	29	ARG
48	m1	30	LEU
48	m1	34	SER
48	m1	35	LYS
48	m1	44	THR
48	m1	46	VAL
48	m1	51	ARG
48	m1	54	VAL
48	m1	56	THR
48	m1	61	ARG
48	m1	82	ARG
48	m1	92	ARG
48	m1	99	THR
48	m1	107	ASP
48	m1	112	LEU
48	m1	129	VAL
48	m1	130	VAL
48	m1	140	ARG

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Mol	Chain	Res	Type
48	m1	142	LYS
48	m1	147	THR
48	m1	148	VAL
48	m1	151	SER
48	m1	158	ASP
48	m1	159	THR
48	m1	161	SER
48	m1	165	GLN
48	m1	166	LYS
48	m1	171	VAL
49	m3	13	HIS
49	m3	54	LEU
49	m3	57	VAL
49	m3	58	VAL
49	m3	59	ARG
49	m3	63	VAL
49	m3	67	ARG
49	m3	69	VAL
49	m3	73	ARG
49	m3	76	THR
49	m3	86	THR
49	m3	104	ARG
49	m3	107	GLU
49	m3	108	ILE
49	m3	114	GLN
49	m3	118	GLU
49	m3	121	SER
49	m3	123	ILE
49	m3	124	ILE
49	m3	131	LYS
49	m3	149	GLN
49	m3	154	VAL
49	m3	157	ARG
49	m3	164	GLU
49	m3	168	ARG
49	m3	171	ARG
49	m3	180	ARG
49	m3	183	ARG
49	m3	184	GLU
49	m3	189	GLU
49	m3	190	LYS
50	m4	3	THR

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Mol	Chain	Res	Type
50	m4	4	ASP
50	m4	6	ILE
50	m4	16	GLU
50	m4	20	VAL
50	m4	53	VAL
50	m4	58	ILE
50	m4	60	LEU
50	m4	63	VAL
50	m4	64	VAL
50	m4	72	LEU
50	m4	82	SER
50	m4	107	GLU
50	m4	108	ARG
50	m4	126	GLN
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	7	LEU
51	m5	8	GLU
51	m5	12	ARG
51	m5	19	LEU
51	m5	20	ARG
51	m5	24	ARG
51	m5	49	ARG
51	m5	64	VAL
51	m5	66	VAL
51	m5	67	ARG
51	m5	68	ARG
51	m5	75	VAL
51	m5	76	PRO
51	m5	80	THR
51	m5	85	THR
51	m5	90	ASN
51	m5	91	GLU
51	m5	97	SER
51	m5	98	LEU
51	m5	105	ARG
51	m5	106	VAL
51	m5	117	ASN
51	m5	138	GLN
51	m5	142	ILE
51	m5	153	ASP

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Mol	Chain	Res	Type
51	m5	159	ARG
51	m5	171	SER
51	m5	175	ASN
51	m5	176	LYS
51	m5	183	THR
51	m5	188	ARG
51	m5	190	THR
51	m5	194	GLN
51	m5	198	SER
51	m5	204	LYS
52	m6	3	VAL
52	m6	18	ARG
52	m6	22	VAL
52	m6	34	VAL
52	m6	58	LEU
52	m6	59	ARG
52	m6	67	THR
52	m6	74	ARG
52	m6	84	LEU
52	m6	85	ARG
52	m6	100	GLU
52	m6	106	GLU
52	m6	108	ILE
52	m6	110	PRO
52	m6	115	LYS
52	m6	117	ARG
52	m6	122	GLN
52	m6	124	LEU
52	m6	134	LYS
52	m6	136	THR
52	m6	143	THR
52	m6	160	ARG
52	m6	166	GLU
52	m6	171	LYS
52	m6	180	SER
52	m6	182	ASN
52	m6	184	THR
52	m6	188	SER
52	m6	190	VAL
53	m7	9	THR
53	m7	16	SER
53	m7	31	GLU

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Mol	Chain	Res	Type
53	m7	32	THR
53	m7	42	THR
53	m7	52	LEU
53	m7	53	ASP
53	m7	55	GLN
53	m7	56	ARG
53	m7	78	VAL
53	m7	89	LYS
53	m7	105	LYS
53	m7	114	VAL
53	m7	124	LYS
53	m7	126	ARG
53	m7	127	ARG
53	m7	144	SER
53	m7	148	LEU
53	m7	155	GLU
54	m8	7	SER
54	m8	8	LYS
54	m8	9	GLN
54	m8	17	THR
54	m8	22	ASP
54	m8	26	LEU
54	m8	31	LYS
54	m8	32	LEU
54	m8	34	THR
54	m8	41	ASP
54	m8	49	LEU
54	m8	63	SER
54	m8	64	VAL
54	m8	80	THR
54	m8	81	VAL
54	m8	93	ILE
54	m8	98	LYS
54	m8	113	LYS
54	m8	122	ILE
54	m8	135	GLN
54	m8	138	LEU
54	m8	147	ARG
54	m8	165	ILE
54	m8	166	LEU
54	m8	167	SER
54	m8	170	ARG

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Mol	Chain	Res	Type
54	m8	178	ARG
54	m8	186	VAL
55	m9	5	ARG
55	m9	7	GLN
55	m9	8	LYS
55	m9	20	ARG
55	m9	24	LEU
55	m9	27	ASN
55	m9	29	THR
55	m9	30	SER
55	m9	36	ASN
55	m9	37	SER
55	m9	43	LYS
55	m9	49	THR
55	m9	52	LYS
55	m9	56	THR
55	m9	57	VAL
55	m9	63	THR
55	m9	70	LYS
55	m9	74	ARG
55	m9	98	ARG
55	m9	99	LEU
55	m9	105	LEU
55	m9	106	LEU
55	m9	119	LEU
55	m9	126	GLU
55	m9	128	LYS
55	m9	130	ASN
55	m9	133	LYS
55	m9	134	HIS
55	m9	138	LEU
55	m9	139	VAL
55	m9	148	ASP
55	m9	152	GLU
55	m9	153	LYS
55	m9	156	ASN
55	m9	158	GLU
55	m9	167	ARG
55	m9	170	ARG
55	m9	186	LYS
56	n0	1	MET
56	n0	13	ARG

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Mol	Chain	Res	Type
56	n0	17	GLU
56	n0	21	GLU
56	n0	23	LYS
56	n0	32	SER
56	n0	45	LEU
56	n0	51	VAL
56	n0	53	LYS
56	n0	55	SER
56	n0	58	ILE
56	n0	73	LYS
56	n0	74	ASN
56	n0	77	VAL
56	n0	84	ARG
56	n0	87	THR
56	n0	96	ASP
56	n0	97	VAL
56	n0	104	GLU
56	n0	115	ARG
56	n0	117	ARG
56	n0	125	LYS
56	n0	130	GLU
56	n0	132	THR
56	n0	137	ARG
56	n0	145	THR
56	n0	148	LEU
56	n0	149	LYS
56	n0	155	ARG
56	n0	160	THR
56	n0	162	THR
56	n0	164	SER
56	n0	172	TYR
57	n1	3	LYS
57	n1	22	HIS
57	n1	32	LYS
57	n1	35	LYS
57	n1	36	VAL
57	n1	52	MET
57	n1	55	LYS
57	n1	71	SER
57	n1	80	VAL
57	n1	83	ARG
57	n1	88	ARG

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Mol	Chain	Res	Type
57	n1	89	LEU
57	n1	93	VAL
57	n1	96	ILE
57	n1	102	ARG
57	n1	104	GLU
57	n1	126	VAL
57	n1	131	GLN
57	n1	139	ARG
57	n1	141	VAL
57	n1	143	THR
57	n1	149	GLN
57	n1	150	THR
57	n1	154	VAL
58	n2	13	LYS
58	n2	16	THR
58	n2	21	SER
58	n2	23	THR
58	n2	27	VAL
58	n2	37	LEU
58	n2	43	VAL
58	n2	47	VAL
58	n2	50	LEU
58	n2	54	VAL
58	n2	55	THR
58	n2	58	GLU
58	n2	63	VAL
58	n2	68	THR
58	n2	72	SER
58	n2	74	LYS
58	n2	90	ARG
58	n2	98	THR
59	n3	4	ASN
59	n3	13	ILE
59	n3	45	ARG
59	n3	48	ARG
59	n3	66	LYS
59	n3	69	LEU
59	n3	88	ARG
59	n3	115	THR
59	n3	120	LYS
60	n4	1	MET
60	n4	26	SER

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Mol	Chain	Res	Type
60	n4	39	LEU
60	n4	63	ILE
60	n4	82	ILE
60	n4	89	LEU
60	n4	96	LEU
60	n4	105	ARG
60	n4	119	GLU
60	n4	126	GLU
60	n4	127	LYS
61	n5	24	LEU
61	n5	27	ARG
61	n5	33	ARG
61	n5	34	LEU
61	n5	37	THR
61	n5	38	LEU
61	n5	45	LYS
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	71	THR
61	n5	78	ASP
61	n5	86	VAL
61	n5	88	MET
61	n5	108	LEU
61	n5	115	ARG
61	n5	117	ASN
61	n5	125	ARG
61	n5	135	ILE
62	n6	3	LYS
62	n6	7	ASP
62	n6	11	ASP
62	n6	12	ARG
62	n6	13	ARG
62	n6	14	LYS
62	n6	25	SER
62	n6	32	SER
62	n6	35	LEU
62	n6	37	LYS
62	n6	38	GLU
62	n6	39	LEU
62	n6	40	ARG
62	n6	45	ILE

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Mol	Chain	Res	Type
62	n6	50	ILE
62	n6	51	ARG
62	n6	55	GLU
62	n6	56	VAL
62	n6	57	LEU
62	n6	66	GLN
62	n6	67	GLU
62	n6	69	LYS
62	n6	74	TYR
62	n6	76	LEU
62	n6	83	ASP
62	n6	89	LYS
62	n6	90	VAL
62	n6	91	ASN
62	n6	94	SER
62	n6	99	LEU
62	n6	105	VAL
62	n6	115	ARG
62	n6	119	ILE
62	n6	120	GLN
62	n6	122	LYS
62	n6	126	LEU
63	n7	5	LEU
63	n7	17	ARG
63	n7	24	VAL
63	n7	26	VAL
63	n7	33	SER
63	n7	34	LYS
63	n7	36	HIS
63	n7	42	LEU
63	n7	46	ILE
63	n7	52	LYS
63	n7	56	LYS
63	n7	72	ILE
63	n7	73	LYS
63	n7	81	LEU
63	n7	83	THR
63	n7	86	THR
63	n7	90	GLU
63	n7	95	VAL
63	n7	97	SER
63	n7	99	GLU

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Mol	Chain	Res	Type
63	n7	103	GLN
63	n7	121	ARG
63	n7	126	LYS
63	n7	127	ASN
63	n7	128	GLN
63	n7	132	SER
63	n7	134	LEU
63	n7	135	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	10	LYS
64	n8	15	VAL
64	n8	24	LYS
64	n8	27	LYS
64	n8	34	MET
64	n8	42	ARG
64	n8	45	MET
64	n8	46	ASP
64	n8	56	VAL
64	n8	60	TYR
64	n8	65	GLN
64	n8	67	HIS
64	n8	73	LEU
64	n8	78	LEU
64	n8	82	ILE
64	n8	85	ASP
64	n8	88	ASP
64	n8	89	GLN
64	n8	91	LEU
64	n8	97	GLU
64	n8	98	THR
64	n8	115	LYS
64	n8	124	ILE
64	n8	128	ARG
64	n8	133	LEU
65	n9	10	HIS
65	n9	14	ARG
65	n9	21	ILE
65	n9	22	LYS
65	n9	23	LYS
65	n9	26	THR
65	n9	33	LYS

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Mol	Chain	Res	Type
65	n9	38	LYS
65	n9	50	THR
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	14	LEU
66	o0	30	THR
66	o0	32	LYS
66	o0	33	SER
66	o0	34	LEU
66	o0	40	LYS
66	o0	41	LEU
66	o0	61	MET
66	o0	65	THR
66	o0	76	GLU
66	o0	81	VAL
66	o0	83	LYS
66	o0	86	ARG
66	o0	87	VAL
66	o0	89	VAL
66	o0	92	ILE
67	o1	6	ASP
67	o1	8	VAL
67	o1	16	LEU
67	o1	26	LYS
67	o1	28	ARG
67	o1	31	ARG
67	o1	34	LYS
67	o1	36	ILE
67	o1	42	LEU
67	o1	44	MET
67	o1	46	THR
67	o1	50	ARG
67	o1	55	LEU
67	o1	64	VAL
67	o1	70	ARG
67	o1	76	SER
67	o1	82	GLU
67	o1	90	PHE

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Mol	Chain	Res	Type
67	o1	96	VAL
67	o1	98	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
67	o1	112	ASP
68	o2	16	LYS
68	o2	19	ARG
68	o2	21	HIS
68	o2	24	ARG
68	o2	33	ARG
68	o2	34	LYS
68	o2	35	GLN
68	o2	40	SER
68	o2	41	VAL
68	o2	51	SER
68	o2	52	GLN
68	o2	54	LYS
68	o2	61	LYS
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	86	THR
68	o2	89	THR
68	o2	109	LEU
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	10	LYS
69	o3	20	LYS
69	o3	21	ARG
69	o3	28	SER
69	o3	31	LYS
69	o3	33	GLU
69	o3	37	THR
69	o3	49	ILE
69	o3	56	SER
69	o3	58	GLU
69	o3	59	VAL

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Mol	Chain	Res	Type
69	o3	73	ARG
69	o3	74	THR
69	o3	81	VAL
69	o3	84	THR
69	o3	90	PRO
69	o3	93	THR
69	o3	98	VAL
70	o4	6	THR
70	o4	9	ARG
70	o4	10	ARG
70	o4	20	ILE
70	o4	23	VAL
70	o4	24	LYS
70	o4	25	THR
70	o4	31	ARG
70	o4	33	GLN
70	o4	46	ASP
70	o4	47	CYS
70	o4	58	ARG
70	o4	71	THR
70	o4	79	SER
70	o4	85	VAL
70	o4	88	ARG
70	o4	95	ILE
70	o4	98	GLN
70	o4	101	VAL
71	o5	4	VAL
71	o5	20	GLN
71	o5	21	LEU
71	o5	27	GLU
71	o5	31	LEU
71	o5	38	ARG
71	o5	41	LEU
71	o5	44	ILE
71	o5	45	LYS
71	o5	46	THR
71	o5	47	VAL
71	o5	62	GLN
71	o5	69	LEU
71	o5	79	ASP
71	o5	84	LYS
71	o5	85	THR

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Mol	Chain	Res	Type
71	o5	86	ARG
71	o5	88	LEU
71	o5	98	SER
71	o5	100	VAL
71	o5	107	LYS
71	o5	113	GLN
71	o5	118	ILE
72	o6	7	ILE
72	o6	9	ILE
72	o6	12	ASN
72	o6	15	LYS
72	o6	16	LYS
72	o6	17	VAL
72	o6	21	THR
72	o6	26	ILE
72	o6	27	SER
72	o6	29	LYS
72	o6	34	SER
72	o6	35	ASN
72	o6	36	ARG
72	o6	37	THR
72	o6	38	LYS
72	o6	42	SER
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	68	ARG
72	o6	76	ARG
72	o6	89	GLU
72	o6	93	ILE
72	o6	94	ILE
72	o6	98	ARG
73	o7	7	SER
73	o7	25	ARG
73	o7	36	SER
73	o7	54	LYS
73	o7	55	ARG
73	o7	58	THR
73	o7	59	THR
73	o7	67	LEU
73	o7	70	VAL

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Mol	Chain	Res	Type
73	o7	80	THR
73	o7	84	SER
74	o8	5	ILE
74	o8	6	THR
74	o8	12	LEU
74	o8	13	GLU
74	o8	14	LEU
74	o8	16	ARG
74	o8	19	ASP
74	o8	20	VAL
74	o8	22	THR
74	o8	24	THR
74	o8	31	LEU
74	o8	40	GLN
74	o8	41	THR
74	o8	48	SER
74	o8	50	SER
74	o8	53	THR
74	o8	63	LYS
74	o8	64	LYS
74	o8	65	LEU
75	o9	4	GLN
75	o9	5	LYS
75	o9	11	GLN
75	o9	21	ARG
75	o9	23	LEU
75	o9	29	LEU
75	o9	31	THR
75	o9	51	ILE
76	q0	78	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	127	LEU
77	q1	2	ARG
77	q1	6	ARG
77	q1	9	ARG
77	q1	13	LEU
77	q1	16	LYS

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Mol	Chain	Res	Type
77	q1	21	ARG
77	q1	23	ARG
77	q1	24	SER
78	q2	7	THR
78	q2	8	ARG
78	q2	17	CYS
78	q2	20	HIS
78	q2	26	THR
78	q2	35	LEU
78	q2	45	ARG
78	q2	46	LYS
78	q2	61	LYS
78	q2	71	ARG
78	q2	72	LEU
78	q2	78	LYS
78	q2	79	THR
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	87	ARG
78	q2	93	LEU
78	q2	105	GLN
78	q2	106	PHE
79	q3	10	ILE
79	q3	20	SER
79	q3	24	ARG
79	q3	40	SER
79	q3	41	PHE
79	q3	45	LYS
79	q3	48	LYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	59	CYS
79	q3	72	SER
79	q3	78	THR
79	q3	79	VAL
79	q3	81	SER
81	p0	4	ILE
81	p0	5	ARG
81	p0	14	LYS
81	p0	15	LEU

