Full wwPDB EM Validation Report

Nov 19, 2022 – 10:20 pm GMT

PDB ID	:	5K0Y
EMDB ID	:	EMD-8190
Title	:	m48S late-stage initiation complex, purified from rabbit reticulocytes lysates, displaying eIF2 ternary complex and eIF3 i and g subunits relocated to the intersubunit face
Authors	:	Simonetti, A.; Brito Querido, J.; Myasnikov, A.G.; Mancera-Martinez, E.; Renaud, A.; Kuhn, L.; Hashem, Y.
Deposited on	:	2016-05-17
Resolution	:	5.80 Å(reported)
Based on initial model	:	4KZY

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

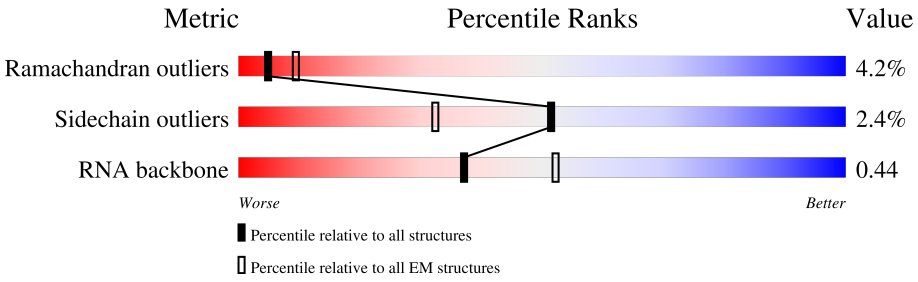
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.80 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)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	N	75	73% 24%
2	A	1776	67% 31%
3	F	30	57% 40%
4	P	266	46% 85% 12%
5	G	158	5% 93% 7%
6	H	141	91% 8%
7	I	263	92% 7%
8	J	53	96%

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Mol	Chain	Length	Quality of chain
9	K	182	94% 5%
10	L	137	91% 8%
11	M	38	89% 97%
12	O	77	78% 99%
13	Q	142	94% 6%
14	R	141	92% 7%
15	S	422	75% 92% 7%
16	T	329	89% 94% 5%
17	U	191	93% 6%
18	V	59	7% 92% 8%
19	W	75	93% 7%
20	X	190	7% 89% 9%
21	Y	84	88% 11%
22	Z	150	97%
23	a	129	95% 5%
24	b	82	82% 17%
25	c	226	95%
26	d	17	88% 100%
27	e	126	6% 96%
28	f	208	93% 7%
29	g	227	94% 6%
30	h	104	88% 12%
31	i	215	94% 6%
32	j	136	93% 5%
33	k	99	92% 8%

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Mol	Chain	Length	Quality of chain
34	l	64	97%
35	m	313	92% 7%
36	n	127	84% 13%
37	o	206	94% 6%
38	p	71	80% 17%
39	q	237	94% 6%
40	r	124	90% 10%
41	s	131	89% 10%
42	t	98	81% 17%

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 88157 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	73	C	-	expression tag	REF 655840029
N	74	C	-	expression tag	REF 655840029
N	75	A	-	expression tag	REF 655840029

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1776	Total	C	N	O	P	0	0
			37881	16910	6782	12414	1775		