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Mol	Chain	Res	Type
81	p0	25	LEU
81	p0	28	VAL
81	p0	32	ASN
81	p0	42	ARG
81	p0	44	GLU
81	p0	51	VAL
81	p0	57	THR
81	p0	63	ILE
81	p0	67	LEU
81	p0	68	SER
81	p0	70	LEU
81	p0	76	LEU
81	p0	81	LYS
81	p0	83	ASN
81	p0	84	VAL
81	p0	91	GLU
81	p0	93	LEU
81	p0	97	LYS
81	p0	103	ASN
81	p0	104	ARG

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

Mol	Chain	Res	Type
3	S1	149	GLN
3	S1	177	GLN
3	S1	209	ASN
6	S4	259	GLN
7	S5	139	ASN
8	S6	59	GLN
9	S7	74	GLN
9	S7	170	GLN
11	S9	110	GLN
12	C0	12	HIS
14	C2	70	ASN
21	C9	25	GLN
23	D1	74	GLN
24	D2	56	HIS
27	D5	95	HIS
31	D9	48	ASN
32	E0	17	GLN
41	L4	320	ASN

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Mol	Chain	Res	Type
42	L5	40	HIS
44	L7	244	ASN
46	L9	49	ASN
47	M0	95	HIS
47	M0	144	ASN
51	M5	37	HIS
54	M8	145	ASN
56	N0	154	HIS
57	N1	146	ASN
59	N3	98	ASN
62	N6	42	GLN
63	N7	127	ASN
65	N9	6	ASN
78	Q2	22	GLN
11	s9	110	GLN
11	s9	124	HIS
11	s9	142	ASN
12	c0	32	HIS
14	c2	125	ASN
20	c8	89	GLN
20	c8	90	ASN
22	d0	12	GLN
22	d0	72	ASN
24	d2	56	HIS
25	d3	48	HIS
29	d7	19	HIS
29	d7	42	ASN
40	l3	211	GLN
42	l5	40	HIS
52	m6	31	GLN
52	m6	72	HIS
57	n1	26	HIS
61	n5	111	ASN
63	n7	103	GLN
64	n8	49	HIS
69	o3	5	HIS
70	o4	3	GLN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1800 (98%)	496 (27%)	62 (3%)
1	6	1793/1800 (99%)	470 (26%)	50 (2%)
36	1	3145/3396 (92%)	697 (22%)	82 (2%)
36	5	3145/3396 (92%)	693 (22%)	83 (2%)
37	3	120/121 (99%)	17 (14%)	2 (1%)
37	7	120/121 (99%)	18 (15%)	1 (0%)
38	4	157/158 (99%)	38 (24%)	4 (2%)
38	8	157/158 (99%)	35 (22%)	5 (3%)
All	All	10414/10950 (95%)	2464 (23%)	289 (2%)

All (2464) 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	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
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	99	C
1	2	101	U
1	2	104	A
1	2	111	U
1	2	114	C

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Mol	Chain	Res	Type
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	175	G
1	2	178	U
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	189	C
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	200	A
1	2	214	G
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	233	C
1	2	234	G

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Mol	Chain	Res	Type
1	2	235	G
1	2	236	A
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	242	U
1	2	246	G
1	2	250	C
1	2	261	U
1	2	262	U
1	2	265	A
1	2	267	U
1	2	269	G
1	2	271	A
1	2	272	U
1	2	274	G
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	288	A
1	2	290	G
1	2	299	A
1	2	308	C
1	2	309	C
1	2	313	U
1	2	314	C
1	2	316	A
1	2	319	U
1	2	321	C
1	2	322	G
1	2	337	G
1	2	338	C
1	2	341	A
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	387	A

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Mol	Chain	Res	Type
1	2	397	A
1	2	399	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	403	G
1	2	404	G
1	2	416	A
1	2	418	G
1	2	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	446	A
1	2	447	U
1	2	448	C
1	2	454	U
1	2	459	G
1	2	468	A
1	2	483	A
1	2	484	C
1	2	485	A
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G

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Mol	Chain	Res	Type
1	2	511	A
1	2	512	A
1	2	513	U
1	2	514	G
1	2	515	A
1	2	516	G
1	2	519	C
1	2	520	A
1	2	525	A
1	2	527	A
1	2	532	U
1	2	534	A
1	2	536	C
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	548	G
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	579	A
1	2	580	A
1	2	594	A
1	2	595	G
1	2	597	G
1	2	606	A
1	2	617	U
1	2	619	A
1	2	620	A
1	2	621	A
1	2	622	A
1	2	623	A
1	2	639	U
1	2	640	U
1	2	650	U
1	2	653	C
1	2	655	G

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Mol	Chain	Res	Type
1	2	656	G
1	2	657	U
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C
1	2	692	C
1	2	694	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	709	C
1	2	710	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	729	G
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A

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Mol	Chain	Res	Type
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	744	U
1	2	745	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	776	G
1	2	778	G
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	785	U
1	2	787	G
1	2	789	A
1	2	793	A
1	2	794	U
1	2	795	U
1	2	796	A
1	2	806	A
1	2	807	A
1	2	811	A
1	2	812	A
1	2	813	U
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	830	U
1	2	831	U

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Mol	Chain	Res	Type
1	2	833	U
1	2	837	G
1	2	854	U
1	2	856	A
1	2	860	U
1	2	862	A
1	2	863	A
1	2	865	A
1	2	876	G
1	2	886	U
1	2	896	U
1	2	898	A
1	2	911	U
1	2	912	U
1	2	913	G
1	2	914	G
1	2	915	A
1	2	916	U
1	2	921	U
1	2	933	A
1	2	935	U
1	2	942	G
1	2	949	C
1	2	951	A
1	2	959	U
1	2	960	U
1	2	966	A
1	2	988	A
1	2	991	G
1	2	992	A
1	2	993	A
1	2	995	A
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1020	A
1	2	1021	C
1	2	1026	A
1	2	1028	C
1	2	1029	U
1	2	1031	U
1	2	1039	A

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Mol	Chain	Res	Type
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1066	C
1	2	1076	A
1	2	1079	U
1	2	1080	U
1	2	1082	C
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1111	G
1	2	1117	U
1	2	1138	A
1	2	1139	A
1	2	1146	G
1	2	1150	G
1	2	1151	A
1	2	1154	G
1	2	1155	G
1	2	1157	A
1	2	1158	C
1	2	1160	A
1	2	1163	A
1	2	1164	G
1	2	1165	G
1	2	1167	G
1	2	1168	U
1	2	1176	G
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G

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Mol	Chain	Res	Type
1	2	1200	G
1	2	1202	A
1	2	1207	C
1	2	1208	A
1	2	1217	A
1	2	1218	G
1	2	1226	A
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1257	U
1	2	1258	U
1	2	1260	U
1	2	1286	U
1	2	1287	A
1	2	1301	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	1354	G
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	1383	G
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1400	A

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Mol	Chain	Res	Type
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	1447	C
1	2	1457	C
1	2	1458	G
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	1477	G
1	2	1482	C
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1499	G
1	2	1506	G
1	2	1516	A
1	2	1517	U
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	1542	G
1	2	1550	A
1	2	1557	U
1	2	1559	A
1	2	1569	A

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Mol	Chain	Res	Type
1	2	1573	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	1624	C
1	2	1631	A
1	2	1634	C
1	2	1639	C
1	2	1657	U
1	2	1658	G
1	2	1681	A
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1692	G
1	2	1697	G
1	2	1698	G
1	2	1699	G
1	2	1700	C
1	2	1701	A
1	2	1702	A
1	2	1703	C
1	2	1711	C
1	2	1712	A
1	2	1713	G
1	2	1715	G
1	2	1729	C
1	2	1730	A
1	2	1747	G
1	2	1750	A
1	2	1756	A
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

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Mol	Chain	Res	Type
1	2	1789	G
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	26	A
36	1	40	A
36	1	43	A
36	1	49	A
36	1	56	G
36	1	57	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	68	C
36	1	76	G
36	1	92	G
36	1	93	C
36	1	94	G
36	1	99	A
36	1	109	A
36	1	110	G
36	1	111	C
36	1	121	A
36	1	122	A
36	1	133	U
36	1	136	G
36	1	143	G
36	1	147	U
36	1	156	G
36	1	157	A
36	1	160	G
36	1	163	C
36	1	166	C
36	1	169	U
36	1	173	G
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C

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Mol	Chain	Res	Type
36	1	200	C
36	1	210	U
36	1	213	A
36	1	218	G
36	1	219	A
36	1	238	A
36	1	240	U
36	1	241	G
36	1	243	G
36	1	245	U
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	266	A
36	1	269	G
36	1	278	U
36	1	282	G
36	1	283	G
36	1	284	A
36	1	286	U
36	1	295	A
36	1	298	U
36	1	323	A
36	1	326	U
36	1	329	U
36	1	339	C
36	1	344	A
36	1	349	A
36	1	350	C
36	1	351	A
36	1	352	A
36	1	375	A
36	1	376	G
36	1	395	A
36	1	397	A
36	1	398	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	419	G
36	1	421	G

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Mol	Chain	Res	Type
36	1	422	A
36	1	439	C
36	1	440	A
36	1	495	G
36	1	498	A
36	1	520	U
36	1	521	A
36	1	523	A
36	1	531	G
36	1	535	G
36	1	536	U
36	1	541	U
36	1	543	C
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	556	U
36	1	557	A
36	1	558	U
36	1	559	A
36	1	569	A
36	1	578	A
36	1	579	G
36	1	589	A
36	1	592	A
36	1	594	U
36	1	595	G
36	1	601	U
36	1	604	G
36	1	609	G
36	1	611	A
36	1	620	U
36	1	621	A
36	1	625	G
36	1	636	C
36	1	649	A
36	1	651	G
36	1	658	G

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Mol	Chain	Res	Type
36	1	660	A
36	1	677	A
36	1	679	U
36	1	681	U
36	1	691	A
36	1	705	A
36	1	708	G
36	1	709	A
36	1	712	G
36	1	715	A
36	1	716	A
36	1	719	U
36	1	725	G
36	1	733	G
36	1	735	A
36	1	758	C
36	1	759	U
36	1	763	G
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	768	C
36	1	776	U
36	1	777	U
36	1	780	A
36	1	781	G
36	1	784	A
36	1	785	G
36	1	786	A
36	1	806	A
36	1	817	A
36	1	830	A
36	1	837	A
36	1	849	C
36	1	861	C
36	1	865	U
36	1	872	U
36	1	874	U
36	1	879	U
36	1	890	C
36	1	894	G

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Mol	Chain	Res	Type
36	1	896	A
36	1	907	G
36	1	908	G
36	1	910	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	923	C
36	1	924	G
36	1	937	G
36	1	944	C
36	1	947	G
36	1	959	C
36	1	960	U
36	1	973	A
36	1	974	G
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	991	G
36	1	994	G
36	1	1000	C
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1021	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1037	C
36	1	1047	A
36	1	1049	C
36	1	1057	A
36	1	1064	A
36	1	1065	A

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Mol	Chain	Res	Type
36	1	1068	C
36	1	1069	C
36	1	1071	U
36	1	1072	G
36	1	1079	A
36	1	1081	U
36	1	1082	U
36	1	1087	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1121	U
36	1	1128	U
36	1	1131	G
36	1	1144	U
36	1	1148	G
36	1	1153	A
36	1	1154	A
36	1	1159	A
36	1	1160	C
36	1	1165	A
36	1	1179	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1185	C
36	1	1190	A
36	1	1191	U
36	1	1192	C
36	1	1196	C
36	1	1201	C
36	1	1202	A
36	1	1205	A
36	1	1206	G
36	1	1209	G
36	1	1212	A

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Mol	Chain	Res	Type
36	1	1213	G
36	1	1216	C
36	1	1217	A
36	1	1218	U
36	1	1222	G
36	1	1225	A
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	1242	G
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1251	A
36	1	1258	U
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
36	1	1267	U
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1274	A
36	1	1278	A
36	1	1279	C
36	1	1280	C
36	1	1285	G
36	1	1286	A
36	1	1287	A
36	1	1292	C
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1313	G

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Mol	Chain	Res	Type
36	1	1330	A
36	1	1345	G
36	1	1348	U
36	1	1349	G
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1363	A
36	1	1379	G
36	1	1380	G
36	1	1386	A
36	1	1399	A
36	1	1400	G
36	1	1417	G
36	1	1418	A
36	1	1419	A
36	1	1425	U
36	1	1429	G
36	1	1431	G
36	1	1434	G
36	1	1437	C
36	1	1446	A
36	1	1450	G
36	1	1455	U
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1487	G
36	1	1495	U
36	1	1496	C
36	1	1508	C
36	1	1524	A
36	1	1527	C
36	1	1529	A
36	1	1536	G
36	1	1556	C
36	1	1558	A
36	1	1560	G
36	1	1562	C

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Mol	Chain	Res	Type
36	1	1563	C
36	1	1564	U
36	1	1565	G
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1572	U
36	1	1576	G
36	1	1578	C
36	1	1579	C
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1605	A
36	1	1607	U
36	1	1620	U
36	1	1629	U
36	1	1639	C
36	1	1641	U
36	1	1643	A
36	1	1645	U
36	1	1655	G
36	1	1657	C
36	1	1677	G
36	1	1683	A
36	1	1716	U
36	1	1717	U
36	1	1725	C
36	1	1727	G
36	1	1736	G
36	1	1741	A
36	1	1742	U
36	1	1750	A
36	1	1751	G
36	1	1762	C
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1770	G

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Mol	Chain	Res	Type
36	1	1779	C
36	1	1780	G
36	1	1797	A
36	1	1809	A
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	1835	A
36	1	1839	A
36	1	1841	A
36	1	1842	A
36	1	1845	G
36	1	1846	C
36	1	1849	C
36	1	1855	U
36	1	1863	G
36	1	1864	A
36	1	1866	C
36	1	1871	U
36	1	1879	A
36	1	1880	U
36	1	1886	A
36	1	1901	A
36	1	1906	G
36	1	1931	U
36	1	1935	G
36	1	1948	G
36	1	1951	C
36	1	1952	G
36	1	1954	G
36	1	2094	C
36	1	2097	U
36	1	2101	C
36	1	2102	U
36	1	2111	G
36	1	2112	U
36	1	2113	A

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Mol	Chain	Res	Type
36	1	2114	C
36	1	2116	G
36	1	2121	G
36	1	2122	G
36	1	2123	G
36	1	2124	G
36	1	2131	A
36	1	2138	A
36	1	2139	A
36	1	2140	U
36	1	2146	C
36	1	2158	A
36	1	2168	A
36	1	2169	G
36	1	2187	G
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	2226	U
36	1	2239	G
36	1	2244	A
36	1	2249	G
36	1	2250	G
36	1	2252	A
36	1	2255	A
36	1	2256	A
36	1	2267	C
36	1	2272	G
36	1	2273	G
36	1	2282	U
36	1	2284	C
36	1	2288	G
36	1	2298	U
36	1	2303	A
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2314	U

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Mol	Chain	Res	Type
36	1	2315	G
36	1	2319	U
36	1	2334	U
36	1	2336	U
36	1	2339	C
36	1	2363	A
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2388	U
36	1	2393	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2404	A
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2424	A
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2507	C
36	1	2514	U
36	1	2515	A
36	1	2522	G
36	1	2523	A
36	1	2532	U
36	1	2533	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2544	U
36	1	2549	G
36	1	2552	C
36	1	2554	A

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Mol	Chain	Res	Type
36	1	2555	G
36	1	2561	A
36	1	2567	C
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
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	2619	G
36	1	2621	G
36	1	2626	A
36	1	2628	A
36	1	2637	A
36	1	2638	C
36	1	2651	G
36	1	2652	U
36	1	2653	C
36	1	2656	A
36	1	2674	A
36	1	2677	G
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	2705	A
36	1	2714	G
36	1	2720	G
36	1	2725	U
36	1	2728	G
36	1	2732	G
36	1	2752	U

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Mol	Chain	Res	Type
36	1	2753	G
36	1	2762	A
36	1	2771	U
36	1	2772	C
36	1	2777	G
36	1	2778	G
36	1	2779	A
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2802	A
36	1	2810	C
36	1	2816	G
36	1	2817	A
36	1	2818	U
36	1	2819	A
36	1	2829	U
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2849	C
36	1	2853	A
36	1	2860	U
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2875	U
36	1	2876	C
36	1	2883	U
36	1	2887	A
36	1	2889	C
36	1	2898	G
36	1	2899	C
36	1	2904	U
36	1	2914	G
36	1	2922	G
36	1	2923	U
36	1	2924	U
36	1	2925	C
36	1	2927	C
36	1	2935	U

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Mol	Chain	Res	Type
36	1	2936	A
36	1	2942	C
36	1	2943	G
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	2996	U
36	1	2997	G
36	1	3012	A
36	1	3018	C
36	1	3025	C
36	1	3030	G
36	1	3037	U
36	1	3056	U
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3086	A
36	1	3087	A
36	1	3092	C
36	1	3093	C
36	1	3113	A
36	1	3116	G
36	1	3119	U
36	1	3122	A
36	1	3130	A
36	1	3131	U
36	1	3139	A
36	1	3141	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

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Mol	Chain	Res	Type
36	1	3158	G
36	1	3164	C
36	1	3165	A
36	1	3166	C
36	1	3168	A
36	1	3169	U
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3185	U
36	1	3187	A
36	1	3195	U
36	1	3196	U
36	1	3198	U
36	1	3202	G
36	1	3207	U
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3228	C
36	1	3229	G
36	1	3235	C
36	1	3239	G
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3257	C
36	1	3259	U
36	1	3270	U
36	1	3271	G
36	1	3273	A
36	1	3276	G
36	1	3281	U
36	1	3282	U
36	1	3286	G
36	1	3287	U
36	1	3289	G

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Mol	Chain	Res	Type
36	1	3293	U
36	1	3294	A
36	1	3295	A
36	1	3304	U
36	1	3307	A
36	1	3313	U
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3335	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3350	C
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3360	C
36	1	3369	G
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3386	G
36	1	3389	U
36	1	3390	G
37	3	13	A
37	3	14	U
37	3	22	A
37	3	32	U
37	3	42	A
37	3	50	U
37	3	54	U
37	3	65	G
37	3	73	C
37	3	74	C
37	3	76	A

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Mol	Chain	Res	Type
37	3	91	G
37	3	92	A
37	3	102	A
37	3	104	A
37	3	112	G
37	3	121	U
38	4	13	A
38	4	21	C
38	4	26	U
38	4	34	U
38	4	35	C
38	4	47	C
38	4	51	G
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	82	U
38	4	83	C
38	4	84	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	97	A
38	4	104	A
38	4	105	A
38	4	106	C
38	4	108	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	142	C
38	4	148	G

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Mol	Chain	Res	Type
38	4	152	G
38	4	158	U
1	6	2	A
1	6	4	C
1	6	17	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	39	A
1	6	44	U
1	6	46	A
1	6	47	A
1	6	57	G
1	6	60	U
1	6	63	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	103	A
1	6	104	A
1	6	114	C
1	6	125	U
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	142	G
1	6	143	G
1	6	144	U
1	6	145	A
1	6	146	U
1	6	159	U
1	6	166	C
1	6	175	G

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Mol	Chain	Res	Type
1	6	178	U
1	6	179	A
1	6	185	U
1	6	187	G
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	194	U
1	6	195	G
1	6	197	A
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	222	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	229	U
1	6	230	C
1	6	232	U
1	6	233	C
1	6	234	G
1	6	235	G
1	6	240	U
1	6	241	U
1	6	246	G
1	6	249	U
1	6	250	C
1	6	260	U
1	6	261	U
1	6	262	U
1	6	265	A
1	6	271	A
1	6	272	U
1	6	273	G

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Mol	Chain	Res	Type
1	6	275	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	285	G
1	6	287	G
1	6	299	A
1	6	301	A
1	6	308	C
1	6	313	U
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	323	A
1	6	337	G
1	6	338	C
1	6	352	A
1	6	357	G
1	6	359	A
1	6	360	A
1	6	361	C
1	6	369	A
1	6	370	A
1	6	381	C
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	417	A
1	6	418	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	439	U
1	6	444	C
1	6	448	C
1	6	454	U

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Mol	Chain	Res	Type
1	6	464	A
1	6	469	C
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
1	6	496	G
1	6	497	G
1	6	500	C
1	6	501	U
1	6	502	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	508	U
1	6	510	G
1	6	511	A
1	6	513	U
1	6	514	G
1	6	515	A
1	6	519	C
1	6	527	A
1	6	536	C
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	555	A
1	6	556	A
1	6	557	G

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Mol	Chain	Res	Type
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	594	A
1	6	595	G
1	6	597	G
1	6	609	U
1	6	611	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	637	C
1	6	639	U
1	6	640	U
1	6	651	G
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	668	C
1	6	669	G
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	680	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	691	C

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Mol	Chain	Res	Type
1	6	696	C
1	6	698	U
1	6	709	C
1	6	710	U
1	6	711	U
1	6	714	G
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	723	G
1	6	726	C
1	6	730	G
1	6	739	G
1	6	742	U
1	6	751	G
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	766	U
1	6	774	A
1	6	775	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G
1	6	789	A
1	6	793	A
1	6	803	A
1	6	806	A
1	6	811	A
1	6	812	A
1	6	814	A
1	6	815	G
1	6	816	G
1	6	821	U
1	6	823	G
1	6	825	U
1	6	826	U

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Mol	Chain	Res	Type
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	847	A
1	6	856	A
1	6	861	U
1	6	863	A
1	6	864	U
1	6	865	A
1	6	898	A
1	6	906	A
1	6	910	C
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	959	U
1	6	960	U
1	6	966	A
1	6	970	A
1	6	971	A
1	6	991	G
1	6	992	A
1	6	993	A
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1020	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	1056	U
1	6	1057	U

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Mol	Chain	Res	Type
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1072	C
1	6	1076	A
1	6	1082	C
1	6	1083	G
1	6	1084	A
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
1	6	1108	G
1	6	1109	G
1	6	1138	A
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1160	A
1	6	1164	G
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	1203	A
1	6	1206	U
1	6	1208	A
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	1239	U

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Mol	Chain	Res	Type
1	6	1240	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	1261	G
1	6	1275	A
1	6	1286	U
1	6	1297	G
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A
1	6	1338	C
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1348	A
1	6	1352	G
1	6	1354	G
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1367	G
1	6	1371	A
1	6	1372	U
1	6	1373	C
1	6	1384	A
1	6	1388	A
1	6	1390	U
1	6	1391	A
1	6	1398	U
1	6	1399	C
1	6	1400	A

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Mol	Chain	Res	Type
1	6	1402	G
1	6	1413	U
1	6	1415	U
1	6	1424	A
1	6	1425	A
1	6	1427	A
1	6	1428	G
1	6	1429	G
1	6	1431	C
1	6	1433	G
1	6	1435	G
1	6	1445	G
1	6	1446	A
1	6	1448	G
1	6	1458	G
1	6	1459	C
1	6	1460	A
1	6	1461	C
1	6	1469	A
1	6	1471	A
1	6	1478	G
1	6	1482	C
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1506	G
1	6	1514	U
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	1526	A
1	6	1527	C
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1548	G
1	6	1554	U
1	6	1557	U

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Mol	Chain	Res	Type
1	6	1559	A
1	6	1569	A
1	6	1573	A
1	6	1574	G
1	6	1575	G
1	6	1584	G
1	6	1590	G
1	6	1600	A
1	6	1601	G
1	6	1616	G
1	6	1618	C
1	6	1620	C
1	6	1621	U
1	6	1631	A
1	6	1634	C
1	6	1657	U
1	6	1658	G
1	6	1680	G
1	6	1683	C
1	6	1696	G
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1703	C
1	6	1710	U
1	6	1712	A
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1730	A
1	6	1736	G
1	6	1750	A
1	6	1760	G
1	6	1762	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A

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Mol	Chain	Res	Type
1	6	1783	C
1	6	1788	G
1	6	1789	G
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1795	U
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	15	C
36	5	26	A
36	5	40	A
36	5	44	U
36	5	49	A
36	5	52	A
36	5	54	C
36	5	57	A
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	76	G
36	5	89	A
36	5	92	G
36	5	96	G
36	5	99	A
36	5	109	A
36	5	110	G
36	5	111	C
36	5	116	A
36	5	117	U
36	5	118	U
36	5	120	G
36	5	121	A
36	5	122	A
36	5	133	U
36	5	134	U
36	5	136	G
36	5	150	A
36	5	152	U
36	5	156	G

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Mol	Chain	Res	Type
36	5	157	A
36	5	161	G
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	181	U
36	5	182	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	210	U
36	5	211	A
36	5	218	G
36	5	219	A
36	5	221	A
36	5	234	G
36	5	235	A
36	5	236	G
36	5	237	G
36	5	239	G
36	5	240	U
36	5	244	G
36	5	247	C
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	259	C
36	5	269	G
36	5	270	U
36	5	271	C
36	5	284	A
36	5	286	U
36	5	294	U

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Mol	Chain	Res	Type
36	5	295	A
36	5	311	C
36	5	315	C
36	5	323	A
36	5	326	U
36	5	329	U
36	5	334	A
36	5	339	C
36	5	349	A
36	5	350	C
36	5	376	G
36	5	377	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	404	G
36	5	421	G
36	5	422	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	492	U
36	5	495	G
36	5	507	U
36	5	516	A
36	5	521	A
36	5	532	A
36	5	535	G
36	5	538	G
36	5	542	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	551	A
36	5	553	U
36	5	555	U
36	5	557	A

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Mol	Chain	Res	Type
36	5	559	A
36	5	569	A
36	5	578	A
36	5	579	G
36	5	585	A
36	5	592	A
36	5	600	G
36	5	604	G
36	5	608	A
36	5	609	G
36	5	611	A
36	5	612	U
36	5	619	A
36	5	620	U
36	5	621	A
36	5	630	A
36	5	636	C
36	5	640	U
36	5	649	A
36	5	660	A
36	5	677	A
36	5	681	U
36	5	683	U
36	5	691	A
36	5	705	A
36	5	709	A
36	5	712	G
36	5	715	A
36	5	716	A
36	5	725	G
36	5	727	G
36	5	735	A
36	5	736	A
36	5	737	G
36	5	747	A
36	5	758	C
36	5	763	G
36	5	766	U
36	5	776	U
36	5	777	U
36	5	780	A
36	5	781	G

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Mol	Chain	Res	Type
36	5	785	G
36	5	786	A
36	5	806	A
36	5	809	G
36	5	817	A
36	5	830	A
36	5	846	A
36	5	851	C
36	5	854	G
36	5	861	C
36	5	874	U
36	5	879	U
36	5	880	G
36	5	881	C
36	5	882	A
36	5	884	A
36	5	890	C
36	5	896	A
36	5	897	U
36	5	907	G
36	5	908	G
36	5	913	A
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	923	C
36	5	924	G
36	5	926	A
36	5	937	G
36	5	938	C
36	5	944	C
36	5	947	G
36	5	959	C
36	5	960	U
36	5	961	C
36	5	963	G
36	5	979	U
36	5	984	G
36	5	986	U
36	5	993	G
36	5	994	G

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Mol	Chain	Res	Type
36	5	1000	C
36	5	1001	G
36	5	1002	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	1022	U
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1027	A
36	5	1028	U
36	5	1029	G
36	5	1032	C
36	5	1034	U
36	5	1035	G
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1072	G
36	5	1081	U
36	5	1082	U
36	5	1087	G
36	5	1093	A
36	5	1094	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	1129	A
36	5	1131	G
36	5	1144	U
36	5	1152	G
36	5	1153	A
36	5	1154	A

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Mol	Chain	Res	Type
36	5	1159	A
36	5	1174	G
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1191	U
36	5	1192	C
36	5	1193	A
36	5	1196	C
36	5	1201	C
36	5	1202	A
36	5	1209	G
36	5	1222	G
36	5	1223	A
36	5	1232	C
36	5	1233	G
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1243	G
36	5	1245	A
36	5	1246	G
36	5	1252	A
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	1294	A
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1313	G
36	5	1330	A
36	5	1331	U
36	5	1349	G
36	5	1351	U
36	5	1352	A

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Mol	Chain	Res	Type
36	5	1353	U
36	5	1356	U
36	5	1357	G
36	5	1386	A
36	5	1399	A
36	5	1400	G
36	5	1403	C
36	5	1419	A
36	5	1421	G
36	5	1429	G
36	5	1431	G
36	5	1434	G
36	5	1435	A
36	5	1437	C
36	5	1450	G
36	5	1454	A
36	5	1465	A
36	5	1480	G
36	5	1481	A
36	5	1482	A
36	5	1484	U
36	5	1488	G
36	5	1503	A
36	5	1508	C
36	5	1519	G
36	5	1527	C
36	5	1528	G
36	5	1531	C
36	5	1536	G
36	5	1539	A
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1564	U
36	5	1565	G
36	5	1566	A
36	5	1567	U
36	5	1569	U
36	5	1570	U

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Mol	Chain	Res	Type
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	1593	A
36	5	1605	A
36	5	1620	U
36	5	1621	A
36	5	1629	U
36	5	1632	A
36	5	1635	G
36	5	1639	C
36	5	1641	U
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1657	C
36	5	1682	U
36	5	1687	U
36	5	1702	U
36	5	1713	G
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1725	C
36	5	1750	A
36	5	1751	G
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1769	G
36	5	1770	G

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Mol	Chain	Res	Type
36	5	1780	G
36	5	1794	G
36	5	1795	U
36	5	1797	A
36	5	1812	G
36	5	1813	A
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1821	U
36	5	1839	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1847	A
36	5	1849	C
36	5	1850	A
36	5	1851	G
36	5	1858	A
36	5	1859	A
36	5	1876	U
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1886	A
36	5	1892	G
36	5	1893	A
36	5	1906	G
36	5	1918	C
36	5	1935	G
36	5	1952	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	2117	A
36	5	2121	G
36	5	2122	G

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Mol	Chain	Res	Type
36	5	2131	A
36	5	2157	G
36	5	2158	A
36	5	2169	G
36	5	2170	U
36	5	2184	U
36	5	2187	G
36	5	2205	U
36	5	2208	A
36	5	2209	U
36	5	2210	G
36	5	2222	A
36	5	2223	A
36	5	2225	U
36	5	2244	A
36	5	2246	G
36	5	2250	G
36	5	2251	G
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2258	U
36	5	2273	G
36	5	2278	C
36	5	2279	A
36	5	2280	A
36	5	2281	A
36	5	2288	G
36	5	2298	U
36	5	2303	A
36	5	2304	C
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2318	U
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2364	G
36	5	2366	C

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Mol	Chain	Res	Type
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2386	A
36	5	2393	G
36	5	2394	G
36	5	2397	A
36	5	2399	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	2438	A
36	5	2439	A
36	5	2441	A
36	5	2443	A
36	5	2444	C
36	5	2504	U
36	5	2505	U
36	5	2506	U
36	5	2507	C
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2512	C
36	5	2514	U
36	5	2515	A
36	5	2522	G
36	5	2523	A
36	5	2524	A
36	5	2525	G
36	5	2526	C
36	5	2530	G
36	5	2531	C
36	5	2532	U
36	5	2537	U

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Mol	Chain	Res	Type
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2544	U
36	5	2549	G
36	5	2552	C
36	5	2555	G
36	5	2559	U
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2574	G
36	5	2580	A
36	5	2584	G
36	5	2585	G
36	5	2589	G
36	5	2593	A
36	5	2594	C
36	5	2606	G
36	5	2607	G
36	5	2614	G
36	5	2618	G
36	5	2626	A
36	5	2638	C
36	5	2639	G
36	5	2652	U
36	5	2656	A
36	5	2674	A
36	5	2677	G
36	5	2683	U
36	5	2689	A
36	5	2690	G
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2705	A
36	5	2714	G

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Mol	Chain	Res	Type
36	5	2728	G
36	5	2729	U
36	5	2752	U
36	5	2753	G
36	5	2755	C
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2780	A
36	5	2796	G
36	5	2797	C
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2802	A
36	5	2810	C
36	5	2814	G
36	5	2817	A
36	5	2818	U
36	5	2819	A
36	5	2826	U
36	5	2834	G
36	5	2839	G
36	5	2843	U
36	5	2845	A
36	5	2847	A
36	5	2849	C
36	5	2853	A
36	5	2860	U
36	5	2871	G
36	5	2872	A
36	5	2873	U
36	5	2876	C
36	5	2887	A
36	5	2889	C
36	5	2896	A
36	5	2899	C
36	5	2900	A
36	5	2901	G
36	5	2922	G

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Mol	Chain	Res	Type
36	5	2923	U
36	5	2924	U
36	5	2935	U
36	5	2936	A
36	5	2941	A
36	5	2942	C
36	5	2943	G
36	5	2947	G
36	5	2957	G
36	5	2971	A
36	5	2972	G
36	5	2976	A
36	5	2977	G
36	5	2979	U
36	5	2983	C
36	5	2990	G
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3046	A
36	5	3049	A
36	5	3050	U
36	5	3056	U
36	5	3057	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3084	C
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	3153	U
36	5	3154	C
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G

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Mol	Chain	Res	Type
36	5	3164	C
36	5	3165	A
36	5	3168	A
36	5	3171	U
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3175	U
36	5	3176	G
36	5	3177	G
36	5	3179	U
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3224	G
36	5	3229	G
36	5	3238	G
36	5	3239	G
36	5	3243	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3270	U
36	5	3273	A
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3279	A
36	5	3281	U
36	5	3282	U
36	5	3283	U
36	5	3284	G
36	5	3285	C
36	5	3286	G
36	5	3288	G

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Mol	Chain	Res	Type
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3302	U
36	5	3304	U
36	5	3313	U
36	5	3314	A
36	5	3316	A
36	5	3317	U
36	5	3318	G
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	3343	G
36	5	3345	G
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3356	G
36	5	3358	U
36	5	3369	G
36	5	3376	A
36	5	3378	C
36	5	3382	U
36	5	3389	U
36	5	3391	A
36	5	3393	U
36	5	3396	U
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	60	G
37	7	65	G
37	7	73	C
37	7	74	C

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Mol	Chain	Res	Type
37	7	76	A
37	7	79	A
37	7	99	G
37	7	101	G
37	7	102	A
37	7	103	A
37	7	112	G
38	8	14	C
38	8	34	U
38	8	35	C
38	8	41	A
38	8	48	A
38	8	59	A
38	8	62	C
38	8	63	G
38	8	80	A
38	8	81	U
38	8	82	U
38	8	83	C
38	8	84	C
38	8	86	U
38	8	87	G
38	8	90	U
38	8	95	G
38	8	96	A
38	8	97	A
38	8	99	C
38	8	101	U
38	8	104	A
38	8	105	A
38	8	106	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	138	A
38	8	152	G
38	8	156	U
38	8	157	U
38	8	158	U