There are 685 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	U	-	expression tag	REF 283837872
A	2	A	-	expression tag	REF 283837872
A	3	C	-	expression tag	REF 283837872
A	4	C	-	expression tag	REF 283837872
A	5	U	-	expression tag	REF 283837872
A	6	G	-	expression tag	REF 283837872
A	7	G	-	expression tag	REF 283837872
A	8	U	-	expression tag	REF 283837872
A	9	U	-	expression tag	REF 283837872
A	10	G	-	expression tag	REF 283837872
A	11	A	-	expression tag	REF 283837872
A	12	U	-	expression tag	REF 283837872
A	13	C	-	expression tag	REF 283837872
A	14	C	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	U	-	expression tag	REF 283837872
A	16	G	-	expression tag	REF 283837872
A	17	C	-	expression tag	REF 283837872
A	18	C	-	expression tag	REF 283837872
A	19	A	-	expression tag	REF 283837872
A	20	G	-	expression tag	REF 283837872
A	21	U	-	expression tag	REF 283837872
A	22	A	-	expression tag	REF 283837872
A	23	G	-	expression tag	REF 283837872
A	24	C	-	expression tag	REF 283837872
A	25	A	-	expression tag	REF 283837872
A	26	U	-	expression tag	REF 283837872
A	27	A	-	expression tag	REF 283837872
A	28	U	-	expression tag	REF 283837872
A	29	G	-	expression tag	REF 283837872
A	30	C	-	expression tag	REF 283837872
A	31	U	-	expression tag	REF 283837872
A	32	U	-	expression tag	REF 283837872
A	33	G	-	expression tag	REF 283837872
A	34	U	-	expression tag	REF 283837872
A	35	C	-	expression tag	REF 283837872
A	36	U	-	expression tag	REF 283837872
A	37	C	-	expression tag	REF 283837872
A	38	A	-	expression tag	REF 283837872
A	39	A	-	expression tag	REF 283837872
A	40	A	-	expression tag	REF 283837872
A	41	G	-	expression tag	REF 283837872
A	42	A	-	expression tag	REF 283837872
A	43	U	-	expression tag	REF 283837872
A	44	U	-	expression tag	REF 283837872
A	45	A	-	expression tag	REF 283837872
A	46	A	-	expression tag	REF 283837872
A	47	G	-	expression tag	REF 283837872
A	48	C	-	expression tag	REF 283837872
A	49	C	-	expression tag	REF 283837872
A	50	A	-	expression tag	REF 283837872
A	51	U	-	expression tag	REF 283837872
A	52	G	-	expression tag	REF 283837872
A	53	C	-	expression tag	REF 283837872
A	54	A	-	expression tag	REF 283837872
A	55	U	-	expression tag	REF 283837872
A	56	G	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	57	U	-	expression tag	REF 283837872
A	58	C	-	expression tag	REF 283837872
A	59	U	-	expression tag	REF 283837872
A	60	A	-	expression tag	REF 283837872
A	61	A	-	expression tag	REF 283837872
A	62	G	-	expression tag	REF 283837872
A	63	U	-	expression tag	REF 283837872
A	64	A	-	expression tag	REF 283837872
A	65	C	-	expression tag	REF 283837872
A	66	G	-	expression tag	REF 283837872
A	67	C	-	expression tag	REF 283837872
A	68	A	-	expression tag	REF 283837872
A	69	C	-	expression tag	REF 283837872
A	70	G	-	expression tag	REF 283837872
A	71	G	-	expression tag	REF 283837872
A	72	C	-	expression tag	REF 283837872
A	73	C	-	expression tag	REF 283837872
A	74	G	-	expression tag	REF 283837872
A	75	G	-	expression tag	REF 283837872
A	76	U	-	expression tag	REF 283837872
A	77	A	-	expression tag	REF 283837872
A	78	C	-	expression tag	REF 283837872
A	79	A	-	expression tag	REF 283837872
A	80	G	-	expression tag	REF 283837872
A	81	U	-	expression tag	REF 283837872
A	82	G	-	expression tag	REF 283837872
A	83	A	-	expression tag	REF 283837872
A	84	A	-	expression tag	REF 283837872
A	85	A	-	expression tag	REF 283837872
A	86	C	-	expression tag	REF 283837872
A	87	U	-	expression tag	REF 283837872
A	88	G	-	expression tag	REF 283837872
A	89	C	-	expression tag	REF 283837872
A	90	G	-	expression tag	REF 283837872
A	91	A	-	expression tag	REF 283837872
A	92	A	-	expression tag	REF 283837872
A	93	U	-	expression tag	REF 283837872
A	94	G	-	expression tag	REF 283837872
A	95	G	-	expression tag	REF 283837872
A	96	C	-	expression tag	REF 283837872
A	97	U	-	expression tag	REF 283837872
A	98	C	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	99	A	-	expression tag	REF 283837872
A	100	U	-	expression tag	REF 283837872
A	101	U	-	expression tag	REF 283837872
A	102	A	-	expression tag	REF 283837872
A	103	A	-	expression tag	REF 283837872
A	104	A	-	expression tag	REF 283837872
A	105	U	-	expression tag	REF 283837872
A	106	C	-	expression tag	REF 283837872
A	107	A	-	expression tag	REF 283837872
A	108	G	-	expression tag	REF 283837872
A	109	U	-	expression tag	REF 283837872
A	110	U	-	expression tag	REF 283837872
A	111	A	-	expression tag	REF 283837872
A	112	U	-	expression tag	REF 283837872
A	113	G	-	expression tag	REF 283837872
A	114	G	-	expression tag	REF 283837872
A	115	U	-	expression tag	REF 283837872
A	116	U	-	expression tag	REF 283837872
A	117	C	-	expression tag	REF 283837872
A	118	C	-	expression tag	REF 283837872
A	119	U	-	expression tag	REF 283837872
A	120	U	-	expression tag	REF 283837872
A	121	U	-	expression tag	REF 283837872
A	122	G	-	expression tag	REF 283837872
A	123	G	-	expression tag	REF 283837872
A	124	U	-	expression tag	REF 283837872
A	125	C	-	expression tag	REF 283837872
A	126	G	-	expression tag	REF 283837872
A	127	C	-	expression tag	REF 283837872
A	128	U	-	expression tag	REF 283837872
A	129	C	-	expression tag	REF 283837872
A	130	G	-	expression tag	REF 283837872
A	131	C	-	expression tag	REF 283837872
A	132	U	-	expression tag	REF 283837872
A	133	C	-	expression tag	REF 283837872
A	134	C	-	expression tag	REF 283837872
A	135	U	-	expression tag	REF 283837872
A	136	C	-	expression tag	REF 283837872
A	137	U	-	expression tag	REF 283837872
A	138	C	-	expression tag	REF 283837872
A	139	C	-	expression tag	REF 283837872
A	140	U	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	141	A	-	expression tag	REF 283837872
A	142	C	-	expression tag	REF 283837872
A	143	U	-	expression tag	REF 283837872
A	144	U	-	expression tag	REF 283837872
A	145	G	-	expression tag	REF 283837872
A	146	G	-	expression tag	REF 283837872
A	147	A	-	expression tag	REF 283837872
A	148	U	-	expression tag	REF 283837872
A	149	A	-	expression tag	REF 283837872
A	150	A	-	expression tag	REF 283837872
A	151	C	-	expression tag	REF 283837872
A	152	U	-	expression tag	REF 283837872
A	153	G	-	expression tag	REF 283837872
A	154	U	-	expression tag	REF 283837872
A	155	G	-	expression tag	REF 283837872
A	156	G	-	expression tag	REF 283837872
A	157	U	-	expression tag	REF 283837872
A	158	A	-	expression tag	REF 283837872
A	159	A	-	expression tag	REF 283837872
A	160	U	-	expression tag	REF 283837872
A	161	U	-	expression tag	REF 283837872
A	162	C	-	expression tag	REF 283837872
A	163	U	-	expression tag	REF 283837872
A	164	A	-	expression tag	REF 283837872
A	165	G	-	expression tag	REF 283837872
A	166	A	-	expression tag	REF 283837872
A	167	G	-	expression tag	REF 283837872
A	168	C	-	expression tag	REF 283837872
A	169	U	-	expression tag	REF 283837872
A	170	A	-	expression tag	REF 283837872
A	171	A	-	expression tag	REF 283837872
A	172	U	-	expression tag	REF 283837872
A	173	A	-	expression tag	REF 283837872
A	174	C	-	expression tag	REF 283837872
A	175	A	-	expression tag	REF 283837872
A	176	U	-	expression tag	REF 283837872
A	177	G	-	expression tag	REF 283837872
A	178	C	-	expression tag	REF 283837872
A	179	C	-	expression tag	REF 283837872
A	180	G	-	expression tag	REF 283837872
A	181	A	-	expression tag	REF 283837872
A	182	C	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	183	G	-	expression tag	REF 283837872
A	184	G	-	expression tag	REF 283837872
A	185	C	-	expression tag	REF 283837872
A	186	G	-	expression tag	REF 283837872
A	187	C	-	expression tag	REF 283837872
A	188	U	-	expression tag	REF 283837872
A	189	G	-	expression tag	REF 283837872
A	190	A	-	expression tag	REF 283837872
A	191	C	-	expression tag	REF 283837872
A	192	U	-	expression tag	REF 283837872
A	193	C	-	expression tag	REF 283837872
A	194	C	-	expression tag	REF 283837872
A	195	C	-	expression tag	REF 283837872
A	196	U	-	expression tag	REF 283837872
A	197	U	-	expression tag	REF 283837872
A	198	U	-	expression tag	REF 283837872
A	199	G	-	expression tag	REF 283837872
A	200	U	-	expression tag	REF 283837872
A	201	G	-	expression tag	REF 283837872
A	202	U	-	expression tag	REF 283837872
A	203	G	-	expression tag	REF 283837872
A	204	G	-	expression tag	REF 283837872
A	205	G	-	expression tag	REF 283837872
A	206	A	-	expression tag	REF 283837872
A	207	U	-	expression tag	REF 283837872
A	208	G	-	expression tag	REF 283837872
A	209	C	-	expression tag	REF 283837872
A	210	G	-	expression tag	REF 283837872
A	211	U	-	expression tag	REF 283837872
A	212	G	-	expression tag	REF 283837872
A	213	C	-	expression tag	REF 283837872
A	214	A	-	expression tag	REF 283837872
A	215	U	-	expression tag	REF 283837872
A	216	U	-	expression tag	REF 283837872
A	217	U	-	expression tag	REF 283837872
A	218	A	-	expression tag	REF 283837872
A	219	U	-	expression tag	REF 283837872
A	220	C	-	expression tag	REF 283837872
A	221	A	-	expression tag	REF 283837872
A	222	G	-	expression tag	REF 283837872
A	223	A	-	expression tag	REF 283837872
A	224	U	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	225	C	-	expression tag	REF 283837872
A	226	A	-	expression tag	REF 283837872
A	227	A	-	expression tag	REF 283837872
A	228	A	-	expression tag	REF 283837872
A	229	A	-	expression tag	REF 283837872
A	230	C	-	expression tag	REF 283837872
A	231	C	-	expression tag	REF 283837872
A	232	A	-	expression tag	REF 283837872
A	233	A	-	expression tag	REF 283837872
A	234	C	-	expression tag	REF 283837872
A	235	C	-	expression tag	REF 283837872
A	236	C	-	expression tag	REF 283837872
A	237	G	-	expression tag	REF 283837872
A	238	G	-	expression tag	REF 283837872
A	239	U	-	expression tag	REF 283837872
A	240	C	-	expression tag	REF 283837872
A	241	A	-	expression tag	REF 283837872
A	242	G	-	expression tag	REF 283837872
A	243	C	-	expression tag	REF 283837872
A	267	G	-	expression tag	REF 283837872
A	268	G	-	expression tag	REF 283837872
A	269	C	-	expression tag	REF 283837872
A	270	G	-	expression tag	REF 283837872
A	271	G	-	expression tag	REF 283837872
A	272	C	-	expression tag	REF 283837872
A	273	G	-	expression tag	REF 283837872
A	274	G	-	expression tag	REF 283837872
A	275	C	-	expression tag	REF 283837872
A	276	U	-	expression tag	REF 283837872
A	277	U	-	expression tag	REF 283837872
A	278	U	-	expression tag	REF 283837872
A	279	G	-	expression tag	REF 283837872
A	280	G	-	expression tag	REF 283837872
A	281	U	-	expression tag	REF 283837872
A	282	G	-	expression tag	REF 283837872
A	283	A	-	expression tag	REF 283837872
A	284	C	-	expression tag	REF 283837872
A	285	U	-	expression tag	REF 283837872
A	286	C	-	expression tag	REF 283837872
A	287	U	-	expression tag	REF 283837872
A	288	A	-	expression tag	REF 283837872
A	289	G	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	290	A	-	expression tag	REF 283837872
A	291	U	-	expression tag	REF 283837872
A	292	A	-	expression tag	REF 283837872
A	293	A	-	expression tag	REF 283837872
A	294	C	-	expression tag	REF 283837872
A	295	C	-	expression tag	REF 283837872
A	296	U	-	expression tag	REF 283837872
A	297	C	-	expression tag	REF 283837872
A	298	G	-	expression tag	REF 283837872
A	299	G	-	expression tag	REF 283837872
A	300	G	-	expression tag	REF 283837872
A	301	C	-	expression tag	REF 283837872
A	302	C	-	expression tag	REF 283837872
A	303	G	-	expression tag	REF 283837872
A	304	A	-	expression tag	REF 283837872
A	305	U	-	expression tag	REF 283837872
A	306	C	-	expression tag	REF 283837872
A	307	G	-	expression tag	REF 283837872
A	308	C	-	expression tag	REF 283837872
A	309	A	-	expression tag	REF 283837872
A	310	G	-	expression tag	REF 283837872
A	311	C	-	expression tag	REF 283837872
A	312	C	-	expression tag	REF 283837872
A	313	C	-	expression tag	REF 283837872
A	314	U	-	expression tag	REF 283837872
A	315	C	-	expression tag	REF 283837872
A	316	C	-	expression tag	REF 283837872
A	317	G	-	expression tag	REF 283837872
A	318	U	-	expression tag	REF 283837872
A	319	G	-	expression tag	REF 283837872
A	320	G	-	expression tag	REF 283837872
A	321	C	-	expression tag	REF 283837872
A	322	G	-	expression tag	REF 283837872
A	323	G	-	expression tag	REF 283837872
A	324	C	-	expression tag	REF 283837872
A	325	G	-	expression tag	REF 283837872
A	326	A	-	expression tag	REF 283837872
A	327	C	-	expression tag	REF 283837872
A	328	G	-	expression tag	REF 283837872
A	329	A	-	expression tag	REF 283837872
A	330	C	-	expression tag	REF 283837872
A	331	C	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	332	C	-	expression tag	REF 283837872
A	333	A	-	expression tag	REF 283837872
A	334	U	-	expression tag	REF 283837872
A	335	U	-	expression tag	REF 283837872
A	336	C	-	expression tag	REF 283837872
A	337	G	-	expression tag	REF 283837872
A	338	A	-	expression tag	REF 283837872
A	339	A	-	expression tag	REF 283837872
A	340	C	-	expression tag	REF 283837872
A	341	G	-	expression tag	REF 283837872
A	342	U	-	expression tag	REF 283837872
A	343	C	-	expression tag	REF 283837872
A	344	U	-	expression tag	REF 283837872
A	345	G	-	expression tag	REF 283837872
A	346	C	-	expression tag	REF 283837872
A	347	C	-	expression tag	REF 283837872
A	348	C	-	expression tag	REF 283837872
A	349	U	-	expression tag	REF 283837872
A	350	A	-	expression tag	REF 283837872
A	351	U	-	expression tag	REF 283837872
A	352	C	-	expression tag	REF 283837872
A	353	A	-	expression tag	REF 283837872
A	354	A	-	expression tag	REF 283837872
A	355	C	-	expression tag	REF 283837872
A	356	U	-	expression tag	REF 283837872
A	357	U	-	expression tag	REF 283837872
A	358	U	-	expression tag	REF 283837872
A	359	C	-	expression tag	REF 283837872
A	360	G	-	expression tag	REF 283837872
A	361	A	-	expression tag	REF 283837872
A	362	U	-	expression tag	REF 283837872
A	363	G	-	expression tag	REF 283837872
A	364	G	-	expression tag	REF 283837872
A	365	U	-	expression tag	REF 283837872
A	366	A	-	expression tag	REF 283837872
A	367	G	-	expression tag	REF 283837872
A	368	U	-	expression tag	REF 283837872
A	369	C	-	expression tag	REF 283837872
A	370	G	-	expression tag	REF 283837872
A	371	C	-	expression tag	REF 283837872
A	372	C	-	expression tag	REF 283837872
A	373	G	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	374	U	-	expression tag	REF 283837872
A	375	G	-	expression tag	REF 283837872
A	376	C	-	expression tag	REF 283837872
A	377	C	-	expression tag	REF 283837872
A	378	U	-	expression tag	REF 283837872
A	379	A	-	expression tag	REF 283837872
A	380	C	-	expression tag	REF 283837872
A	381	C	-	expression tag	REF 283837872
A	382	A	-	expression tag	REF 283837872
A	383	U	-	expression tag	REF 283837872
A	384	G	-	expression tag	REF 283837872
A	385	G	-	expression tag	REF 283837872
A	386	U	-	expression tag	REF 283837872
A	387	G	-	expression tag	REF 283837872
A	388	A	-	expression tag	REF 283837872
A	389	C	-	expression tag	REF 283837872
A	390	C	-	expression tag	REF 283837872
A	391	A	-	expression tag	REF 283837872
A	392	C	-	expression tag	REF 283837872
A	393	G	-	expression tag	REF 283837872
A	394	G	-	expression tag	REF 283837872
A	395	G	-	expression tag	REF 283837872
A	396	U	-	expression tag	REF 283837872
A	397	G	-	expression tag	REF 283837872
A	398	A	-	expression tag	REF 283837872
A	399	C	-	expression tag	REF 283837872
A	400	G	-	expression tag	REF 283837872
A	401	G	-	expression tag	REF 283837872
A	402	G	-	expression tag	REF 283837872
A	403	G	-	expression tag	REF 283837872
A	404	A	-	expression tag	REF 283837872
A	405	A	-	expression tag	REF 283837872
A	406	U	-	expression tag	REF 283837872
A	407	C	-	expression tag	REF 283837872
A	408	A	-	expression tag	REF 283837872
A	409	G	-	expression tag	REF 283837872
A	410	G	-	expression tag	REF 283837872
A	411	G	-	expression tag	REF 283837872
A	412	U	-	expression tag	REF 283837872
A	413	U	-	expression tag	REF 283837872
A	414	C	-	expression tag	REF 283837872
A	415	G	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	416	A	-	expression tag	REF 283837872
A	417	U	-	expression tag	REF 283837872
A	418	U	-	expression tag	REF 283837872
A	419	C	-	expression tag	REF 283837872
A	420	C	-	expression tag	REF 283837872
A	421	G	-	expression tag	REF 283837872
A	422	G	-	expression tag	REF 283837872
A	423	A	-	expression tag	REF 283837872
A	424	G	-	expression tag	REF 283837872
A	425	A	-	expression tag	REF 283837872
A	426	G	-	expression tag	REF 283837872
A	427	G	-	expression tag	REF 283837872
A	428	G	-	expression tag	REF 283837872
A	429	A	-	expression tag	REF 283837872
A	430	G	-	expression tag	REF 283837872
A	431	C	-	expression tag	REF 283837872
A	432	C	-	expression tag	REF 283837872
A	433	U	-	expression tag	REF 283837872
A	434	G	-	expression tag	REF 283837872
A	435	A	-	expression tag	REF 283837872
A	436	G	-	expression tag	REF 283837872
A	437	A	-	expression tag	REF 283837872
A	438	A	-	expression tag	REF 283837872
A	439	A	-	expression tag	REF 283837872
A	440	C	-	expression tag	REF 283837872
A	441	G	-	expression tag	REF 283837872
A	442	G	-	expression tag	REF 283837872
A	443	C	-	expression tag	REF 283837872
A	444	U	-	expression tag	REF 283837872
A	445	A	-	expression tag	REF 283837872
A	446	C	-	expression tag	REF 283837872
A	447	C	-	expression tag	REF 283837872
A	448	A	-	expression tag	REF 283837872
A	449	C	-	expression tag	REF 283837872
A	450	A	-	expression tag	REF 283837872
A	451	U	-	expression tag	REF 283837872
A	452	C	-	expression tag	REF 283837872
A	453	C	-	expression tag	REF 283837872
A	454	A	-	expression tag	REF 283837872
A	455	A	-	expression tag	REF 283837872
A	456	G	-	expression tag	REF 283837872
A	457	G	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	458	A	-	expression tag	REF 283837872
A	459	A	-	expression tag	REF 283837872
A	460	G	-	expression tag	REF 283837872
A	461	G	-	expression tag	REF 283837872
A	462	C	-	expression tag	REF 283837872
A	463	A	-	expression tag	REF 283837872
A	464	G	-	expression tag	REF 283837872
A	465	C	-	expression tag	REF 283837872
A	466	A	-	expression tag	REF 283837872
A	467	G	-	expression tag	REF 283837872
A	468	G	-	expression tag	REF 283837872
A	469	C	-	expression tag	REF 283837872
A	470	G	-	expression tag	REF 283837872
A	471	C	-	expression tag	REF 283837872
A	472	G	-	expression tag	REF 283837872
A	473	C	-	expression tag	REF 283837872
A	474	A	-	expression tag	REF 283837872
A	475	A	-	expression tag	REF 283837872
A	476	A	-	expression tag	REF 283837872
A	477	U	-	expression tag	REF 283837872
A	478	U	-	expression tag	REF 283837872
A	479	A	-	expression tag	REF 283837872
A	480	C	-	expression tag	REF 283837872
A	481	C	-	expression tag	REF 283837872
A	482	C	-	expression tag	REF 283837872
A	483	A	-	expression tag	REF 283837872
A	484	C	-	expression tag	REF 283837872
A	485	U	-	expression tag	REF 283837872
A	486	C	-	expression tag	REF 283837872
A	487	C	-	expression tag	REF 283837872
A	488	C	-	expression tag	REF 283837872
A	489	G	-	expression tag	REF 283837872
A	490	A	-	expression tag	REF 283837872
A	491	C	-	expression tag	REF 283837872
A	492	C	-	expression tag	REF 283837872
A	493	C	-	expression tag	REF 283837872
A	494	G	-	expression tag	REF 283837872
A	495	G	-	expression tag	REF 283837872
A	496	G	-	expression tag	REF 283837872
A	497	G	-	expression tag	REF 283837872
A	498	A	-	expression tag	REF 283837872
A	499	G	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	500	G	-	expression tag	REF 283837872
A	501	U	-	expression tag	REF 283837872
A	502	A	-	expression tag	REF 283837872
A	503	G	-	expression tag	REF 283837872
A	504	U	-	expression tag	REF 283837872
A	505	G	-	expression tag	REF 283837872
A	506	A	-	expression tag	REF 283837872
A	507	C	-	expression tag	REF 283837872
A	508	G	-	expression tag	REF 283837872
A	509	A	-	expression tag	REF 283837872
A	510	A	-	expression tag	REF 283837872
A	511	A	-	expression tag	REF 283837872
A	512	A	-	expression tag	REF 283837872
A	513	A	-	expression tag	REF 283837872
A	514	U	-	expression tag	REF 283837872
A	515	A	-	expression tag	REF 283837872
A	516	A	-	expression tag	REF 283837872
A	517	C	-	expression tag	REF 283837872
A	518	A	-	expression tag	REF 283837872
A	519	A	-	expression tag	REF 283837872
A	520	U	-	expression tag	REF 283837872
A	521	A	-	expression tag	REF 283837872
A	522	C	-	expression tag	REF 283837872
A	523	A	-	expression tag	REF 283837872
A	524	G	-	expression tag	REF 283837872
A	525	G	-	expression tag	REF 283837872
A	526	A	-	expression tag	REF 283837872
A	527	C	-	expression tag	REF 283837872
A	528	U	-	expression tag	REF 283837872
A	529	C	-	expression tag	REF 283837872
A	530	U	-	expression tag	REF 283837872
A	531	U	-	expression tag	REF 283837872
A	532	U	-	expression tag	REF 283837872
A	533	C	-	expression tag	REF 283837872
A	534	G	-	expression tag	REF 283837872
A	535	A	-	expression tag	REF 283837872
A	536	G	-	expression tag	REF 283837872
A	537	G	-	expression tag	REF 283837872
A	538	C	-	expression tag	REF 283837872
A	539	C	-	expression tag	REF 283837872
A	540	C	-	expression tag	REF 283837872
A	541	U	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	542	G	-	expression tag	REF 283837872
A	543	U	-	expression tag	REF 283837872
A	544	A	-	expression tag	REF 283837872
A	545	A	-	expression tag	REF 283837872
A	546	U	-	expression tag	REF 283837872
A	547	U	-	expression tag	REF 283837872
A	548	G	-	expression tag	REF 283837872
A	549	G	-	expression tag	REF 283837872
A	550	A	-	expression tag	REF 283837872
A	551	A	-	expression tag	REF 283837872
A	552	U	-	expression tag	REF 283837872
A	553	G	-	expression tag	REF 283837872
A	554	A	-	expression tag	REF 283837872
A	555	G	-	expression tag	REF 283837872
A	556	U	-	expression tag	REF 283837872
A	557	C	-	expression tag	REF 283837872
A	558	C	-	expression tag	REF 283837872
A	559	A	-	expression tag	REF 283837872
A	560	C	-	expression tag	REF 283837872
A	561	U	-	expression tag	REF 283837872
A	562	U	-	expression tag	REF 283837872
A	563	U	-	expression tag	REF 283837872
A	564	A	-	expression tag	REF 283837872
A	565	A	-	expression tag	REF 283837872
A	566	A	-	expression tag	REF 283837872
A	567	U	-	expression tag	REF 283837872
A	568	C	-	expression tag	REF 283837872
A	569	C	-	expression tag	REF 283837872
A	570	U	-	expression tag	REF 283837872
A	571	U	-	expression tag	REF 283837872
A	572	U	-	expression tag	REF 283837872
A	573	A	-	expression tag	REF 283837872
A	574	A	-	expression tag	REF 283837872
A	575	C	-	expression tag	REF 283837872
A	576	G	-	expression tag	REF 283837872
A	577	A	-	expression tag	REF 283837872
A	578	G	-	expression tag	REF 283837872
A	579	G	-	expression tag	REF 283837872
A	580	A	-	expression tag	REF 283837872
A	581	U	-	expression tag	REF 283837872
A	582	C	-	expression tag	REF 283837872
A	583	C	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	584	A	-	expression tag	REF 283837872
A	585	U	-	expression tag	REF 283837872
A	586	U	-	expression tag	REF 283837872
A	587	G	-	expression tag	REF 283837872
A	588	G	-	expression tag	REF 283837872
A	589	A	-	expression tag	REF 283837872
A	590	G	-	expression tag	REF 283837872
A	591	G	-	expression tag	REF 283837872
A	592	G	-	expression tag	REF 283837872
A	593	C	-	expression tag	REF 283837872
A	594	A	-	expression tag	REF 283837872
A	595	A	-	expression tag	REF 283837872
A	596	G	-	expression tag	REF 283837872
A	597	U	-	expression tag	REF 283837872
A	598	C	-	expression tag	REF 283837872
A	599	U	-	expression tag	REF 283837872
A	600	G	-	expression tag	REF 283837872
A	601	G	-	expression tag	REF 283837872
A	602	U	-	expression tag	REF 283837872
A	603	C	-	expression tag	REF 283837872
A	604	G	-	expression tag	REF 283837872
A	605	C	-	expression tag	REF 283837872
A	606	A	-	expression tag	REF 283837872
A	607	G	-	expression tag	REF 283837872
A	608	C	-	expression tag	REF 283837872
A	609	A	-	expression tag	REF 283837872
A	610	G	-	expression tag	REF 283837872
A	611	C	-	expression tag	REF 283837872
A	612	C	-	expression tag	REF 283837872
A	613	G	-	expression tag	REF 283837872
A	614	C	-	expression tag	REF 283837872
A	615	G	-	expression tag	REF 283837872
A	616	G	-	expression tag	REF 283837872
A	617	U	-	expression tag	REF 283837872
A	618	A	-	expression tag	REF 283837872
A	619	A	-	expression tag	REF 283837872
A	620	U	-	expression tag	REF 283837872
A	621	U	-	expression tag	REF 283837872
A	622	C	-	expression tag	REF 283837872
A	623	C	-	expression tag	REF 283837872
A	624	A	-	expression tag	REF 283837872
A	625	G	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	626	C	-	expression tag	REF 283837872
A	627	U	-	expression tag	REF 283837872
A	628	C	-	expression tag	REF 283837872
A	629	C	-	expression tag	REF 283837872
A	630	A	-	expression tag	REF 283837872
A	631	A	-	expression tag	REF 283837872
A	632	U	-	expression tag	REF 283837872
A	633	A	-	expression tag	REF 283837872
A	634	G	-	expression tag	REF 283837872
A	635	C	-	expression tag	REF 283837872
A	636	G	-	expression tag	REF 283837872
A	637	U	-	expression tag	REF 283837872
A	638	A	-	expression tag	REF 283837872
A	639	U	-	expression tag	REF 283837872
A	640	A	-	expression tag	REF 283837872
A	641	U	-	expression tag	REF 283837872
A	642	U	-	expression tag	REF 283837872
A	643	A	-	expression tag	REF 283837872
A	644	A	-	expression tag	REF 283837872
A	645	A	-	expression tag	REF 283837872
A	646	G	-	expression tag	REF 283837872
A	647	U	-	expression tag	REF 283837872
A	648	U	-	expression tag	REF 283837872
A	649	G	-	expression tag	REF 283837872
A	650	C	-	expression tag	REF 283837872
A	651	U	-	expression tag	REF 283837872
A	652	G	-	expression tag	REF 283837872
A	653	C	-	expression tag	REF 283837872
A	654	A	-	expression tag	REF 283837872
A	655	G	-	expression tag	REF 283837872
A	656	U	-	expression tag	REF 283837872
A	657	U	-	expression tag	REF 283837872
A	658	A	-	expression tag	REF 283837872
A	659	A	-	expression tag	REF 283837872
A	660	A	-	expression tag	REF 283837872
A	661	A	-	expression tag	REF 283837872
A	662	A	-	expression tag	REF 283837872
A	663	G	-	expression tag	REF 283837872
A	664	C	-	expression tag	REF 283837872
A	665	U	-	expression tag	REF 283837872
A	666	C	-	expression tag	REF 283837872
A	667	G	-	expression tag	REF 283837872