All (289) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A
1	2	73	U
1	2	74	U
1	2	103	A
1	2	114	C
1	2	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	192	U
1	2	218	A
1	2	240	U
1	2	278	U
1	2	280	U
1	2	400	A
1	2	417	A
1	2	497	G
1	2	498	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	510	G
1	2	512	A
1	2	558	U
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	734	A
1	2	755	A
1	2	782	U
1	2	794	U
1	2	811	A
1	2	829	A
1	2	1051	G
1	2	1058	U
1	2	1081	A

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Mol	Chain	Res	Type
1	2	1157	A
1	2	1196	A
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1339	C
1	2	1344	A
1	2	1370	U
1	2	1481	C
1	2	1489	U
1	2	1517	U
1	2	1568	C
1	2	1573	A
1	2	1600	A
1	2	1615	C
1	2	1657	U
1	2	1696	G
1	2	1698	G
1	2	1711	C
1	2	1761	U
36	1	43	A
36	1	65	A
36	1	93	C
36	1	217	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	715	A
36	1	763	G
36	1	764	U
36	1	816	A
36	1	873	C
36	1	916	G
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A

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Mol	Chain	Res	Type
36	1	1181	U
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	1484	U
36	1	1507	G
36	1	1562	C
36	1	1716	U
36	1	1724	U
36	1	1751	G
36	1	1815	U
36	1	1816	A
36	1	1820	U
36	1	1846	C
36	1	1849	C
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2249	G
36	1	2281	A
36	1	2297	U
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2418	G
36	1	2513	U
36	1	2537	U
36	1	2538	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	2656	A
36	1	2689	A
36	1	2704	A
36	1	2728	G
36	1	2801	A
36	1	2818	U

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Mol	Chain	Res	Type
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3157	U
36	1	3169	U
36	1	3195	U
36	1	3207	U
36	1	3217	C
36	1	3218	A
36	1	3228	C
36	1	3269	U
36	1	3275	U
36	1	3316	A
36	1	3319	U
36	1	3333	G
36	1	3350	C
36	1	3351	U
36	1	3353	G
37	3	13	A
37	3	49	G
38	4	85	G
38	4	90	U
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	136	C
1	6	139	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	272	U
1	6	277	U
1	6	322	G
1	6	400	A
1	6	417	A
1	6	468	A

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Mol	Chain	Res	Type
1	6	512	A
1	6	539	G
1	6	542	A
1	6	555	A
1	6	558	U
1	6	651	G
1	6	667	U
1	6	678	A
1	6	717	C
1	6	755	A
1	6	829	A
1	6	834	G
1	6	1051	G
1	6	1058	U
1	6	1081	A
1	6	1097	U
1	6	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	1696	G
1	6	1698	G
1	6	1700	C
36	5	43	A
36	5	151	A
36	5	210	U
36	5	217	U
36	5	218	G
36	5	238	A
36	5	438	A
36	5	546	C
36	5	594	U
36	5	647	A

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Mol	Chain	Res	Type
36	5	715	A
36	5	735	A
36	5	765	C
36	5	816	A
36	5	873	C
36	5	896	A
36	5	916	G
36	5	937	G
36	5	960	U
36	5	993	G
36	5	1027	A
36	5	1033	U
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1222	G
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1317	A
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1481	A
36	5	1507	G
36	5	1560	G
36	5	1589	A
36	5	1716	U
36	5	1815	U
36	5	1816	A
36	5	1846	C
36	5	1878	G
36	5	2101	C
36	5	2112	U
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2256	A
36	5	2372	A

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Mol	Chain	Res	Type
36	5	2418	G
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2539	C
36	5	2593	A
36	5	2689	A
36	5	2704	A
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2818	U
36	5	2872	A
36	5	2887	A
36	5	2896	A
36	5	2971	A
36	5	2996	U
36	5	3056	U
36	5	3078	U
36	5	3154	C
36	5	3167	A
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3242	G
36	5	3269	U
36	5	3275	U
36	5	3289	G
36	5	3340	G
36	5	3341	U
36	5	3357	U
37	7	49	G
38	8	83	C
38	8	89	A
38	8	111	A
38	8	126	A
38	8	156	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2558 ligands modelled in this entry, 1425 are monoatomic - leaving 1133 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	6	2072	-	0,6,6	0.00	-	-		
86	OHX	1	4199	-	0,6,6	0.00	-	-		
86	OHX	5	3930	-	0,6,6	0.00	-	-		
86	OHX	6	2099	-	0,6,6	0.00	-	-		
86	OHX	5	4060	-	0,6,6	0.00	-	-		
86	OHX	1	4085	-	0,6,6	0.00	-	-		
86	OHX	6	2050	-	0,6,6	0.00	-	-		
86	OHX	8	221	-	0,6,6	0.00	-	-		
86	OHX	5	4078	-	0,6,6	0.00	-	-		
86	OHX	1	4200	-	0,6,6	0.00	-	-		
86	OHX	5	4058	-	0,6,6	0.00	-	-		
86	OHX	5	4057	-	0,6,6	0.00	-	-		
86	OHX	1	4107	-	0,6,6	0.00	-	-		
86	OHX	1	4093	-	0,6,6	0.00	-	-		
86	OHX	5	4191	-	0,6,6	0.00	-	-		
86	OHX	1	4128	-	0,6,6	0.00	-	-		
86	OHX	5	4109	-	0,6,6	0.00	-	-		
86	OHX	5	3970	-	0,6,6	0.00	-	-		
86	OHX	1	4144	-	0,6,6	0.00	-	-		
86	OHX	6	2088	-	0,6,6	0.00	-	-		
86	OHX	6	2113	-	0,6,6	0.00	-	-		
86	OHX	1	4002	-	0,6,6	0.00	-	-		
86	OHX	5	4095	-	0,6,6	0.00	-	-		
86	OHX	2	2065	-	0,6,6	0.00	-	-		
86	OHX	D9	102	-	0,6,6	0.00	-	-		
86	OHX	1	3915	-	0,6,6	0.00	-	-		
86	OHX	5	4037	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4145	-	0,6,6	0.00	-	-		
86	OHX	5	4032	-	0,6,6	0.00	-	-		
86	OHX	6	2102	-	0,6,6	0.00	-	-		
86	OHX	1	4040	-	0,6,6	0.00	-	-		
86	OHX	1	4187	-	0,6,6	0.00	-	-		
86	OHX	1	4074	-	0,6,6	0.00	-	-		
86	OHX	5	4206	-	0,6,6	0.00	-	-		
86	OHX	1	3872	-	0,6,6	0.00	-	-		
86	OHX	2	2031	-	0,6,6	0.00	-	-		
86	OHX	1	3902	-	0,6,6	0.00	-	-		
86	OHX	2	2061	-	0,6,6	0.00	-	-		
86	OHX	1	4025	-	0,6,6	0.00	-	-		
86	OHX	1	4017	-	0,6,6	0.00	-	-		
86	OHX	1	4188	-	0,6,6	0.00	-	-		
86	OHX	5	4062	-	0,6,6	0.00	-	-		
86	OHX	6	2184	-	0,6,6	0.00	-	-		
86	OHX	1	3913	-	0,6,6	0.00	-	-		
86	OHX	5	4038	-	0,6,6	0.00	-	-		
86	OHX	1	4036	-	0,6,6	0.00	-	-		
86	OHX	1	3898	-	0,6,6	0.00	-	-		
86	OHX	1	4121	-	0,6,6	0.00	-	-		
86	OHX	2	2056	-	0,6,6	0.00	-	-		
86	OHX	5	3967	-	0,6,6	0.00	-	-		
86	OHX	1	4058	-	0,6,6	0.00	-	-		
86	OHX	6	2100	-	0,6,6	0.00	-	-		
86	OHX	6	2090	-	0,6,6	0.00	-	-		
86	OHX	6	2055	-	0,6,6	0.00	-	-		
86	OHX	2	2048	-	0,6,6	0.00	-	-		
86	OHX	2	2097	-	0,6,6	0.00	-	-		
86	OHX	1	4043	-	0,6,6	0.00	-	-		
86	OHX	1	3899	-	0,6,6	0.00	-	-		
86	OHX	5	4081	-	0,6,6	0.00	-	-		
86	OHX	2	2054	-	0,6,6	0.00	-	-		
86	OHX	6	2144	-	0,6,6	0.00	-	-		
86	OHX	5	3904	-	0,6,6	0.00	-	-		
86	OHX	5	4103	-	0,6,6	0.00	-	-		
86	OHX	5	3913	-	0,6,6	0.00	-	-		
86	OHX	5	4075	-	0,6,6	0.00	-	-		
86	OHX	1	4083	-	0,6,6	0.00	-	-		
86	OHX	6	2052	-	0,6,6	0.00	-	-		
86	OHX	1	3947	-	0,6,6	0.00	-	-		
86	OHX	L3	405	-	0,6,6	0.00	-	-		
86	OHX	5	4029	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3966	-	0,6,6	0.00	-	-		
86	OHX	1	4060	-	0,6,6	0.00	-	-		
86	OHX	6	2110	-	0,6,6	0.00	-	-		
86	OHX	1	3984	-	0,6,6	0.00	-	-		
86	OHX	O3	202	-	0,6,6	0.00	-	-		
86	OHX	1	3940	-	0,6,6	0.00	-	-		
86	OHX	6	2160	-	0,6,6	0.00	-	-		
86	OHX	6	2074	-	0,6,6	0.00	-	-		
86	OHX	5	4207	-	0,6,6	0.00	-	-		
86	OHX	2	2145	-	0,6,6	0.00	-	-		
86	OHX	2	2140	-	0,6,6	0.00	-	-		
86	OHX	6	2207	-	0,6,6	0.00	-	-		
86	OHX	2	2173	-	0,6,6	0.00	-	-		
86	OHX	1	4022	-	0,6,6	0.00	-	-		
86	OHX	1	3909	-	0,6,6	0.00	-	-		
86	OHX	2	2028	-	0,6,6	0.00	-	-		
86	OHX	6	2076	-	0,6,6	0.00	-	-		
86	OHX	1	3965	-	0,6,6	0.00	-	-		
86	OHX	1	3957	-	0,6,6	0.00	-	-		
86	OHX	1	4148	-	0,6,6	0.00	-	-		
86	OHX	1	3982	-	0,6,6	0.00	-	-		
86	OHX	5	4255	-	0,6,6	0.00	-	-		
86	OHX	5	4056	-	0,6,6	0.00	-	-		
86	OHX	2	2155	-	0,6,6	0.00	-	-		
86	OHX	6	2071	-	0,6,6	0.00	-	-		
86	OHX	5	4211	-	0,6,6	0.00	-	-		
86	OHX	6	2087	-	0,6,6	0.00	-	-		
86	OHX	6	2158	-	0,6,6	0.00	-	-		
86	OHX	6	2122	-	0,6,6	0.00	-	-		
86	OHX	2	2084	-	0,6,6	0.00	-	-		
86	OHX	1	3919	-	0,6,6	0.00	-	-		
86	OHX	5	4113	-	0,6,6	0.00	-	-		
86	OHX	6	2147	-	0,6,6	0.00	-	-		
86	OHX	5	4116	-	0,6,6	0.00	-	-		
86	OHX	2	2152	-	0,6,6	0.00	-	-		
86	OHX	6	2164	-	0,6,6	0.00	-	-		
86	OHX	1	4196	-	0,6,6	0.00	-	-		
86	OHX	5	3941	-	0,6,6	0.00	-	-		
86	OHX	14	403	-	0,6,6	0.00	-	-		
86	OHX	5	3986	-	0,6,6	0.00	-	-		
86	OHX	1	4092	-	0,6,6	0.00	-	-		
86	OHX	6	2176	-	0,6,6	0.00	-	-		
86	OHX	5	4006	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3972	-	0,6,6	0.00	-	-		
86	OHX	1	4080	-	0,6,6	0.00	-	-		
86	OHX	1	4000	-	0,6,6	0.00	-	-		
86	OHX	1	3865	-	0,6,6	0.00	-	-		
86	OHX	5	4005	-	0,6,6	0.00	-	-		
86	OHX	1	4137	-	0,6,6	0.00	-	-		
86	OHX	6	2126	-	0,6,6	0.00	-	-		
86	OHX	1	4030	-	0,6,6	0.00	-	-		
86	OHX	6	2068	-	0,6,6	0.00	-	-		
86	OHX	5	4248	-	0,6,6	0.00	-	-		
86	OHX	S9	201	-	0,6,6	0.00	-	-		
86	OHX	1	4193	-	0,6,6	0.00	-	-		
86	OHX	5	4111	-	0,6,6	0.00	-	-		
86	OHX	2	2068	-	0,6,6	0.00	-	-		
86	OHX	1	4078	-	0,6,6	0.00	-	-		
86	OHX	1	3991	-	0,6,6	0.00	-	-		
86	OHX	5	3944	-	0,6,6	0.00	-	-		
86	OHX	6	2073	-	0,6,6	0.00	-	-		
86	OHX	2	2047	-	0,6,6	0.00	-	-		
86	OHX	1	4079	-	0,6,6	0.00	-	-		
86	OHX	5	4214	-	0,6,6	0.00	-	-		
86	OHX	5	4102	-	0,6,6	0.00	-	-		
86	OHX	1	4062	-	0,6,6	0.00	-	-		
86	OHX	6	2206	-	0,6,6	0.00	-	-		
86	OHX	5	4040	-	0,6,6	0.00	-	-		
86	OHX	5	4133	-	0,6,6	0.00	-	-		
86	OHX	2	2052	-	0,6,6	0.00	-	-		
86	OHX	1	3988	-	0,6,6	0.00	-	-		
86	OHX	1	4094	-	0,6,6	0.00	-	-		
86	OHX	5	3931	-	0,6,6	0.00	-	-		
86	OHX	1	4129	-	0,6,6	0.00	-	-		
86	OHX	1	4115	-	0,6,6	0.00	-	-		
86	OHX	1	4048	-	0,6,6	0.00	-	-		
86	OHX	5	4039	-	0,6,6	0.00	-	-		
86	OHX	8	224	-	0,6,6	0.00	-	-		
86	OHX	1	3860	-	0,6,6	0.00	-	-		
86	OHX	1	4084	-	0,6,6	0.00	-	-		
86	OHX	1	4020	-	0,6,6	0.00	-	-		
86	OHX	2	2178	-	0,6,6	0.00	-	-		
86	OHX	5	4228	-	0,6,6	0.00	-	-		
86	OHX	1	4164	-	0,6,6	0.00	-	-		
86	OHX	5	3928	-	0,6,6	0.00	-	-		
86	OHX	1	4125	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4215	-	0,6,6	0.00	-	-		
86	OHX	2	2119	-	0,6,6	0.00	-	-		
86	OHX	5	3983	-	0,6,6	0.00	-	-		
86	OHX	2	2182	-	0,6,6	0.00	-	-		
86	OHX	5	3921	-	0,6,6	0.00	-	-		
86	OHX	1	4197	-	0,6,6	0.00	-	-		
86	OHX	5	3998	-	0,6,6	0.00	-	-		
86	OHX	1	3931	-	0,6,6	0.00	-	-		
86	OHX	5	3934	-	0,6,6	0.00	-	-		
86	OHX	6	2078	-	0,6,6	0.00	-	-		
86	OHX	2	2171	-	0,6,6	0.00	-	-		
86	OHX	5	4016	-	0,6,6	0.00	-	-		
86	OHX	5	3932	-	0,6,6	0.00	-	-		
86	OHX	2	2064	-	0,6,6	0.00	-	-		
86	OHX	5	3985	-	0,6,6	0.00	-	-		
86	OHX	5	4033	-	0,6,6	0.00	-	-		
86	OHX	1	3976	-	0,6,6	0.00	-	-		
86	OHX	1	3885	-	0,6,6	0.00	-	-		
86	OHX	C8	201	-	0,6,6	0.00	-	-		
86	OHX	8	222	-	0,6,6	0.00	-	-		
86	OHX	2	2153	-	0,6,6	0.00	-	-		
86	OHX	3	222	-	0,6,6	0.00	-	-		
86	OHX	5	4043	-	0,6,6	0.00	-	-		
86	OHX	2	2139	-	0,6,6	0.00	-	-		
86	OHX	5	4055	-	0,6,6	0.00	-	-		
86	OHX	6	2140	-	0,6,6	0.00	-	-		
86	OHX	6	2138	-	0,6,6	0.00	-	-		
86	OHX	1	4055	-	0,6,6	0.00	-	-		
86	OHX	5	3961	-	0,6,6	0.00	-	-		
86	OHX	1	4042	-	0,6,6	0.00	-	-		
86	OHX	5	4178	-	0,6,6	0.00	-	-		
86	OHX	l3	404	-	0,6,6	0.00	-	-		
86	OHX	6	2051	-	0,6,6	0.00	-	-		
86	OHX	1	3879	-	0,6,6	0.00	-	-		
86	OHX	6	2054	-	0,6,6	0.00	-	-		
86	OHX	5	4147	-	0,6,6	0.00	-	-		
86	OHX	6	2095	-	0,6,6	0.00	-	-		
86	OHX	5	4174	-	0,6,6	0.00	-	-		
86	OHX	5	4069	-	0,6,6	0.00	-	-		
86	OHX	5	4051	-	0,6,6	0.00	-	-		
86	OHX	5	4090	-	0,6,6	0.00	-	-		
86	OHX	5	4036	-	0,6,6	0.00	-	-		
86	OHX	1	3908	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4130	-	0,6,6	0.00	-	-		
86	OHX	1	3884	-	0,6,6	0.00	-	-		
86	OHX	2	2104	-	0,6,6	0.00	-	-		
86	OHX	6	2202	-	0,6,6	0.00	-	-		
86	OHX	1	3880	-	0,6,6	0.00	-	-		
86	OHX	5	4209	-	0,6,6	0.00	-	-		
86	OHX	1	4044	-	0,6,6	0.00	-	-		
86	OHX	6	2130	-	0,6,6	0.00	-	-		
86	OHX	5	3977	-	0,6,6	0.00	-	-		
86	OHX	5	4235	-	0,6,6	0.00	-	-		
86	OHX	2	2138	-	0,6,6	0.00	-	-		
86	OHX	2	2090	-	0,6,6	0.00	-	-		
86	OHX	6	2128	-	0,6,6	0.00	-	-		
86	OHX	1	3942	-	0,6,6	0.00	-	-		
86	OHX	2	2046	-	0,6,6	0.00	-	-		
86	OHX	1	3962	-	0,6,6	0.00	-	-		
86	OHX	1	3888	-	0,6,6	0.00	-	-		
86	OHX	5	4165	-	0,6,6	0.00	-	-		
86	OHX	2	2081	-	0,6,6	0.00	-	-		
86	OHX	2	2073	-	0,6,6	0.00	-	-		
86	OHX	5	4019	-	0,6,6	0.00	-	-		
86	OHX	2	2030	-	0,6,6	0.00	-	-		
86	OHX	1	4153	-	0,6,6	0.00	-	-		
86	OHX	5	4017	-	0,6,6	0.00	-	-		
86	OHX	1	3905	-	0,6,6	0.00	-	-		
86	OHX	6	2165	-	0,6,6	0.00	-	-		
86	OHX	6	2166	-	0,6,6	0.00	-	-		
86	OHX	5	4243	-	0,6,6	0.00	-	-		
86	OHX	1	4151	-	0,6,6	0.00	-	-		
86	OHX	1	4010	-	0,6,6	0.00	-	-		
86	OHX	1	4061	-	0,6,6	0.00	-	-		
86	OHX	5	3937	-	0,6,6	0.00	-	-		
86	OHX	1	4034	-	0,6,6	0.00	-	-		
86	OHX	1	4143	-	0,6,6	0.00	-	-		
86	OHX	5	3936	-	0,6,6	0.00	-	-		
86	OHX	1	3881	-	0,6,6	0.00	-	-		
86	OHX	1	4027	-	0,6,6	0.00	-	-		
86	OHX	7	223	-	0,6,6	0.00	-	-		
86	OHX	5	4142	-	0,6,6	0.00	-	-		
86	OHX	1	4150	-	0,6,6	0.00	-	-		
86	OHX	6	2109	-	0,6,6	0.00	-	-		
86	OHX	5	3920	-	0,6,6	0.00	-	-		
86	OHX	5	3907	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	15	303	-	0,6,6	0.00	-	-		
86	OHX	3	224	-	0,6,6	0.00	-	-		
86	OHX	6	2157	-	0,6,6	0.00	-	-		
86	OHX	5	4219	-	0,6,6	0.00	-	-		
86	OHX	1	4166	-	0,6,6	0.00	-	-		
86	OHX	1	3890	-	0,6,6	0.00	-	-		
86	OHX	5	3918	-	0,6,6	0.00	-	-		
86	OHX	6	2170	-	0,6,6	0.00	-	-		
86	OHX	5	4064	-	0,6,6	0.00	-	-		
86	OHX	Q2	503	-	0,6,6	0.00	-	-		
86	OHX	5	3981	-	0,6,6	0.00	-	-		
86	OHX	5	4086	-	0,6,6	0.00	-	-		
86	OHX	3	218	-	0,6,6	0.00	-	-		
86	OHX	5	4100	-	0,6,6	0.00	-	-		
88	ZBA	1	4206	85	36,36,36	1.65	3 (8%)	49,58,58	1.81	4 (8%)
86	OHX	7	218	-	0,6,6	0.00	-	-		
86	OHX	1	4099	-	0,6,6	0.00	-	-		
86	OHX	5	3999	-	0,6,6	0.00	-	-		
86	OHX	5	4197	-	0,6,6	0.00	-	-		
86	OHX	6	2163	-	0,6,6	0.00	-	-		
86	OHX	5	4112	-	0,6,6	0.00	-	-		
86	OHX	2	2026	-	0,6,6	0.00	-	-		
86	OHX	6	2161	-	0,6,6	0.00	-	-		
86	OHX	5	4137	-	0,6,6	0.00	-	-		
86	OHX	6	2133	-	0,6,6	0.00	-	-		
86	OHX	2	2057	-	0,6,6	0.00	-	-		
86	OHX	1	4110	-	0,6,6	0.00	-	-		
86	OHX	6	2085	-	0,6,6	0.00	-	-		
86	OHX	1	3893	-	0,6,6	0.00	-	-		
86	OHX	1	3973	-	0,6,6	0.00	-	-		
86	OHX	1	3896	-	0,6,6	0.00	-	-		
86	OHX	4	236	-	0,6,6	0.00	-	-		
86	OHX	1	4072	-	0,6,6	0.00	-	-		
86	OHX	5	4167	-	0,6,6	0.00	-	-		
86	OHX	5	4212	-	0,6,6	0.00	-	-		
86	OHX	1	3992	-	0,6,6	0.00	-	-		
86	OHX	5	4180	-	0,6,6	0.00	-	-		
86	OHX	1	3862	-	0,6,6	0.00	-	-		
86	OHX	1	3906	-	0,6,6	0.00	-	-		
86	OHX	2	2125	-	0,6,6	0.00	-	-		
86	OHX	1	3983	-	0,6,6	0.00	-	-		
86	OHX	1	4013	-	0,6,6	0.00	-	-		
86	OHX	2	2120	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4073	-	0,6,6	0.00	-	-		
86	OHX	6	2134	-	0,6,6	0.00	-	-		
86	OHX	1	4067	-	0,6,6	0.00	-	-		
86	OHX	5	4025	-	0,6,6	0.00	-	-		
86	OHX	7	229	-	0,6,6	0.00	-	-		
86	OHX	1	3921	-	0,6,6	0.00	-	-		
86	OHX	6	2137	-	0,6,6	0.00	-	-		
86	OHX	5	4136	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	5	4089	-	0,6,6	0.00	-	-		
86	OHX	5	4128	-	0,6,6	0.00	-	-		
86	OHX	5	4192	-	0,6,6	0.00	-	-		
86	OHX	7	220	-	0,6,6	0.00	-	-		
86	OHX	5	3911	-	0,6,6	0.00	-	-		
86	OHX	5	3976	-	0,6,6	0.00	-	-		
86	OHX	1	3901	-	0,6,6	0.00	-	-		
86	OHX	6	2201	-	0,6,6	0.00	-	-		
86	OHX	5	3987	-	0,6,6	0.00	-	-		
86	OHX	1	3943	-	0,6,6	0.00	-	-		
86	OHX	5	3965	-	0,6,6	0.00	-	-		
86	OHX	1	3917	-	0,6,6	0.00	-	-		
86	OHX	2	2044	-	0,6,6	0.00	-	-		
86	OHX	1	4003	-	0,6,6	0.00	-	-		
86	OHX	1	4047	-	0,6,6	0.00	-	-		
86	OHX	2	2041	-	0,6,6	0.00	-	-		
86	OHX	c5	201	-	0,6,6	0.00	-	-		
86	OHX	5	4098	-	0,6,6	0.00	-	-		
86	OHX	1	4201	-	0,6,6	0.00	-	-		
86	OHX	5	4213	-	0,6,6	0.00	-	-		
86	OHX	1	4076	-	0,6,6	0.00	-	-		
86	OHX	1	4176	-	0,6,6	0.00	-	-		
86	OHX	2	2121	-	0,6,6	0.00	-	-		
86	OHX	6	2171	-	0,6,6	0.00	-	-		
86	OHX	6	2189	-	0,6,6	0.00	-	-		
86	OHX	L3	404	-	0,6,6	0.00	-	-		
86	OHX	7	221	-	0,6,6	0.00	-	-		
86	OHX	2	2071	-	0,6,6	0.00	-	-		
86	OHX	5	4118	-	0,6,6	0.00	-	-		
86	OHX	5	3947	-	0,6,6	0.00	-	-		
86	OHX	M8	201	-	0,6,6	0.00	-	-		
86	OHX	2	2100	-	0,6,6	0.00	-	-		
86	OHX	5	4251	-	0,6,6	0.00	-	-		
86	OHX	6	2089	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4103	-	0,6,6	0.00	-	-		
86	OHX	sR	401	-	0,6,6	0.00	-	-		
86	OHX	5	4035	-	0,6,6	0.00	-	-		
86	OHX	6	2114	-	0,6,6	0.00	-	-		
86	OHX	5	4009	-	0,6,6	0.00	-	-		
86	OHX	2	2114	-	0,6,6	0.00	-	-		
86	OHX	5	4236	-	0,6,6	0.00	-	-		
86	OHX	1	4037	-	0,6,6	0.00	-	-		
86	OHX	1	3922	-	0,6,6	0.00	-	-		
86	OHX	5	4014	-	0,6,6	0.00	-	-		
86	OHX	1	4190	-	0,6,6	0.00	-	-		
86	OHX	1	4104	-	0,6,6	0.00	-	-		
86	OHX	5	3942	-	0,6,6	0.00	-	-		
86	OHX	1	4202	-	0,6,6	0.00	-	-		
86	OHX	1	4117	-	0,6,6	0.00	-	-		
86	OHX	2	2146	-	0,6,6	0.00	-	-		
86	OHX	6	2204	-	0,6,6	0.00	-	-		
86	OHX	1	4112	-	0,6,6	0.00	-	-		
86	OHX	6	2079	-	0,6,6	0.00	-	-		
86	OHX	2	2076	-	0,6,6	0.00	-	-		
86	OHX	6	2108	-	0,6,6	0.00	-	-		
86	OHX	2	2149	-	0,6,6	0.00	-	-		
86	OHX	1	3970	-	0,6,6	0.00	-	-		
86	OHX	1	4075	-	0,6,6	0.00	-	-		
86	OHX	1	4139	-	0,6,6	0.00	-	-		
86	OHX	6	2082	-	0,6,6	0.00	-	-		
86	OHX	5	4080	-	0,6,6	0.00	-	-		
86	OHX	5	3978	-	0,6,6	0.00	-	-		
86	OHX	1	3960	-	0,6,6	0.00	-	-		
86	OHX	5	4097	-	0,6,6	0.00	-	-		
86	OHX	5	3923	-	0,6,6	0.00	-	-		
86	OHX	1	3907	-	0,6,6	0.00	-	-		
86	OHX	6	2203	-	0,6,6	0.00	-	-		
86	OHX	2	2088	-	0,6,6	0.00	-	-		
86	OHX	4	226	-	0,6,6	0.00	-	-		
86	OHX	5	4023	-	0,6,6	0.00	-	-		
86	OHX	6	2142	-	0,6,6	0.00	-	-		
86	OHX	5	4223	-	0,6,6	0.00	-	-		
86	OHX	1	4135	-	0,6,6	0.00	-	-		
86	OHX	6	2111	-	0,6,6	0.00	-	-		
86	OHX	1	4001	-	0,6,6	0.00	-	-		
86	OHX	1	4045	-	0,6,6	0.00	-	-		
86	OHX	6	2046	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4224	-	0,6,6	0.00	-	-		
86	OHX	6	2105	-	0,6,6	0.00	-	-		
86	OHX	2	2099	-	0,6,6	0.00	-	-		
86	OHX	1	3929	-	0,6,6	0.00	-	-		
86	OHX	1	3878	-	0,6,6	0.00	-	-		
86	OHX	4	233	-	0,6,6	0.00	-	-		
86	OHX	5	4202	-	0,6,6	0.00	-	-		
86	OHX	5	3945	-	0,6,6	0.00	-	-		
86	OHX	1	4156	-	0,6,6	0.00	-	-		
86	OHX	6	2048	-	0,6,6	0.00	-	-		
86	OHX	6	2183	-	0,6,6	0.00	-	-		
86	OHX	1	4182	-	0,6,6	0.00	-	-		
86	OHX	6	2185	-	0,6,6	0.00	-	-		
86	OHX	1	3995	-	0,6,6	0.00	-	-		
86	OHX	1	4149	-	0,6,6	0.00	-	-		
86	OHX	5	4114	-	0,6,6	0.00	-	-		
86	OHX	5	4084	-	0,6,6	0.00	-	-		
86	OHX	1	4203	-	0,6,6	0.00	-	-		
86	OHX	1	4024	-	0,6,6	0.00	-	-		
86	OHX	1	4090	-	0,6,6	0.00	-	-		
86	OHX	1	4184	-	0,6,6	0.00	-	-		
86	OHX	6	2153	-	0,6,6	0.00	-	-		
86	OHX	5	3909	-	0,6,6	0.00	-	-		
86	OHX	1	3868	-	0,6,6	0.00	-	-		
86	OHX	1	3889	-	0,6,6	0.00	-	-		
86	OHX	5	4063	-	0,6,6	0.00	-	-		
86	OHX	5	4048	-	0,6,6	0.00	-	-		
86	OHX	1	3916	-	0,6,6	0.00	-	-		
86	OHX	1	3873	-	0,6,6	0.00	-	-		
86	OHX	6	2146	-	0,6,6	0.00	-	-		
86	OHX	1	3904	-	0,6,6	0.00	-	-		
86	OHX	1	3996	-	0,6,6	0.00	-	-		
86	OHX	1	3993	-	0,6,6	0.00	-	-		
86	OHX	1	4039	-	0,6,6	0.00	-	-		
86	OHX	1	4136	-	0,6,6	0.00	-	-		
86	OHX	5	4246	-	0,6,6	0.00	-	-		
86	OHX	6	2132	-	0,6,6	0.00	-	-		
86	OHX	1	4035	-	0,6,6	0.00	-	-		
86	OHX	5	4122	-	0,6,6	0.00	-	-		
86	OHX	6	2139	-	0,6,6	0.00	-	-		
86	OHX	2	2059	-	0,6,6	0.00	-	-		
86	OHX	2	2133	-	0,6,6	0.00	-	-		
86	OHX	5	4201	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2108	-	0,6,6	0.00	-	-		
86	OHX	2	2094	-	0,6,6	0.00	-	-		
86	OHX	5	4208	-	0,6,6	0.00	-	-		
86	OHX	1	3961	-	0,6,6	0.00	-	-		
86	OHX	s8	303	-	0,6,6	0.00	-	-		
86	OHX	6	2135	-	0,6,6	0.00	-	-		
86	OHX	5	3951	-	0,6,6	0.00	-	-		
86	OHX	1	4183	-	0,6,6	0.00	-	-		
86	OHX	1	3987	-	0,6,6	0.00	-	-		
86	OHX	6	2097	-	0,6,6	0.00	-	-		
86	OHX	1	3910	-	0,6,6	0.00	-	-		
86	OHX	1	4011	-	0,6,6	0.00	-	-		
86	OHX	5	4198	-	0,6,6	0.00	-	-		
86	OHX	5	4129	-	0,6,6	0.00	-	-		
86	OHX	5	4007	-	0,6,6	0.00	-	-		
86	OHX	1	4205	-	0,6,6	0.00	-	-		
86	OHX	1	3923	-	0,6,6	0.00	-	-		
86	OHX	5	3982	-	0,6,6	0.00	-	-		
86	OHX	1	3900	-	0,6,6	0.00	-	-		
86	OHX	15	304	-	0,6,6	0.00	-	-		
86	OHX	1	4053	-	0,6,6	0.00	-	-		
86	OHX	19	600	-	0,6,6	0.00	-	-		
86	OHX	2	2126	-	0,6,6	0.00	-	-		
86	OHX	5	4194	-	0,6,6	0.00	-	-		
86	OHX	1	4124	-	0,6,6	0.00	-	-		
86	OHX	6	2131	-	0,6,6	0.00	-	-		
86	OHX	5	4182	-	0,6,6	0.00	-	-		
86	OHX	2	2072	-	0,6,6	0.00	-	-		
86	OHX	6	2199	-	0,6,6	0.00	-	-		
86	OHX	5	4126	-	0,6,6	0.00	-	-		
86	OHX	3	221	-	0,6,6	0.00	-	-		
86	OHX	5	3916	-	0,6,6	0.00	-	-		
86	OHX	O7	103	-	0,6,6	0.00	-	-		
86	OHX	7	222	-	0,6,6	0.00	-	-		
86	OHX	5	3917	-	0,6,6	0.00	-	-		
88	ZBA	5	4256	85	36,36,36	1.38	2 (5%)	49,58,58	1.76	7 (14%)
86	OHX	5	4175	-	0,6,6	0.00	-	-		
86	OHX	2	2166	-	0,6,6	0.00	-	-		
86	OHX	6	2077	-	0,6,6	0.00	-	-		
86	OHX	5	3984	-	0,6,6	0.00	-	-		
86	OHX	1	3989	-	0,6,6	0.00	-	-		
86	OHX	13	405	-	0,6,6	0.00	-	-		
86	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
86	OHX	1	3925	-	0,6,6	0.00	-	-		
86	OHX	5	4065	-	0,6,6	0.00	-	-		
86	OHX	1	4102	-	0,6,6	0.00	-	-		
86	OHX	6	2193	-	0,6,6	0.00	-	-		
86	OHX	5	4045	-	0,6,6	0.00	-	-		
86	OHX	6	2047	-	0,6,6	0.00	-	-		
86	OHX	1	4119	-	0,6,6	0.00	-	-		
86	OHX	5	4141	-	0,6,6	0.00	-	-		
86	OHX	6	2205	-	0,6,6	0.00	-	-		
86	OHX	2	2156	-	0,6,6	0.00	-	-		
86	OHX	1	4189	-	0,6,6	0.00	-	-		
86	OHX	1	3969	-	0,6,6	0.00	-	-		
86	OHX	5	3903	-	0,6,6	0.00	-	-		
86	OHX	1	4089	-	0,6,6	0.00	-	-		
86	OHX	1	4014	-	0,6,6	0.00	-	-		
86	OHX	8	226	-	0,6,6	0.00	-	-		
86	OHX	5	3974	-	0,6,6	0.00	-	-		
86	OHX	C1	201	-	0,6,6	0.00	-	-		
86	OHX	5	3968	-	0,6,6	0.00	-	-		
86	OHX	6	2065	-	0,6,6	0.00	-	-		
86	OHX	5	4225	-	0,6,6	0.00	-	-		
86	OHX	1	4160	-	0,6,6	0.00	-	-		
86	OHX	2	2143	-	0,6,6	0.00	-	-		
86	OHX	5	4238	-	0,6,6	0.00	-	-		
86	OHX	2	2167	-	0,6,6	0.00	-	-		
86	OHX	5	4186	-	0,6,6	0.00	-	-		
86	OHX	5	4183	-	0,6,6	0.00	-	-		
86	OHX	5	4066	-	0,6,6	0.00	-	-		
86	OHX	5	3992	-	0,6,6	0.00	-	-		
86	OHX	5	4230	-	0,6,6	0.00	-	-		
86	OHX	5	4050	-	0,6,6	0.00	-	-		
86	OHX	4	230	-	0,6,6	0.00	-	-		
86	OHX	6	2159	-	0,6,6	0.00	-	-		
86	OHX	1	4179	-	0,6,6	0.00	-	-		
86	OHX	1	4095	-	0,6,6	0.00	-	-		
86	OHX	d9	102	-	0,6,6	0.00	-	-		
86	OHX	5	4242	-	0,6,6	0.00	-	-		
86	OHX	1	4174	-	0,6,6	0.00	-	-		
86	OHX	1	3927	-	0,6,6	0.00	-	-		
86	OHX	6	2121	-	0,6,6	0.00	-	-		
86	OHX	1	4088	-	0,6,6	0.00	-	-		
86	OHX	5	4222	-	0,6,6	0.00	-	-		
86	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
86	OHX	1	3985	-	0,6,6	0.00	-	-		
86	OHX	2	2083	-	0,6,6	0.00	-	-		
86	OHX	7	227	-	0,6,6	0.00	-	-		
86	OHX	7	226	-	0,6,6	0.00	-	-		
86	OHX	2	2036	-	0,6,6	0.00	-	-		
86	OHX	5	3969	-	0,6,6	0.00	-	-		
86	OHX	1	4105	-	0,6,6	0.00	-	-		
86	OHX	1	3945	-	0,6,6	0.00	-	-		
86	OHX	5	4083	-	0,6,6	0.00	-	-		
86	OHX	1	4026	-	0,6,6	0.00	-	-		
86	OHX	m4	201	-	0,6,6	0.00	-	-		
86	OHX	3	217	-	0,6,6	0.00	-	-		
86	OHX	5	4021	-	0,6,6	0.00	-	-		
86	OHX	3	215	-	0,6,6	0.00	-	-		
86	OHX	1	4122	-	0,6,6	0.00	-	-		
86	OHX	5	3940	-	0,6,6	0.00	-	-		
86	OHX	1	4068	-	0,6,6	0.00	-	-		
86	OHX	6	2112	-	0,6,6	0.00	-	-		
86	OHX	5	3960	-	0,6,6	0.00	-	-		
86	OHX	1	3963	-	0,6,6	0.00	-	-		
86	OHX	5	4121	-	0,6,6	0.00	-	-		
86	OHX	1	3918	-	0,6,6	0.00	-	-		
86	OHX	6	2200	-	0,6,6	0.00	-	-		
86	OHX	1	3924	-	0,6,6	0.00	-	-		
86	OHX	5	4151	-	0,6,6	0.00	-	-		
86	OHX	1	3935	-	0,6,6	0.00	-	-		
86	OHX	5	3924	-	0,6,6	0.00	-	-		
86	OHX	1	4134	-	0,6,6	0.00	-	-		
86	OHX	5	4020	-	0,6,6	0.00	-	-		
86	OHX	6	2075	-	0,6,6	0.00	-	-		
86	OHX	6	2136	-	0,6,6	0.00	-	-		
86	OHX	6	2188	-	0,6,6	0.00	-	-		
86	OHX	6	2116	-	0,6,6	0.00	-	-		
86	OHX	5	3991	-	0,6,6	0.00	-	-		
86	OHX	1	3939	-	0,6,6	0.00	-	-		
86	OHX	1	3974	-	0,6,6	0.00	-	-		
86	OHX	6	2104	-	0,6,6	0.00	-	-		
86	OHX	1	3950	-	0,6,6	0.00	-	-		
86	OHX	1	3886	-	0,6,6	0.00	-	-		
86	OHX	1	3952	-	0,6,6	0.00	-	-		
86	OHX	C3	201	-	0,6,6	0.00	-	-		
86	OHX	1	4132	-	0,6,6	0.00	-	-		
86	OHX	2	2144	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4091	-	0,6,6	0.00	-	-		
86	OHX	m0	302	-	0,6,6	0.00	-	-		
86	OHX	6	2169	-	0,6,6	0.00	-	-		
86	OHX	1	4185	-	0,6,6	0.00	-	-		
86	OHX	5	4123	-	0,6,6	0.00	-	-		
86	OHX	1	4056	-	0,6,6	0.00	-	-		
86	OHX	o7	502	-	0,6,6	0.00	-	-		
86	OHX	5	3996	-	0,6,6	0.00	-	-		
86	OHX	2	2086	-	0,6,6	0.00	-	-		
86	OHX	6	2162	-	0,6,6	0.00	-	-		
86	OHX	2	2135	-	0,6,6	0.00	-	-		
86	OHX	1	3979	-	0,6,6	0.00	-	-		
86	OHX	5	4240	-	0,6,6	0.00	-	-		
86	OHX	6	2192	-	0,6,6	0.00	-	-		
86	OHX	L4	403	-	0,6,6	0.00	-	-		
86	OHX	s1	302	-	0,6,6	0.00	-	-		
86	OHX	2	2035	-	0,6,6	0.00	-	-		
86	OHX	1	4018	-	0,6,6	0.00	-	-		
86	OHX	1	4004	-	0,6,6	0.00	-	-		
86	OHX	5	4154	-	0,6,6	0.00	-	-		
86	OHX	6	2150	-	0,6,6	0.00	-	-		
86	OHX	2	2137	-	0,6,6	0.00	-	-		
86	OHX	5	4203	-	0,6,6	0.00	-	-		
86	OHX	1	4106	-	0,6,6	0.00	-	-		
86	OHX	4	234	-	0,6,6	0.00	-	-		
86	OHX	7	219	-	0,6,6	0.00	-	-		
86	OHX	6	2187	-	0,6,6	0.00	-	-		