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Chain	Residue	Modelled	Actual	Comment	Reference
A	668	U	-	expression tag	REF 283837872
A	669	A	-	expression tag	REF 283837872
A	670	G	-	expression tag	REF 283837872
A	671	U	-	expression tag	REF 283837872
A	672	U	-	expression tag	REF 283837872
A	673	G	-	expression tag	REF 283837872
A	674	G	-	expression tag	REF 283837872
A	675	A	-	expression tag	REF 283837872
A	676	U	-	expression tag	REF 283837872
A	677	C	-	expression tag	REF 283837872
A	678	U	-	expression tag	REF 283837872
A	679	U	-	expression tag	REF 283837872
A	683	G	-	expression tag	REF 283837872
A	684	A	-	expression tag	REF 283837872
A	685	G	-	expression tag	REF 283837872
A	686	G	-	expression tag	REF 283837872
A	687	G	-	expression tag	REF 283837872
A	730	C	-	expression tag	REF 283837872
A	731	C	-	expression tag	REF 283837872
A	732	C	-	expression tag	REF 283837872
A	733	G	-	expression tag	REF 283837872
A	734	C	-	expression tag	REF 283837872
A	735	C	-	expression tag	REF 283837872
A	736	C	-	expression tag	REF 283837872
A	744	C	-	expression tag	REF 283837872
A	745	U	-	expression tag	REF 283837872
A	746	C	-	expression tag	REF 283837872
A	747	G	-	expression tag	REF 283837872
A	748	G	-	expression tag	REF 283837872
A	749	C	-	expression tag	REF 283837872
A	750	G	-	expression tag	REF 283837872
A	751	C	-	expression tag	REF 283837872
A	752	C	-	expression tag	REF 283837872
A	753	C	-	expression tag	REF 283837872
A	754	C	-	expression tag	REF 283837872
A	755	C	-	expression tag	REF 283837872
A	756	U	-	expression tag	REF 283837872
A	757	C	-	expression tag	REF 283837872
A	758	G	-	expression tag	REF 283837872
A	759	A	-	expression tag	REF 283837872
A	760	U	-	expression tag	REF 283837872