86	OHX	1	4015	-	0,6,6	0.00	-	-		
86	OHX	5	4099	-	0,6,6	0.00	-	-		
86	OHX	1	4168	-	0,6,6	0.00	-	-		
86	OHX	2	2070	-	0,6,6	0.00	-	-		
86	OHX	5	3989	-	0,6,6	0.00	-	-		
86	OHX	5	3919	-	0,6,6	0.00	-	-		
86	OHX	5	3906	-	0,6,6	0.00	-	-		
86	OHX	1	3882	-	0,6,6	0.00	-	-		
86	OHX	5	3988	-	0,6,6	0.00	-	-		
86	OHX	6	2152	-	0,6,6	0.00	-	-		
86	OHX	5	4161	-	0,6,6	0.00	-	-		
86	OHX	1	3874	-	0,6,6	0.00	-	-		
86	OHX	1	4041	-	0,6,6	0.00	-	-		
86	OHX	1	3895	-	0,6,6	0.00	-	-		
86	OHX	2	2034	-	0,6,6	0.00	-	-		
86	OHX	2	2050	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4153	-	0,6,6	0.00	-	-		
86	OHX	5	4115	-	0,6,6	0.00	-	-		
86	OHX	1	4152	-	0,6,6	0.00	-	-		
86	OHX	1	4108	-	0,6,6	0.00	-	-		
86	OHX	6	2067	-	0,6,6	0.00	-	-		
86	OHX	1	4118	-	0,6,6	0.00	-	-		
86	OHX	m5	306	-	0,6,6	0.00	-	-		
86	OHX	6	2172	-	0,6,6	0.00	-	-		
86	OHX	M6	202	-	0,6,6	0.00	-	-		
86	OHX	M9	202	-	0,6,6	0.00	-	-		
86	OHX	1	3891	-	0,6,6	0.00	-	-		
86	OHX	1	4140	-	0,6,6	0.00	-	-		
86	OHX	5	4150	-	0,6,6	0.00	-	-		
86	OHX	5	4177	-	0,6,6	0.00	-	-		
86	OHX	1	4181	-	0,6,6	0.00	-	-		
86	OHX	5	4160	-	0,6,6	0.00	-	-		
86	OHX	1	4141	-	0,6,6	0.00	-	-		
86	OHX	O7	104	-	0,6,6	0.00	-	-		
86	OHX	1	4096	-	0,6,6	0.00	-	-		
86	OHX	6	2120	-	0,6,6	0.00	-	-		
86	OHX	5	4159	-	0,6,6	0.00	-	-		
86	OHX	2	2113	-	0,6,6	0.00	-	-		
86	OHX	2	2158	-	0,6,6	0.00	-	-		
86	OHX	5	4168	-	0,6,6	0.00	-	-		
86	OHX	5	4008	-	0,6,6	0.00	-	-		
86	OHX	5	4052	-	0,6,6	0.00	-	-		
86	OHX	1	4054	-	0,6,6	0.00	-	-		
86	OHX	5	4002	-	0,6,6	0.00	-	-		
86	OHX	1	4059	-	0,6,6	0.00	-	-		
86	OHX	1	4069	-	0,6,6	0.00	-	-		
86	OHX	8	218	-	0,6,6	0.00	-	-		
86	OHX	1	3875	-	0,6,6	0.00	-	-		
86	OHX	1	4116	-	0,6,6	0.00	-	-		
86	OHX	6	2186	-	0,6,6	0.00	-	-		
86	OHX	1	3944	-	0,6,6	0.00	-	-		
86	OHX	2	2042	-	0,6,6	0.00	-	-		
86	OHX	2	2092	-	0,6,6	0.00	-	-		
86	OHX	2	2067	-	0,6,6	0.00	-	-		
86	OHX	2	2105	-	0,6,6	0.00	-	-		
86	OHX	1	4008	-	0,6,6	0.00	-	-		
86	OHX	1	4114	-	0,6,6	0.00	-	-		
86	OHX	1	3892	-	0,6,6	0.00	-	-		
86	OHX	2	2080	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3861	-	0,6,6	0.00	-	-		
86	OHX	5	4026	-	0,6,6	0.00	-	-		
86	OHX	1	4005	-	0,6,6	0.00	-	-		
86	OHX	4	231	-	0,6,6	0.00	-	-		
86	OHX	5	4199	-	0,6,6	0.00	-	-		
86	OHX	5	4176	-	0,6,6	0.00	-	-		
86	OHX	6	2167	-	0,6,6	0.00	-	-		
86	OHX	1	4175	-	0,6,6	0.00	-	-		
86	OHX	5	4250	-	0,6,6	0.00	-	-		
86	OHX	6	2124	-	0,6,6	0.00	-	-		
86	OHX	5	4138	-	0,6,6	0.00	-	-		
86	OHX	2	2127	-	0,6,6	0.00	-	-		
86	OHX	5	3997	-	0,6,6	0.00	-	-		
86	OHX	5	4107	-	0,6,6	0.00	-	-		
86	OHX	1	4006	-	0,6,6	0.00	-	-		
86	OHX	6	2194	-	0,6,6	0.00	-	-		
86	OHX	5	4217	-	0,6,6	0.00	-	-		
86	OHX	1	4100	-	0,6,6	0.00	-	-		
86	OHX	6	2125	-	0,6,6	0.00	-	-		
86	OHX	2	2164	-	0,6,6	0.00	-	-		
86	OHX	6	2145	-	0,6,6	0.00	-	-		
86	OHX	2	2147	-	0,6,6	0.00	-	-		
86	OHX	6	2198	-	0,6,6	0.00	-	-		
86	OHX	5	3962	-	0,6,6	0.00	-	-		
86	OHX	6	2174	-	0,6,6	0.00	-	-		
86	OHX	2	2124	-	0,6,6	0.00	-	-		
86	OHX	4	232	-	0,6,6	0.00	-	-		
86	OHX	2	2087	-	0,6,6	0.00	-	-		
86	OHX	2	2039	-	0,6,6	0.00	-	-		
86	OHX	2	2055	-	0,6,6	0.00	-	-		
86	OHX	5	4181	-	0,6,6	0.00	-	-		
86	OHX	5	4245	-	0,6,6	0.00	-	-		
86	OHX	5	4231	-	0,6,6	0.00	-	-		
86	OHX	5	3954	-	0,6,6	0.00	-	-		
86	OHX	6	2069	-	0,6,6	0.00	-	-		
86	OHX	2	2063	-	0,6,6	0.00	-	-		
86	OHX	1	3914	-	0,6,6	0.00	-	-		
86	OHX	1	4038	-	0,6,6	0.00	-	-		
86	OHX	6	2118	-	0,6,6	0.00	-	-		
86	OHX	2	2122	-	0,6,6	0.00	-	-		
86	OHX	1	4194	-	0,6,6	0.00	-	-		
86	OHX	5	4119	-	0,6,6	0.00	-	-		
86	OHX	1	4063	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4024	-	0,6,6	0.00	-	-		
86	OHX	5	4054	-	0,6,6	0.00	-	-		
86	OHX	1	3953	-	0,6,6	0.00	-	-		
86	OHX	6	2093	-	0,6,6	0.00	-	-		
86	OHX	6	2107	-	0,6,6	0.00	-	-		
86	OHX	1	4071	-	0,6,6	0.00	-	-		
86	OHX	5	4127	-	0,6,6	0.00	-	-		
86	OHX	1	4173	-	0,6,6	0.00	-	-		
86	OHX	6	2070	-	0,6,6	0.00	-	-		
86	OHX	5	4232	-	0,6,6	0.00	-	-		
86	OHX	5	4110	-	0,6,6	0.00	-	-		
86	OHX	5	3925	-	0,6,6	0.00	-	-		
86	OHX	5	4237	-	0,6,6	0.00	-	-		
86	OHX	6	2179	-	0,6,6	0.00	-	-		
86	OHX	1	3864	-	0,6,6	0.00	-	-		
86	OHX	5	3990	-	0,6,6	0.00	-	-		
86	OHX	1	4091	-	0,6,6	0.00	-	-		
86	OHX	5	3959	-	0,6,6	0.00	-	-		
86	OHX	1	4031	-	0,6,6	0.00	-	-		
86	OHX	2	2027	-	0,6,6	0.00	-	-		
86	OHX	5	4085	-	0,6,6	0.00	-	-		
86	OHX	6	2091	-	0,6,6	0.00	-	-		
86	OHX	7	217	-	0,6,6	0.00	-	-		
86	OHX	5	4190	-	0,6,6	0.00	-	-		
86	OHX	1	4178	-	0,6,6	0.00	-	-		
86	OHX	5	4226	-	0,6,6	0.00	-	-		
86	OHX	5	4117	-	0,6,6	0.00	-	-		
86	OHX	2	2134	-	0,6,6	0.00	-	-		
86	OHX	M7	207	-	0,6,6	0.00	-	-		
86	OHX	5	4247	-	0,6,6	0.00	-	-		
86	OHX	1	4070	-	0,6,6	0.00	-	-		
86	OHX	2	2079	-	0,6,6	0.00	-	-		
86	OHX	1	4066	-	0,6,6	0.00	-	-		
86	OHX	1	3883	-	0,6,6	0.00	-	-		
86	OHX	2	2131	-	0,6,6	0.00	-	-		
86	OHX	1	4021	-	0,6,6	0.00	-	-		
86	OHX	2	2172	-	0,6,6	0.00	-	-		
86	OHX	5	3910	-	0,6,6	0.00	-	-		
86	OHX	5	4193	-	0,6,6	0.00	-	-		
86	OHX	5	4195	-	0,6,6	0.00	-	-		
86	OHX	5	3993	-	0,6,6	0.00	-	-		
86	OHX	5	3929	-	0,6,6	0.00	-	-		
86	OHX	1	4051	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4042	-	0,6,6	0.00	-	-		
86	OHX	2	2170	-	0,6,6	0.00	-	-		
86	OHX	5	4092	-	0,6,6	0.00	-	-		
86	OHX	1	3968	-	0,6,6	0.00	-	-		
86	OHX	1	3990	-	0,6,6	0.00	-	-		
86	OHX	5	3938	-	0,6,6	0.00	-	-		
86	OHX	2	2037	-	0,6,6	0.00	-	-		
86	OHX	1	4077	-	0,6,6	0.00	-	-		
86	OHX	5	4139	-	0,6,6	0.00	-	-		
86	OHX	1	4138	-	0,6,6	0.00	-	-		
86	OHX	6	2173	-	0,6,6	0.00	-	-		
86	OHX	1	4130	-	0,6,6	0.00	-	-		
86	OHX	5	4034	-	0,6,6	0.00	-	-		
86	OHX	1	3937	-	0,6,6	0.00	-	-		
86	OHX	1	3994	-	0,6,6	0.00	-	-		
86	OHX	2	2174	-	0,6,6	0.00	-	-		
86	OHX	5	4076	-	0,6,6	0.00	-	-		
86	OHX	2	2096	-	0,6,6	0.00	-	-		
86	OHX	5	4185	-	0,6,6	0.00	-	-		
86	OHX	5	4088	-	0,6,6	0.00	-	-		
86	OHX	3	225	-	0,6,6	0.00	-	-		
86	OHX	1	4195	-	0,6,6	0.00	-	-		
86	OHX	8	213	-	0,6,6	0.00	-	-		
86	OHX	1	3978	-	0,6,6	0.00	-	-		
86	OHX	N9	101	-	0,6,6	0.00	-	-		
86	OHX	5	4087	-	0,6,6	0.00	-	-		
86	OHX	6	2080	-	0,6,6	0.00	-	-		
86	OHX	6	2094	-	0,6,6	0.00	-	-		
86	OHX	6	2066	-	0,6,6	0.00	-	-		
86	OHX	5	3980	-	0,6,6	0.00	-	-		
86	OHX	5	3946	-	0,6,6	0.00	-	-		
86	OHX	1	4019	-	0,6,6	0.00	-	-		
86	OHX	5	4144	-	0,6,6	0.00	-	-		
86	OHX	1	3951	-	0,6,6	0.00	-	-		
86	OHX	5	3975	-	0,6,6	0.00	-	-		
86	OHX	5	4135	-	0,6,6	0.00	-	-		
86	OHX	1	3920	-	0,6,6	0.00	-	-		
86	OHX	5	4013	-	0,6,6	0.00	-	-		
86	OHX	5	3949	-	0,6,6	0.00	-	-		
86	OHX	5	4227	-	0,6,6	0.00	-	-		
86	OHX	2	2148	-	0,6,6	0.00	-	-		
86	OHX	6	2195	-	0,6,6	0.00	-	-		
86	OHX	5	4146	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4171	-	0,6,6	0.00	-	-		
86	OHX	5	3966	-	0,6,6	0.00	-	-		
86	OHX	8	220	-	0,6,6	0.00	-	-		
86	OHX	5	4010	-	0,6,6	0.00	-	-		
86	OHX	1	3997	-	0,6,6	0.00	-	-		
86	OHX	5	4104	-	0,6,6	0.00	-	-		
86	OHX	5	4170	-	0,6,6	0.00	-	-		
86	OHX	4	235	-	0,6,6	0.00	-	-		
86	OHX	1	3911	-	0,6,6	0.00	-	-		
86	OHX	5	4061	-	0,6,6	0.00	-	-		
86	OHX	6	2197	-	0,6,6	0.00	-	-		
86	OHX	5	3956	-	0,6,6	0.00	-	-		
86	OHX	5	4216	-	0,6,6	0.00	-	-		
86	OHX	1	4032	-	0,6,6	0.00	-	-		
86	OHX	5	3935	-	0,6,6	0.00	-	-		
86	OHX	1	4029	-	0,6,6	0.00	-	-		
86	OHX	5	4157	-	0,6,6	0.00	-	-		
86	OHX	5	4108	-	0,6,6	0.00	-	-		
86	OHX	1	3933	-	0,6,6	0.00	-	-		
86	OHX	1	3980	-	0,6,6	0.00	-	-		
86	OHX	2	2032	-	0,6,6	0.00	-	-		
86	OHX	2	2033	-	0,6,6	0.00	-	-		
86	OHX	5	4189	-	0,6,6	0.00	-	-		
86	OHX	6	2098	-	0,6,6	0.00	-	-		
86	OHX	14	402	-	0,6,6	0.00	-	-		
86	OHX	5	4162	-	0,6,6	0.00	-	-		
86	OHX	2	2129	-	0,6,6	0.00	-	-		
86	OHX	2	2075	-	0,6,6	0.00	-	-		
86	OHX	5	4200	-	0,6,6	0.00	-	-		
86	OHX	6	2096	-	0,6,6	0.00	-	-		
86	OHX	5	3912	-	0,6,6	0.00	-	-		
86	OHX	2	2154	-	0,6,6	0.00	-	-		
86	OHX	1	4147	-	0,6,6	0.00	-	-		
86	OHX	5	4166	-	0,6,6	0.00	-	-		
86	OHX	1	4057	-	0,6,6	0.00	-	-		
86	OHX	2	2111	-	0,6,6	0.00	-	-		
86	OHX	3	216	-	0,6,6	0.00	-	-		
86	OHX	8	214	-	0,6,6	0.00	-	-		
86	OHX	6	2117	-	0,6,6	0.00	-	-		
86	OHX	C5	201	-	0,6,6	0.00	-	-		
86	OHX	4	223	-	0,6,6	0.00	-	-		
86	OHX	2	2163	-	0,6,6	0.00	-	-		
86	OHX	4	229	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3975	-	0,6,6	0.00	-	-		
86	OHX	1	4087	-	0,6,6	0.00	-	-		
86	OHX	6	2196	-	0,6,6	0.00	-	-		
86	OHX	6	2049	-	0,6,6	0.00	-	-		
86	OHX	1	3938	-	0,6,6	0.00	-	-		
86	OHX	1	4204	-	0,6,6	0.00	-	-		
86	OHX	5	3994	-	0,6,6	0.00	-	-		
86	OHX	5	4004	-	0,6,6	0.00	-	-		
86	OHX	1	4170	-	0,6,6	0.00	-	-		
86	OHX	6	2059	-	0,6,6	0.00	-	-		
86	OHX	1	3948	-	0,6,6	0.00	-	-		
86	OHX	1	4049	-	0,6,6	0.00	-	-		
86	OHX	2	2165	-	0,6,6	0.00	-	-		
86	OHX	1	3934	-	0,6,6	0.00	-	-		
86	OHX	1	4109	-	0,6,6	0.00	-	-		
86	OHX	2	2169	-	0,6,6	0.00	-	-		
86	OHX	1	3981	-	0,6,6	0.00	-	-		
86	OHX	2	2180	-	0,6,6	0.00	-	-		
86	OHX	1	4161	-	0,6,6	0.00	-	-		
86	OHX	1	4154	-	0,6,6	0.00	-	-		
86	OHX	1	3972	-	0,6,6	0.00	-	-		
86	OHX	5	3908	-	0,6,6	0.00	-	-		
86	OHX	N1	201	-	0,6,6	0.00	-	-		
86	OHX	M5	303	-	0,6,6	0.00	-	-		
86	OHX	1	4155	-	0,6,6	0.00	-	-		
86	OHX	4	227	-	0,6,6	0.00	-	-		
86	OHX	5	4188	-	0,6,6	0.00	-	-		
86	OHX	1	4186	-	0,6,6	0.00	-	-		
86	OHX	1	4016	-	0,6,6	0.00	-	-		
86	OHX	1	4123	-	0,6,6	0.00	-	-		
86	OHX	1	4165	-	0,6,6	0.00	-	-		
86	OHX	6	2062	-	0,6,6	0.00	-	-		
86	OHX	5	4071	-	0,6,6	0.00	-	-		
86	OHX	6	2178	-	0,6,6	0.00	-	-		
86	OHX	5	3964	-	0,6,6	0.00	-	-		
86	OHX	5	4163	-	0,6,6	0.00	-	-		
86	OHX	2	2157	-	0,6,6	0.00	-	-		
86	OHX	1	4086	-	0,6,6	0.00	-	-		
86	OHX	6	2191	-	0,6,6	0.00	-	-		
86	OHX	5	4253	-	0,6,6	0.00	-	-		
86	OHX	m0	301	-	0,6,6	0.00	-	-		
86	OHX	n9	102	-	0,6,6	0.00	-	-		
86	OHX	6	2190	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4131	-	0,6,6	0.00	-	-		
86	OHX	5	4082	-	0,6,6	0.00	-	-		
86	OHX	2	2161	-	0,6,6	0.00	-	-		
86	OHX	5	4000	-	0,6,6	0.00	-	-		
86	OHX	1	3977	-	0,6,6	0.00	-	-		
86	OHX	5	4143	-	0,6,6	0.00	-	-		
86	OHX	5	4196	-	0,6,6	0.00	-	-		
86	OHX	2	2142	-	0,6,6	0.00	-	-		
86	OHX	1	4158	-	0,6,6	0.00	-	-		
86	OHX	5	3926	-	0,6,6	0.00	-	-		
86	OHX	2	2130	-	0,6,6	0.00	-	-		
86	OHX	3	223	-	0,6,6	0.00	-	-		
86	OHX	1	3877	-	0,6,6	0.00	-	-		
86	OHX	6	2177	-	0,6,6	0.00	-	-		
86	OHX	7	224	-	0,6,6	0.00	-	-		
86	OHX	1	3863	-	0,6,6	0.00	-	-		
86	OHX	5	4134	-	0,6,6	0.00	-	-		
86	OHX	1	4131	-	0,6,6	0.00	-	-		
86	OHX	SR	401	-	0,6,6	0.00	-	-		
86	OHX	6	2086	-	0,6,6	0.00	-	-		
86	OHX	1	4064	-	0,6,6	0.00	-	-		
86	OHX	1	3912	-	0,6,6	0.00	-	-		
86	OHX	1	4028	-	0,6,6	0.00	-	-		
86	OHX	1	3870	-	0,6,6	0.00	-	-		
86	OHX	5	4148	-	0,6,6	0.00	-	-		
86	OHX	1	4098	-	0,6,6	0.00	-	-		
86	OHX	1	4097	-	0,6,6	0.00	-	-		
86	OHX	6	2155	-	0,6,6	0.00	-	-		
86	OHX	q2	502	-	0,6,6	0.00	-	-		
86	OHX	2	2053	-	0,6,6	0.00	-	-		
86	OHX	2	2095	-	0,6,6	0.00	-	-		
86	OHX	1	3955	-	0,6,6	0.00	-	-		
86	OHX	O1	201	-	0,6,6	0.00	-	-		
86	OHX	5	3943	-	0,6,6	0.00	-	-		
86	OHX	6	2154	-	0,6,6	0.00	-	-		
86	OHX	1	3928	-	0,6,6	0.00	-	-		
86	OHX	m1	203	-	0,6,6	0.00	-	-		
86	OHX	5	3958	-	0,6,6	0.00	-	-		
86	OHX	5	4179	-	0,6,6	0.00	-	-		
86	OHX	5	4172	-	0,6,6	0.00	-	-		
86	OHX	5	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4047	-	0,6,6	0.00	-	-		
86	OHX	5	3905	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2141	-	0,6,6	0.00	-	-		
86	OHX	1	3986	-	0,6,6	0.00	-	-		
86	OHX	1	4133	-	0,6,6	0.00	-	-		
86	OHX	6	2151	-	0,6,6	0.00	-	-		
86	OHX	2	2151	-	0,6,6	0.00	-	-		
86	OHX	4	237	-	0,6,6	0.00	-	-		
86	OHX	1	4046	-	0,6,6	0.00	-	-		
86	OHX	5	4155	-	0,6,6	0.00	-	-		
86	OHX	5	4149	-	0,6,6	0.00	-	-		
86	OHX	5	3902	-	0,6,6	0.00	-	-		
86	OHX	2	2085	-	0,6,6	0.00	-	-		
86	OHX	5	4171	-	0,6,6	0.00	-	-		
86	OHX	6	2181	-	0,6,6	0.00	-	-		
86	OHX	5	4105	-	0,6,6	0.00	-	-		
86	OHX	6	2061	-	0,6,6	0.00	-	-		
86	OHX	2	2179	-	0,6,6	0.00	-	-		
86	OHX	5	3927	-	0,6,6	0.00	-	-		
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	L3	406	-	0,6,6	0.00	-	-		
86	OHX	1	3964	-	0,6,6	0.00	-	-		
86	OHX	5	4156	-	0,6,6	0.00	-	-		
86	OHX	6	2182	-	0,6,6	0.00	-	-		
86	OHX	2	2177	-	0,6,6	0.00	-	-		
86	OHX	2	2176	-	0,6,6	0.00	-	-		
86	OHX	5	4012	-	0,6,6	0.00	-	-		
86	OHX	6	2081	-	0,6,6	0.00	-	-		
86	OHX	1	3866	-	0,6,6	0.00	-	-		
86	OHX	1	4172	-	0,6,6	0.00	-	-		
86	OHX	2	2107	-	0,6,6	0.00	-	-		
86	OHX	3	214	-	0,6,6	0.00	-	-		
86	OHX	1	4169	-	0,6,6	0.00	-	-		
86	OHX	5	4106	-	0,6,6	0.00	-	-		
86	OHX	2	2082	-	0,6,6	0.00	-	-		
86	OHX	n5	201	-	0,6,6	0.00	-	-		
86	OHX	2	2132	-	0,6,6	0.00	-	-		
86	OHX	2	2112	-	0,6,6	0.00	-	-		
86	OHX	2	2118	-	0,6,6	0.00	-	-		
86	OHX	2	2038	-	0,6,6	0.00	-	-		
86	OHX	6	2123	-	0,6,6	0.00	-	-		
86	OHX	1	3998	-	0,6,6	0.00	-	-		
86	OHX	2	2049	-	0,6,6	0.00	-	-		
86	OHX	5	4027	-	0,6,6	0.00	-	-		
86	OHX	5	4120	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2092	-	0,6,6	0.00	-	-		
86	OHX	5	4125	-	0,6,6	0.00	-	-		
86	OHX	2	2051	-	0,6,6	0.00	-	-		
86	OHX	1	3971	-	0,6,6	0.00	-	-		
86	OHX	1	4012	-	0,6,6	0.00	-	-		
86	OHX	6	2064	-	0,6,6	0.00	-	-		
86	OHX	2	2106	-	0,6,6	0.00	-	-		
86	OHX	1	4177	-	0,6,6	0.00	-	-		
86	OHX	8	216	-	0,6,6	0.00	-	-		
86	OHX	S8	302	-	0,6,6	0.00	-	-		
86	OHX	5	3973	-	0,6,6	0.00	-	-		
86	OHX	5	4011	-	0,6,6	0.00	-	-		
86	OHX	6	2148	-	0,6,6	0.00	-	-		
86	OHX	2	2058	-	0,6,6	0.00	-	-		
86	OHX	5	3915	-	0,6,6	0.00	-	-		
86	OHX	1	3946	-	0,6,6	0.00	-	-		
86	OHX	5	4049	-	0,6,6	0.00	-	-		
86	OHX	1	3954	-	0,6,6	0.00	-	-		
86	OHX	n3	203	-	0,6,6	0.00	-	-		
86	OHX	1	3956	-	0,6,6	0.00	-	-		
86	OHX	1	4142	-	0,6,6	0.00	-	-		
86	OHX	8	215	-	0,6,6	0.00	-	-		
86	OHX	5	4018	-	0,6,6	0.00	-	-		
86	OHX	2	2115	-	0,6,6	0.00	-	-		
86	OHX	1	3941	-	0,6,6	0.00	-	-		
86	OHX	6	2106	-	0,6,6	0.00	-	-		
86	OHX	5	4252	-	0,6,6	0.00	-	-		
86	OHX	o2	201	-	0,6,6	0.00	-	-		
86	OHX	5	3950	-	0,6,6	0.00	-	-		
86	OHX	5	4145	-	0,6,6	0.00	-	-		
86	OHX	2	2062	-	0,6,6	0.00	-	-		
86	OHX	1	4159	-	0,6,6	0.00	-	-		
86	OHX	5	4015	-	0,6,6	0.00	-	-		
86	OHX	5	4229	-	0,6,6	0.00	-	-		
86	OHX	1	3887	-	0,6,6	0.00	-	-		
86	OHX	5	4053	-	0,6,6	0.00	-	-		
86	OHX	6	2057	-	0,6,6	0.00	-	-		
86	OHX	1	4033	-	0,6,6	0.00	-	-		
86	OHX	5	4173	-	0,6,6	0.00	-	-		
86	OHX	2	2043	-	0,6,6	0.00	-	-		
86	OHX	5	4046	-	0,6,6	0.00	-	-		
86	OHX	5	4132	-	0,6,6	0.00	-	-		
86	OHX	1	4009	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2083	-	0,6,6	0.00	-	-		
86	OHX	1	3926	-	0,6,6	0.00	-	-		
86	OHX	5	4164	-	0,6,6	0.00	-	-		
86	OHX	2	2078	-	0,6,6	0.00	-	-		
86	OHX	5	3952	-	0,6,6	0.00	-	-		
86	OHX	6	2180	-	0,6,6	0.00	-	-		
86	OHX	6	2101	-	0,6,6	0.00	-	-		
86	OHX	1	3871	-	0,6,6	0.00	-	-		
86	OHX	6	2143	-	0,6,6	0.00	-	-		
86	OHX	5	4152	-	0,6,6	0.00	-	-		
86	OHX	1	4127	-	0,6,6	0.00	-	-		
86	OHX	15	305	-	0,6,6	0.00	-	-		
86	OHX	8	217	-	0,6,6	0.00	-	-		
86	OHX	5	4221	-	0,6,6	0.00	-	-		
86	OHX	1	4146	-	0,6,6	0.00	-	-		
86	OHX	5	4094	-	0,6,6	0.00	-	-		
86	OHX	2	2168	-	0,6,6	0.00	-	-		
86	OHX	1	4113	-	0,6,6	0.00	-	-		
86	OHX	5	4254	-	0,6,6	0.00	-	-		
86	OHX	5	4093	-	0,6,6	0.00	-	-		
86	OHX	5	3955	-	0,6,6	0.00	-	-		
86	OHX	8	225	-	0,6,6	0.00	-	-		
86	OHX	5	4074	-	0,6,6	0.00	-	-		
86	OHX	2	2029	-	0,6,6	0.00	-	-		
86	OHX	1	3959	-	0,6,6	0.00	-	-		
86	OHX	1	3999	-	0,6,6	0.00	-	-		
86	OHX	1	4162	-	0,6,6	0.00	-	-		
86	OHX	5	4234	-	0,6,6	0.00	-	-		
86	OHX	2	2175	-	0,6,6	0.00	-	-		
86	OHX	7	228	-	0,6,6	0.00	-	-		
86	OHX	4	228	-	0,6,6	0.00	-	-		
86	OHX	1	4163	-	0,6,6	0.00	-	-		
86	OHX	8	223	-	0,6,6	0.00	-	-		
86	OHX	2	2150	-	0,6,6	0.00	-	-		
86	OHX	6	2127	-	0,6,6	0.00	-	-		
86	OHX	5	3995	-	0,6,6	0.00	-	-		
86	OHX	M7	206	-	0,6,6	0.00	-	-		
86	OHX	1	3876	-	0,6,6	0.00	-	-		
86	OHX	1	3932	-	0,6,6	0.00	-	-		
86	OHX	c3	201	-	0,6,6	0.00	-	-		
86	OHX	1	4157	-	0,6,6	0.00	-	-		
86	OHX	2	2136	-	0,6,6	0.00	-	-		
86	OHX	5	4031	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2156	-	0,6,6	0.00	-	-		
86	OHX	1	4120	-	0,6,6	0.00	-	-		
86	OHX	5	4184	-	0,6,6	0.00	-	-		
86	OHX	2	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4067	-	0,6,6	0.00	-	-		
86	OHX	1	4065	-	0,6,6	0.00	-	-		
86	OHX	5	4124	-	0,6,6	0.00	-	-		
86	OHX	1	3897	-	0,6,6	0.00	-	-		
86	OHX	m7	205	-	0,6,6	0.00	-	-		
86	OHX	5	4210	-	0,6,6	0.00	-	-		
86	OHX	2	2077	-	0,6,6	0.00	-	-		
86	OHX	5	4239	-	0,6,6	0.00	-	-		
86	OHX	2	2060	-	0,6,6	0.00	-	-		
86	OHX	5	4068	-	0,6,6	0.00	-	-		
86	OHX	1	4023	-	0,6,6	0.00	-	-		
86	OHX	5	4244	-	0,6,6	0.00	-	-		
86	OHX	5	4241	-	0,6,6	0.00	-	-		
86	OHX	5	3971	-	0,6,6	0.00	-	-		
86	OHX	3	220	-	0,6,6	0.00	-	-		
86	OHX	5	3914	-	0,6,6	0.00	-	-		
86	OHX	1	3867	-	0,6,6	0.00	-	-		
86	OHX	1	4052	-	0,6,6	0.00	-	-		
86	OHX	4	225	-	0,6,6	0.00	-	-		
86	OHX	2	2066	-	0,6,6	0.00	-	-		
86	OHX	5	4204	-	0,6,6	0.00	-	-		
86	OHX	5	3948	-	0,6,6	0.00	-	-		
86	OHX	6	2053	-	0,6,6	0.00	-	-		
86	OHX	1	3930	-	0,6,6	0.00	-	-		
86	OHX	5	3979	-	0,6,6	0.00	-	-		
86	OHX	5	4030	-	0,6,6	0.00	-	-		
86	OHX	5	4158	-	0,6,6	0.00	-	-		
86	OHX	6	2129	-	0,6,6	0.00	-	-		
86	OHX	5	4233	-	0,6,6	0.00	-	-		
86	OHX	1	3967	-	0,6,6	0.00	-	-		
86	OHX	5	4059	-	0,6,6	0.00	-	-		
86	OHX	5	4101	-	0,6,6	0.00	-	-		
86	OHX	M0	303	-	0,6,6	0.00	-	-		
86	OHX	5	4022	-	0,6,6	0.00	-	-		
86	OHX	5	4218	-	0,6,6	0.00	-	-		
86	OHX	7	225	-	0,6,6	0.00	-	-		
86	OHX	O2	201	-	0,6,6	0.00	-	-		
86	OHX	2	2101	-	0,6,6	0.00	-	-		
86	OHX	1	4081	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2091	-	0,6,6	0.00	-	-		
86	OHX	5	4072	-	0,6,6	0.00	-	-		
86	OHX	2	2040	-	0,6,6	0.00	-	-		
86	OHX	8	228	-	0,6,6	0.00	-	-		
86	OHX	5	4187	-	0,6,6	0.00	-	-		
86	OHX	2	2159	-	0,6,6	0.00	-	-		
86	OHX	5	4249	-	0,6,6	0.00	-	-		
86	OHX	2	2123	-	0,6,6	0.00	-	-		
86	OHX	2	2181	-	0,6,6	0.00	-	-		
86	OHX	6	2119	-	0,6,6	0.00	-	-		
86	OHX	5	3922	-	0,6,6	0.00	-	-		
86	OHX	6	2084	-	0,6,6	0.00	-	-		
86	OHX	5	3933	-	0,6,6	0.00	-	-		
86	OHX	2	2102	-	0,6,6	0.00	-	-		
86	OHX	6	2056	-	0,6,6	0.00	-	-		
86	OHX	5	4140	-	0,6,6	0.00	-	-		
86	OHX	2	2069	-	0,6,6	0.00	-	-		
86	OHX	5	3963	-	0,6,6	0.00	-	-		
86	OHX	5	3957	-	0,6,6	0.00	-	-		
86	OHX	5	4096	-	0,6,6	0.00	-	-		
86	OHX	5	4220	-	0,6,6	0.00	-	-		
86	OHX	2	2074	-	0,6,6	0.00	-	-		
86	OHX	3	219	-	0,6,6	0.00	-	-		
86	OHX	4	224	-	0,6,6	0.00	-	-		
86	OHX	6	2175	-	0,6,6	0.00	-	-		
86	OHX	8	227	-	0,6,6	0.00	-	-		
86	OHX	1	3958	-	0,6,6	0.00	-	-		
86	OHX	1	4191	-	0,6,6	0.00	-	-		
86	OHX	1	4198	-	0,6,6	0.00	-	-		
86	OHX	s4	301	-	0,6,6	0.00	-	-		
86	OHX	5	4003	-	0,6,6	0.00	-	-		
86	OHX	2	2045	-	0,6,6	0.00	-	-		
86	OHX	5	4169	-	0,6,6	0.00	-	-		
86	OHX	1	4126	-	0,6,6	0.00	-	-		
86	OHX	2	2093	-	0,6,6	0.00	-	-		
86	OHX	1	3903	-	0,6,6	0.00	-	-		
86	OHX	2	2109	-	0,6,6	0.00	-	-		
86	OHX	6	2115	-	0,6,6	0.00	-	-		
86	OHX	2	2160	-	0,6,6	0.00	-	-		
86	OHX	1	3949	-	0,6,6	0.00	-	-		
86	OHX	5	4041	-	0,6,6	0.00	-	-		
86	OHX	1	4050	-	0,6,6	0.00	-	-		
86	OHX	1	3936	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2162	-	0,6,6	0.00	-	-		
86	OHX	6	2058	-	0,6,6	0.00	-	-		
86	OHX	1	4111	-	0,6,6	0.00	-	-		
86	OHX	1	4101	-	0,6,6	0.00	-	-		
86	OHX	c8	203	-	0,6,6	0.00	-	-		
86	OHX	2	2089	-	0,6,6	0.00	-	-		
86	OHX	2	2098	-	0,6,6	0.00	-	-		
86	OHX	2	2116	-	0,6,6	0.00	-	-		
86	OHX	2	2128	-	0,6,6	0.00	-	-		
86	OHX	1	4073	-	0,6,6	0.00	-	-		
86	OHX	6	2149	-	0,6,6	0.00	-	-		
86	OHX	5	4044	-	0,6,6	0.00	-	-		
86	OHX	5	4001	-	0,6,6	0.00	-	-		
86	OHX	1	4167	-	0,6,6	0.00	-	-		
86	OHX	6	2141	-	0,6,6	0.00	-	-		
86	OHX	1	3869	-	0,6,6	0.00	-	-		
86	OHX	6	2103	-	0,6,6	0.00	-	-		
86	OHX	1	3894	-	0,6,6	0.00	-	-		
86	OHX	2	2110	-	0,6,6	0.00	-	-		
86	OHX	1	4192	-	0,6,6	0.00	-	-		
86	OHX	5	4028	-	0,6,6	0.00	-	-		
86	OHX	5	4070	-	0,6,6	0.00	-	-		
86	OHX	1	4007	-	0,6,6	0.00	-	-		
86	OHX	5	3939	-	0,6,6	0.00	-	-		
86	OHX	6	2168	-	0,6,6	0.00	-	-		
86	OHX	5	4205	-	0,6,6	0.00	-	-		
86	OHX	5	4077	-	0,6,6	0.00	-	-		
86	OHX	1	4180	-	0,6,6	0.00	-	-		
86	OHX	5	4079	-	0,6,6	0.00	-	-		
86	OHX	2	2103	-	0,6,6	0.00	-	-		
86	OHX	1	4082	-	0,6,6	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	ZBA	5	4256	85	-	3/18/83/83	0/5/4/4
88	ZBA	1	4206	85	1/1/13/14	4/18/83/83	0/5/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4206	ZBA	C28-C27	-6.52	1.47	1.55
88	5	4256	ZBA	C48-C46	6.42	1.51	1.33
88	1	4206	ZBA	C48-C46	6.36	1.51	1.33
88	5	4256	ZBA	C45-C46	-4.28	1.46	1.50
88	1	4206	ZBA	C45-C46	-2.44	1.48	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4206	ZBA	C45-C46-C48	-8.84	108.62	121.74
88	5	4256	ZBA	C45-C46-C48	-8.25	109.48	121.74
88	1	4206	ZBA	C47-C46-C48	-5.07	110.81	121.98
88	5	4256	ZBA	C47-C46-C48	-4.62	111.81	121.98
88	1	4206	ZBA	C46-C45-C44	4.54	123.94	113.26
88	5	4256	ZBA	C47-C46-C45	-3.40	110.30	116.09
88	5	4256	ZBA	O10-C34-C29	3.06	116.44	112.54
88	5	4256	ZBA	C37-C28-C27	3.02	117.03	112.12
88	1	4206	ZBA	C47-C46-C45	-2.98	111.02	116.09
88	5	4256	ZBA	C37-C28-C35	-2.17	108.32	113.12
88	5	4256	ZBA	O14-C27-C26	2.11	115.91	109.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
88	1	4206	ZBA	C35

All (7) torsion outliers are listed below:

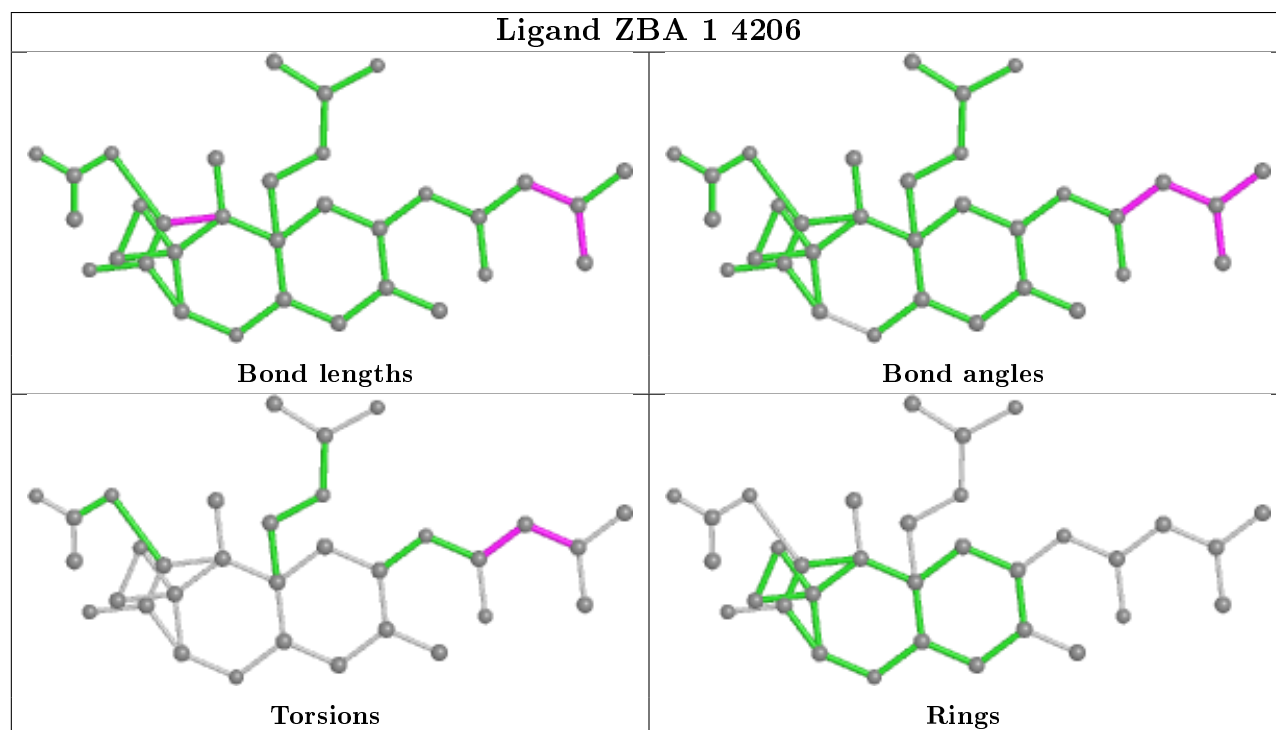
Mol	Chain	Res	Type	Atoms
88	1	4206	ZBA	C44-C45-C46-C48
88	5	4256	ZBA	C44-C45-C46-C48
88	5	4256	ZBA	C43-C42-O14-C27
88	5	4256	ZBA	O15-C42-O14-C27
88	1	4206	ZBA	O17-C44-C45-C46
88	1	4206	ZBA	C44-C45-C46-C47
88	1	4206	ZBA	O18-C44-C45-C46