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	30	Total	C	N	O	P	0	0
			635	285	115	206	29		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	266	Total	C	N	O	S	0	0
			2147	1354	376	406	11		

- Molecule 5 is a protein called ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 6 is a protein called ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 7 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

- Molecule 8 is a protein called ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 9 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	182	Total	C	N	O	S	0	0
			1499	952	300	245	2		

- Molecule 10 is a protein called ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	137	Total	C	N	O	S	0	0
			1140	714	231	194	1		

- Molecule 11 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	38	Total	C	N	O	S	0	0
			288	177	45	64	2		

- Molecule 12 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	77	Total	C	N	O	0	0
			614	388	110	116		

- Molecule 13 is a protein called ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	142	Total	C	N	O	S	0	0
			1107	698	220	185	4		

- Molecule 14 is a protein called ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	141	Total	C	N	O	S	0	0
			1113	701	213	196	3		

- Molecule 15 is a protein called eukaryotic initiation factor 2 Gamma subunit (eIF2-Gamma).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	422	Total	C	N	O	S	0	0
			3214	2044	561	592	17		

- Molecule 16 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	329	Total	C	N	O	S	0	0
			2605	1640	447	503	15		

- Molecule 17 is a protein called ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 18 is a protein called ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	59	Total	C	N	O	S	0	0
			473	293	104	75	1		

- Molecule 19 is a protein called ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	75	Total	C	N	O	S	0	0
			599	382	111	105	1		

- Molecule 20 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	190	Total	C	N	O	S	0	0
			1530	975	281	273	1		

- Molecule 21 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

- Molecule 22 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 23 is a protein called ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 24 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	82	Total	C	N	O	S	0	0
			620	378	117	120	5		

- Molecule 25 is a protein called ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	226	Total	C	N	O	S	0	0
			1743	1127	300	307	9		

- Molecule 26 is a protein called eukaryotic initiation factor 2 subunit Beta (eIF2-Beta).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	17	Total	C	N	O	S	0	0
			147	94	22	30	1		

- Molecule 27 is a protein called ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	126	Total	C	N	O	S	0	0
			1020	639	188	188	5		

- Molecule 28 is a protein called ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	208	Total	C	N	O	S	0	0
			1643	1045	289	301	8		

- Molecule 29 is a protein called ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	227	Total	C	N	O	S	0	0
			1765	1124	317	316	8		

- Molecule 30 is a protein called ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 31 is a protein called ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	215	Total	C	N	O	S	0	0
			1742	1107	309	311	15		

- Molecule 32 is a protein called ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 33 is a protein called ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	k	99	Total	C	N	O	S	0	0
			790	491	162	131	6		

- Molecule 34 is a protein called ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	64	Total	C	N	O	S	0	0
			507	308	102	95	2		

- Molecule 35 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	m	313	Total	C	N	O	S	0	0
			2437	1535	424	466	12		

- Molecule 36 is a protein called ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	n	127	Total	C	N	O	S	0	0
			1061	673	201	180	7		

- Molecule 37 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	o	206	Total	C	N	O	S	0	0
			1680	1054	329	292	5		

- Molecule 38 is a protein called ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	p	71	Total	C	N	O	S	0	0
			582	367	109	99	7		

- Molecule 39 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	q	237	Total	C	N	O	S	0	0
			1924	1200	387	330	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 41 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	131	Total	C	N	O	S	0	0
			1065	673	206	181	5		

- Molecule 42 is a protein called ribosomal protein eS10.