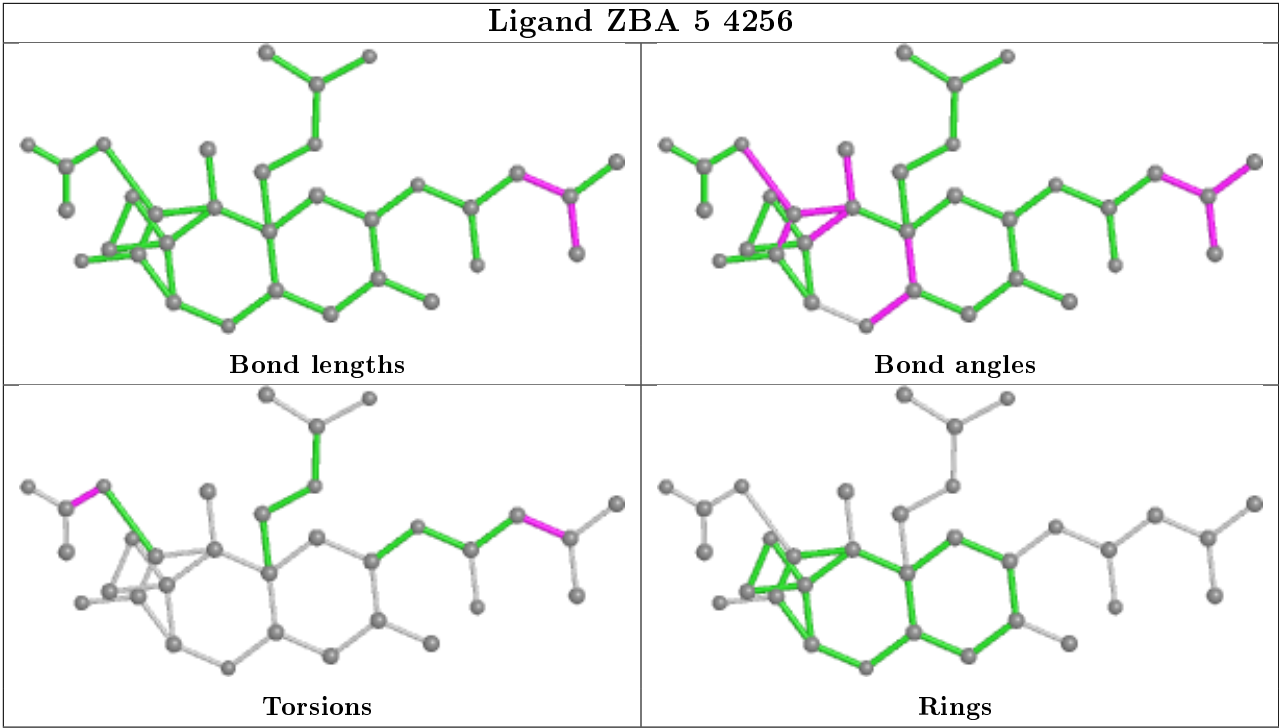
There are no ring outliers.

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
1	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	4.21
1	2	1685:G	O3'	1686:C	P	2.96

6 Fit of model and data [i](#)

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

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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