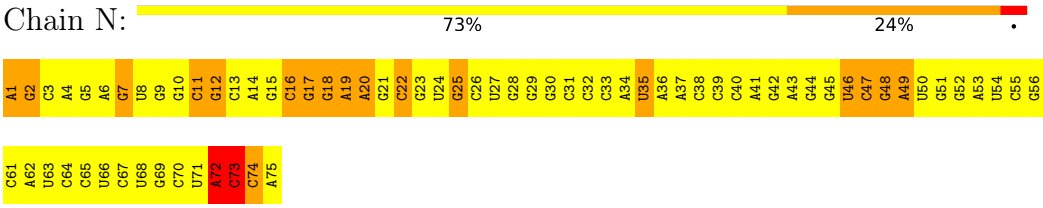
Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	98	Total	C	N	O	S	0	0
			828	539	148	135	6		

3 Residue-property plots (i)

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

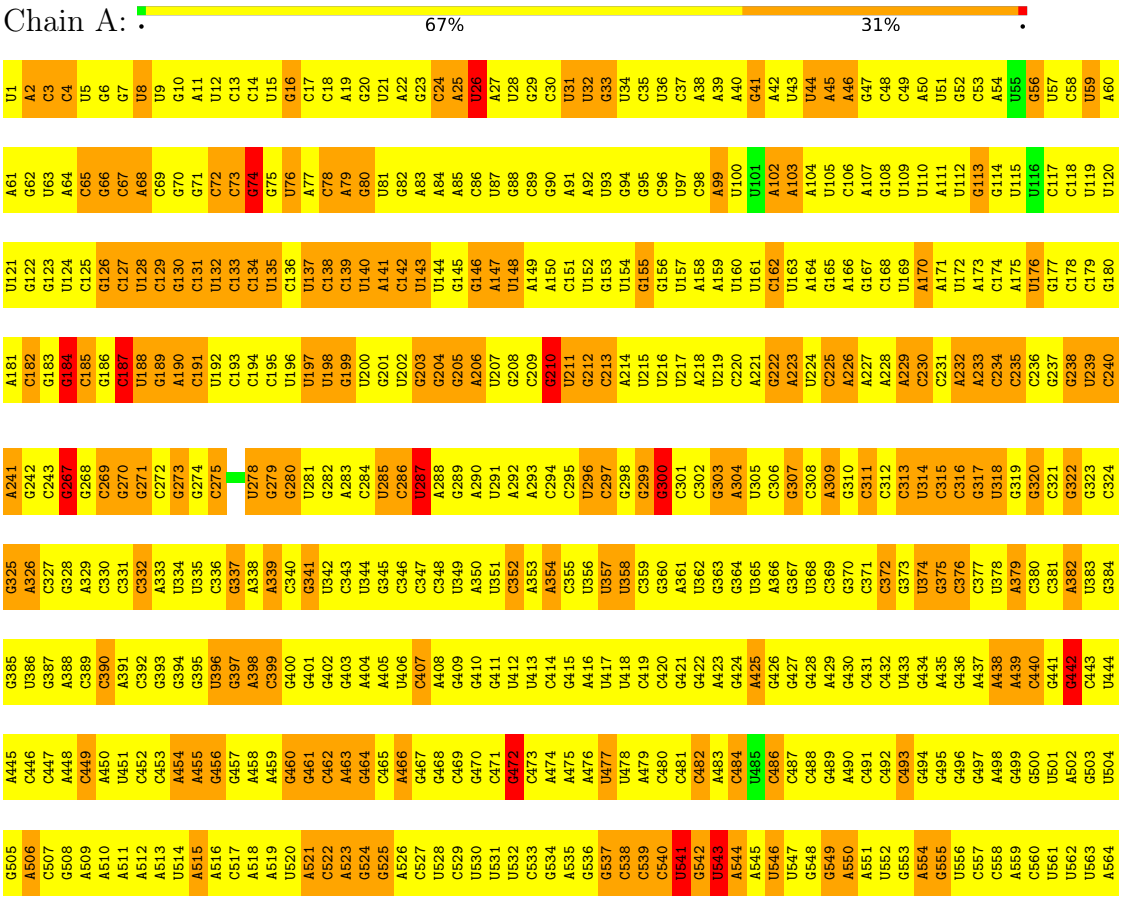
- Molecule 1: tRNA

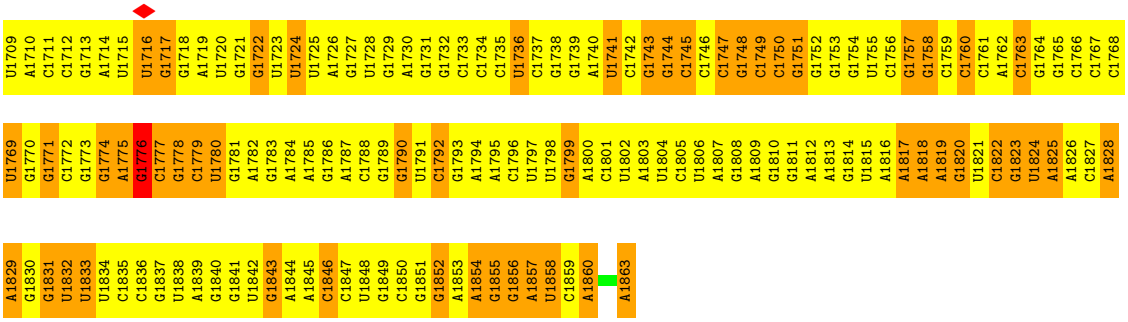
Chain N:



- Molecule 2: 18S ribosomal RNA

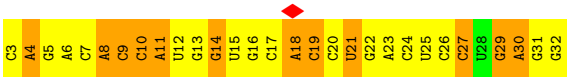
Chain A:





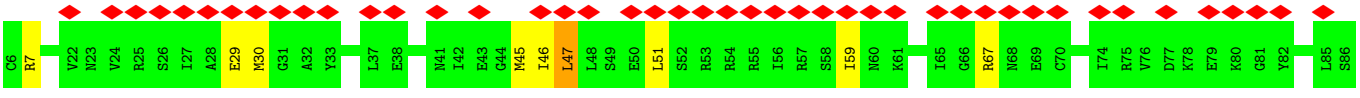
• Molecule 3: mRNA

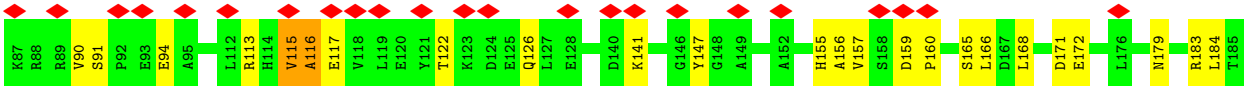
Chain F:

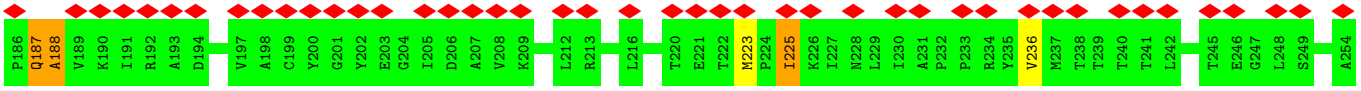


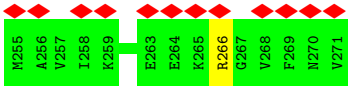
• Molecule 4: Eukaryotic translation initiation factor 2 subunit 1

Chain P:



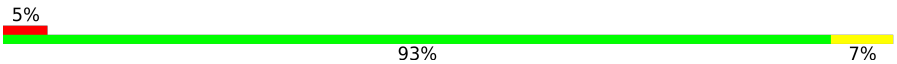


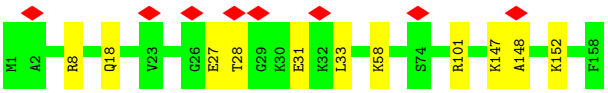




• Molecule 5: ribosomal protein uS17

Chain G:



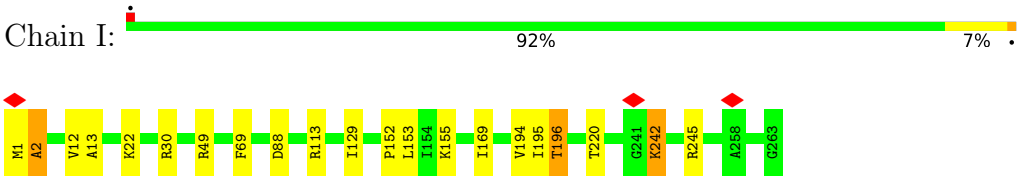


• Molecule 6: ribosomal protein uS9

Chain H:

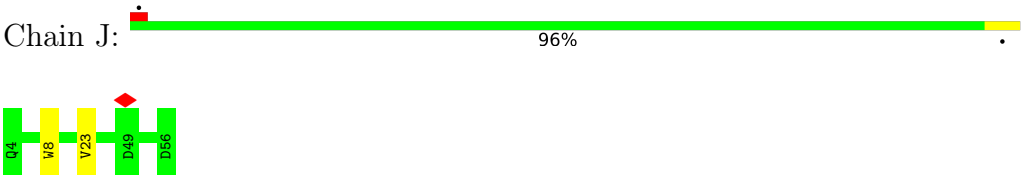
• Molecule 7: 40S ribosomal protein S4

Chain I:



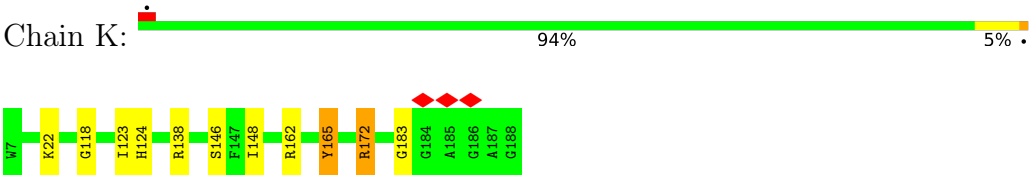
• Molecule 8: ribosomal protein uS14

Chain J:



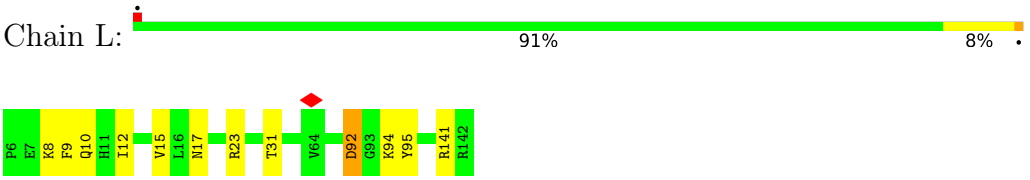
• Molecule 9: Ribosomal protein S9 (Predicted)

Chain K:



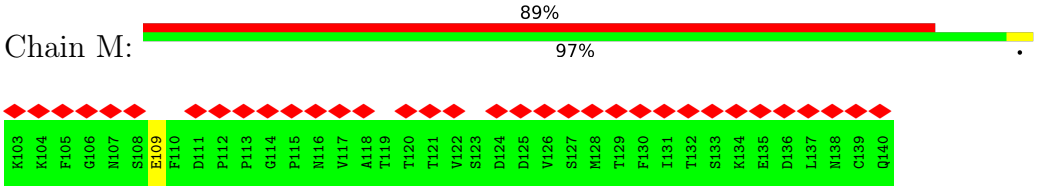
• Molecule 10: ribosomal protein uS13

Chain L:



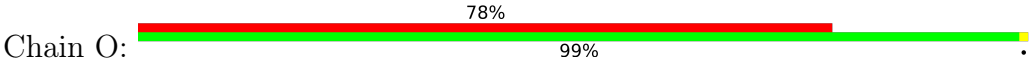
• Molecule 11: Eukaryotic translation initiation factor 3 subunit G

Chain M:



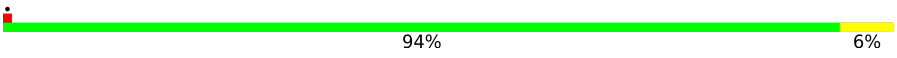
• Molecule 12: Eukaryotic translation initiation factor 3 subunit G

Chain O:



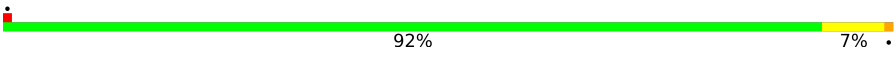
• Molecule 13: ribosomal protein uS12

Chain Q:



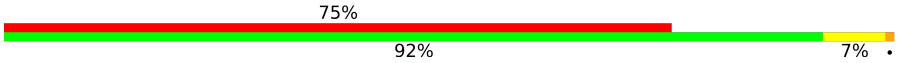
• Molecule 14: ribosomal protein eS19

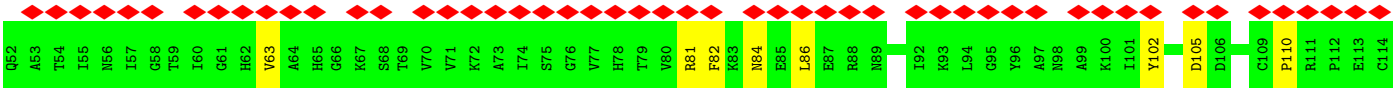
Chain R:

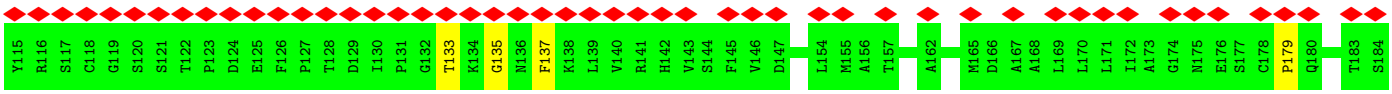


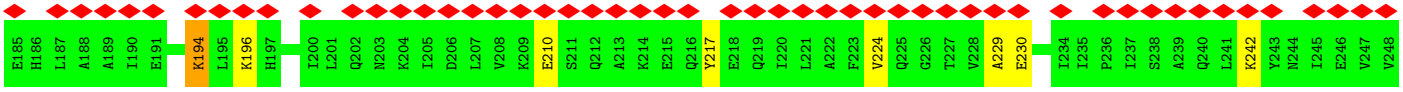
• Molecule 15: eukaryotic initiation factor 2 Gamma subunit (eIF2-Gamma)

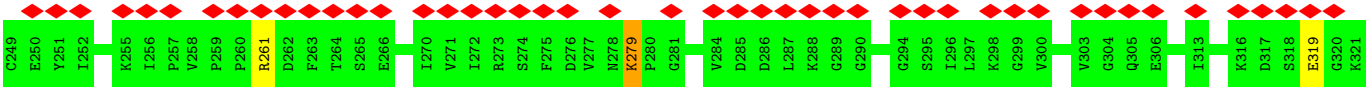
Chain S:

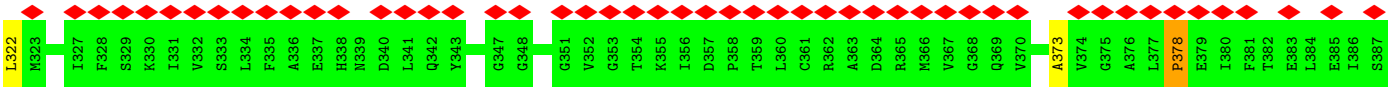


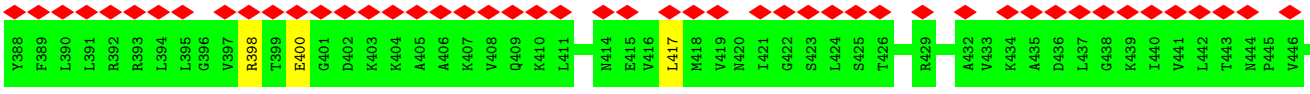


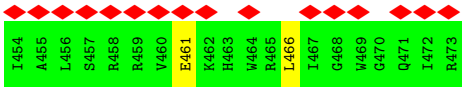






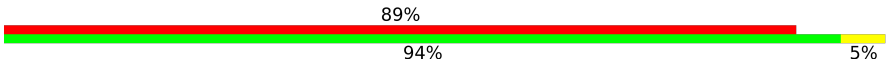


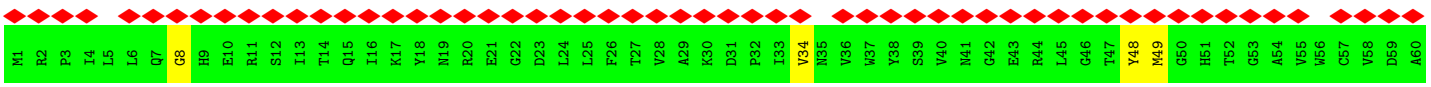


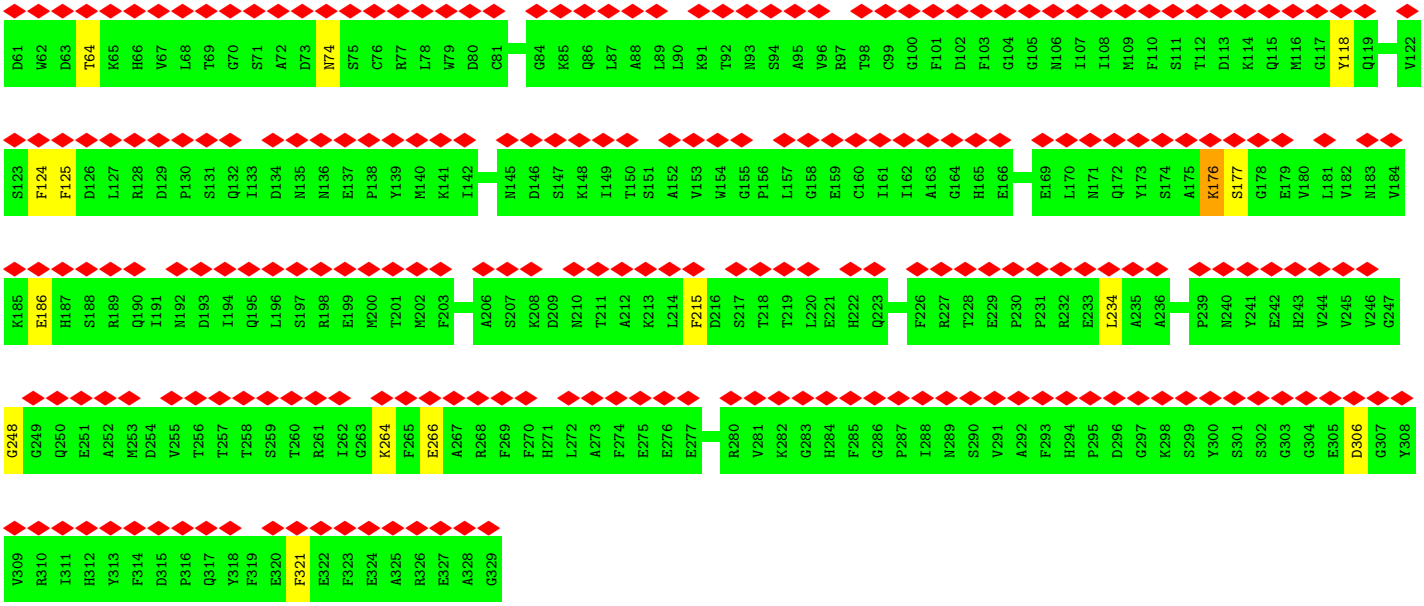


• Molecule 16: Eukaryotic translation initiation factor 3 subunit I

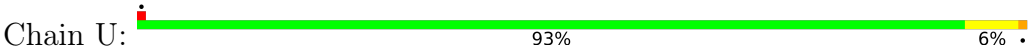
Chain T:

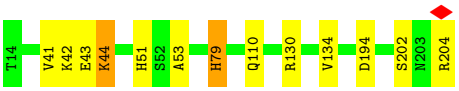




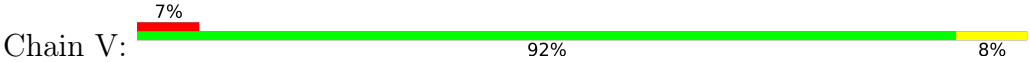


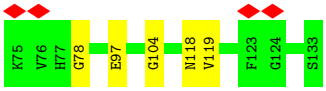
• Molecule 17: ribosomal protein uS7



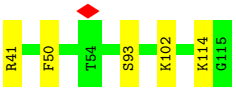


• Molecule 18: ribosomal protein eS30

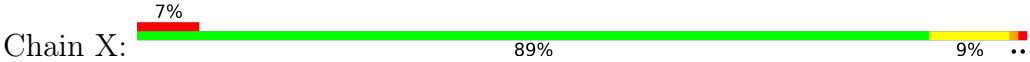


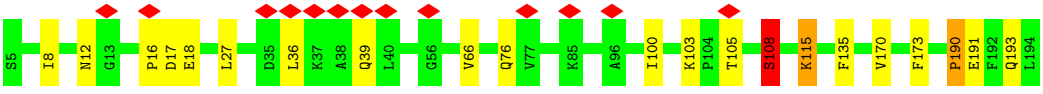


• Molecule 19: ribosomal protein eS25



• Molecule 20: ribosomal protein eS7



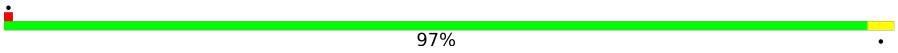


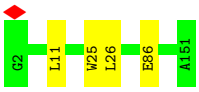
• Molecule 21: 40S ribosomal protein S27

Chain Y:

• Molecule 22: ribosomal protein uS15

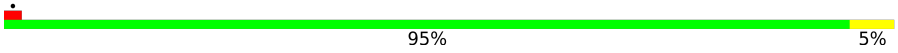
Chain Z:

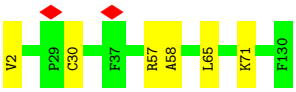




• Molecule 23: ribosomal protein uS8

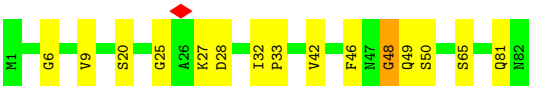
Chain a:





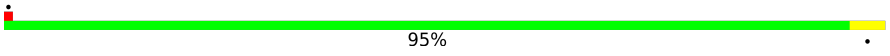
• Molecule 24: 40S ribosomal protein S21

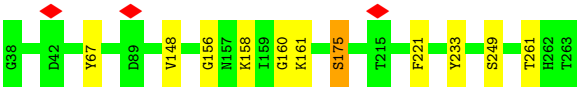
Chain b:



• Molecule 25: ribosomal protein uS5

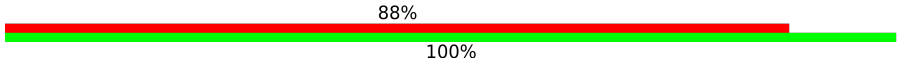
Chain c:

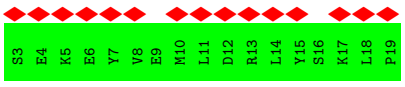




• Molecule 26: eukaryotic initiation factor 2 subunit Beta (eIF2-Beta)

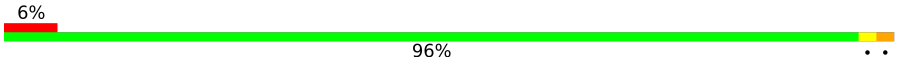
Chain d:

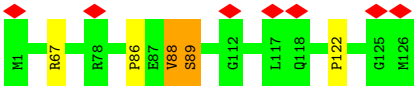




• Molecule 27: ribosomal protein eS17

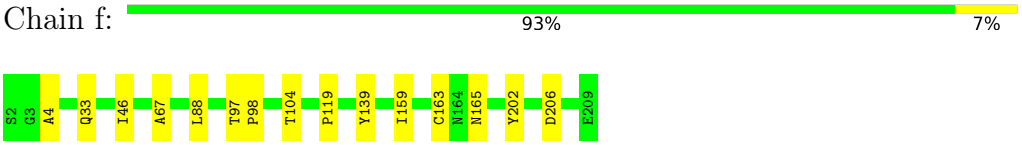
Chain e:





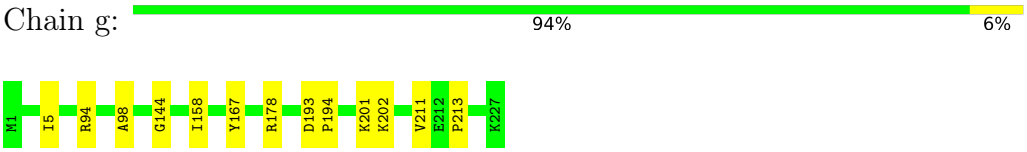
• Molecule 28: ribosomal protein uS2

Chain f:



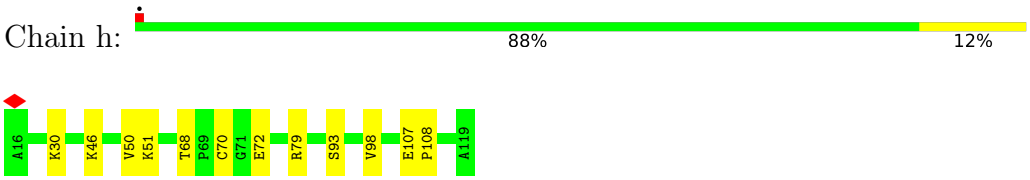
• Molecule 29: ribosomal protein uS3

Chain g:



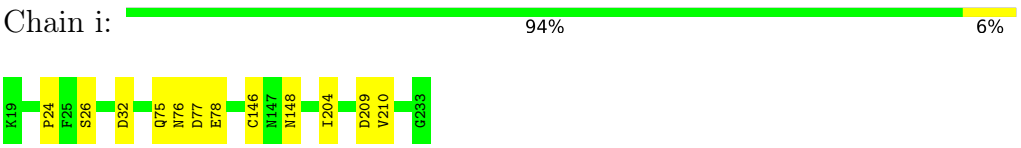
• Molecule 30: ribosomal protein uS10

Chain h:



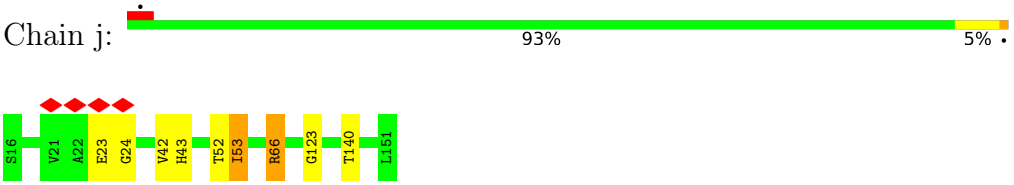
• Molecule 31: ribosomal protein eS1

Chain i:



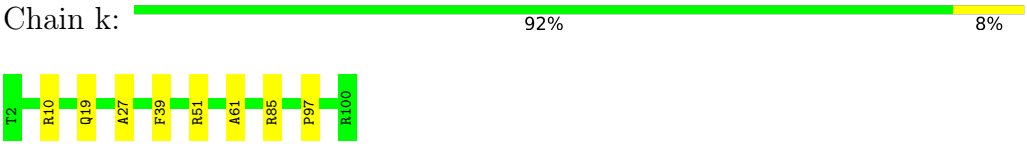
• Molecule 32: ribosomal protein uS11

Chain j:



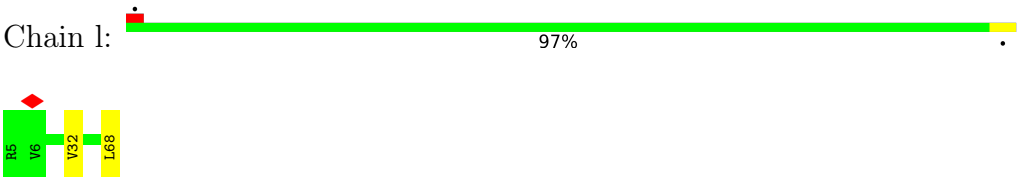
• Molecule 33: ribosomal protein eS26

Chain k:



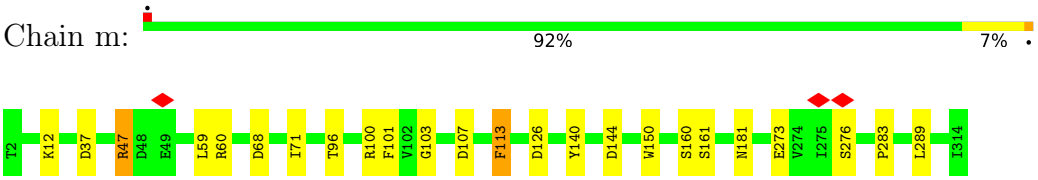
• Molecule 34: ribosomal protein eS28

Chain l:



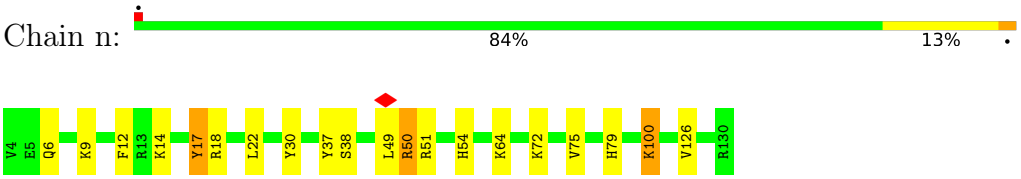
• Molecule 35: ribosomal protein RACK1

Chain m:



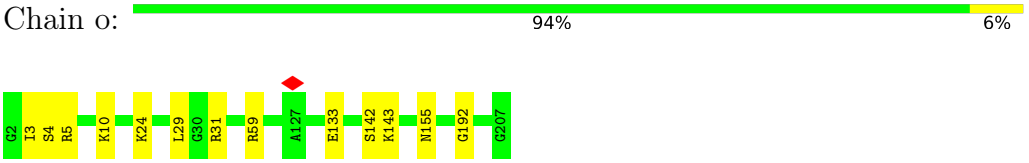
• Molecule 36: ribosomal protein uS19

Chain n:



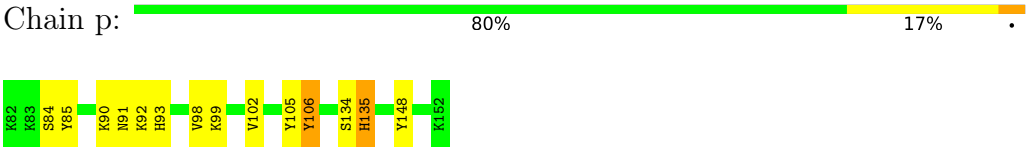
• Molecule 37: 40S ribosomal protein S8

Chain o:



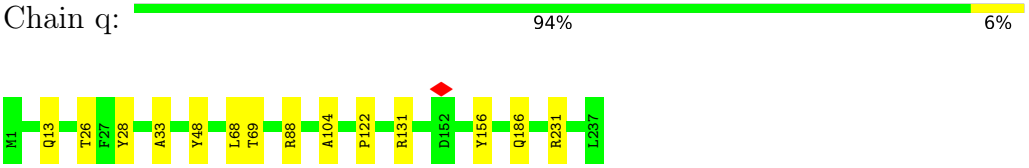
• Molecule 38: ribosomal protein eS31

Chain p:



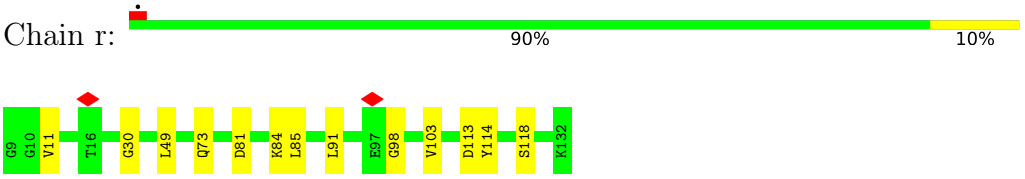
• Molecule 39: 40S ribosomal protein S6

Chain q:



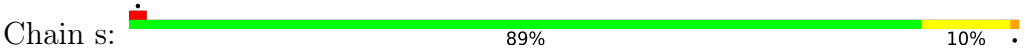
• Molecule 40: 40S ribosomal protein S12

Chain r:

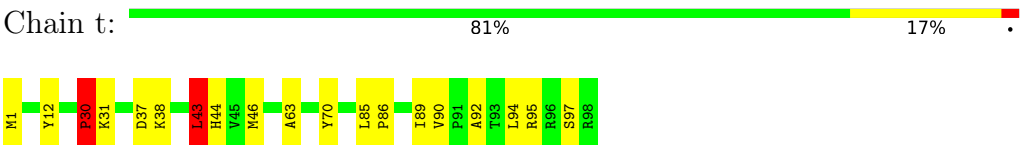


• Molecule 41: 40S ribosomal protein S24

Chain s:



• Molecule 42: ribosomal protein eS10



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	475000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	24	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.400	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.2, 2.2, 2.2	Depositor

5 Model quality

5.1 Standard geometry

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	N	1.68	9/1795 (0.5%)	2.61	215/2798 (7.7%)
2	A	1.62	35/42353 (0.1%)	2.56	5098/66010 (7.7%)
3	F	1.59	0/709	2.51	91/1103 (8.3%)
4	P	1.00	0/2178	1.08	3/2935 (0.1%)
5	G	1.02	0/1319	1.01	0/1761
6	H	1.04	0/1142	1.07	3/1528 (0.2%)
7	I	0.98	0/2125	1.06	5/2856 (0.2%)
8	J	1.12	0/455	0.98	0/603
9	K	1.08	0/1523	1.00	2/2031 (0.1%)
10	L	1.06	0/1158	1.04	1/1548 (0.1%)
11	M	0.81	0/293	0.94	0/396
12	O	1.03	0/626	1.01	0/842
13	Q	0.99	0/1125	0.98	0/1500
14	R	0.99	0/1133	1.05	5/1517 (0.3%)
15	S	0.91	0/3267	1.01	2/4415 (0.0%)
16	T	0.96	0/2669	1.07	8/3608 (0.2%)
17	U	0.99	0/1531	0.98	0/2059
18	V	1.10	0/478	1.04	1/628 (0.2%)
19	W	0.97	0/605	1.04	0/810
20	X	0.96	0/1553	1.04	4/2079 (0.2%)
21	Y	0.94	0/673	1.01	0/902
22	Z	0.98	0/1232	0.94	0/1656
23	a	1.01	0/1051	0.98	0/1406
24	b	0.98	0/627	1.08	0/839
25	c	0.91	0/1779	1.02	3/2399 (0.1%)
26	d	0.98	0/149	0.79	0/197
27	e	0.99	0/1032	1.03	0/1383
28	f	0.96	0/1680	1.05	2/2283 (0.1%)
29	g	0.99	0/1793	1.04	2/2412 (0.1%)
30	h	0.99	0/832	1.08	0/1117
31	i	0.91	0/1770	1.02	0/2367
32	j	1.04	0/1029	1.08	0/1380
33	k	1.07	0/803	1.06	1/1076 (0.1%)
34	l	1.13	0/509	1.05	0/680

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	m	0.92	0/2494	1.13	3/3394 (0.1%)
36	n	1.03	0/1080	1.04	0/1437
37	o	1.04	0/1709	1.05	1/2278 (0.0%)
38	p	0.99	0/594	1.09	1/786 (0.1%)
39	q	1.07	0/1947	1.08	4/2590 (0.2%)
40	r	0.89	0/968	1.04	2/1296 (0.2%)
41	s	0.99	0/1083	1.10	0/1437
42	t	0.96	0/852	1.13	4/1147 (0.3%)
All	All	1.33	44/93723 (0.0%)	1.98	5461/135489 (4.0%)

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
1	N	0	6
2	A	1	68
4	P	0	17
5	G	0	4
6	H	0	2
7	I	1	2
9	K	0	3
10	L	0	6
14	R	0	1
15	S	0	5
16	T	0	1
17	U	0	3
18	V	0	1
19	W	0	2
20	X	0	6
21	Y	0	3
23	a	0	1
24	b	0	5
25	c	0	1
27	e	0	3
28	f	0	2
29	g	0	1
30	h	0	5
31	i	0	3
32	j	0	1
35	m	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	n	0	3
37	o	0	4
38	p	0	7
40	r	0	1
41	s	1	4
42	t	0	7
All	All	3	185

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	211	U	C2-N3	6.75	1.42	1.37
2	A	524	G	O3'-P	-6.71	1.53	1.61
2	A	1186	A	N7-C5	-6.68	1.35	1.39
2	A	749	C	O3'-P	-6.62	1.53	1.61
1	N	14	A	N7-C5	-6.52	1.35	1.39
2	A	184	G	N1-C2	6.28	1.42	1.37
2	A	227	A	N7-C5	-6.21	1.35	1.39
1	N	23	G	N1-C2	5.90	1.42	1.37
2	A	1794	A	N7-C5	-5.86	1.35	1.39
1	N	7	G	N1-C2	5.81	1.42	1.37
2	A	1785	A	N7-C5	-5.73	1.35	1.39
1	N	57	A	N7-C5	-5.72	1.35	1.39
2	A	273	G	C2-N3	5.65	1.37	1.32
2	A	1659	A	N7-C5	-5.63	1.35	1.39
1	N	12	G	N1-C2	5.57	1.42	1.37
1	N	23	G	N9-C4	-5.54	1.33	1.38
2	A	1589	A	N7-C5	-5.54	1.35	1.39
2	A	1683	C	C2'-C1'	-5.47	1.47	1.53
2	A	1283	A	N7-C5	-5.40	1.36	1.39
2	A	1645	A	N7-C5	-5.39	1.36	1.39
2	A	1697	G	C2-N3	5.35	1.37	1.32
2	A	208	G	C2-N3	5.34	1.37	1.32
2	A	1044	G	C2-N3	5.32	1.37	1.32
2	A	437	A	N7-C5	-5.29	1.36	1.39
2	A	66	G	N7-C5	-5.29	1.36	1.39
2	A	1852	G	C2-N3	5.28	1.36	1.32
2	A	1024	A	N7-C5	-5.23	1.36	1.39
2	A	1635	A	N7-C5	-5.22	1.36	1.39
1	N	52	G	N1-C2	5.17	1.41	1.37
2	A	80	G	C2-N3	5.15	1.36	1.32
2	A	1629	A	N7-C5	-5.14	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1783	G	C2-N3	5.14	1.36	1.32
2	A	749	C	C2'-C1'	-5.13	1.47	1.53
2	A	120	U	C2-N3	5.13	1.41	1.37
1	N	29	G	N1-C2	5.11	1.41	1.37
2	A	887	G	C2-N3	5.10	1.36	1.32
2	A	783	G	C2-N3	5.09	1.36	1.32
1	N	60	C	N3-C4	5.09	1.37	1.33
2	A	185	C	N3-C4	5.07	1.37	1.33
2	A	1489	C	N3-C4	5.02	1.37	1.33
2	A	1185	A	N7-C5	-5.02	1.36	1.39
2	A	189	G	C2-N3	5.02	1.36	1.32
2	A	748	G	O3'-P	-5.01	1.55	1.61
2	A	1142	C	N3-C4	5.00	1.37	1.33

All (5461) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	730	C	P-O3'-C3'	22.13	146.25	119.70
2	A	883	U	P-O3'-C3'	21.96	146.05	119.70
2	A	748	G	P-O3'-C3'	21.66	145.69	119.70
2	A	524	G	P-O3'-C3'	21.53	145.53	119.70
2	A	1627	G	P-O3'-C3'	21.22	145.16	119.70
2	A	749	C	P-O5'-C5'	21.08	154.63	120.90
2	A	140	U	P-O3'-C3'	21.04	144.95	119.70
2	A	1471	G	P-O3'-C3'	20.59	144.41	119.70
2	A	747	G	P-O3'-C3'	20.22	143.97	119.70
2	A	24	C	P-O3'-C3'	19.98	143.68	119.70
2	A	1133	U	P-O3'-C3'	18.44	141.82	119.70
2	A	749	C	P-O3'-C3'	18.37	141.74	119.70
2	A	542	G	P-O3'-C3'	18.34	141.70	119.70
2	A	1594	U	P-O3'-C3'	18.31	141.67	119.70
2	A	317	G	P-O3'-C3'	17.95	141.24	119.70
2	A	685	G	P-O3'-C3'	17.85	141.12	119.70
2	A	521	A	P-O3'-C3'	17.83	141.10	119.70
2	A	1470	A	P-O3'-C3'	17.45	140.64	119.70
2	A	1390	G	P-O3'-C3'	17.39	140.56	119.70
2	A	1391	C	P-O3'-C3'	17.31	140.47	119.70
2	A	1774	G	P-O3'-C3'	17.08	140.20	119.70
2	A	319	G	P-O3'-C3'	16.78	139.84	119.70
2	A	189	G	P-O3'-C3'	16.54	139.55	119.70
2	A	313	C	P-O3'-C3'	16.47	139.47	119.70
2	A	1392	A	P-O3'-C3'	16.29	139.25	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1674	A	P-O3'-C3'	15.94	138.83	119.70
2	A	1538	U	P-O3'-C3'	15.66	138.49	119.70
2	A	522	C	P-O3'-C3'	15.49	138.29	119.70
2	A	132	U	O4'-C1'-N1	15.49	120.59	108.20
2	A	1552	C	P-O3'-C3'	15.41	138.19	119.70
2	A	787	C	P-O3'-C3'	15.25	138.00	119.70
2	A	211	U	P-O3'-C3'	15.23	137.98	119.70
2	A	1544	U	P-O3'-C3'	15.00	137.70	119.70
2	A	750	G	P-O3'-C3'	14.89	137.57	119.70
2	A	137	U	O4'-C1'-N1	14.87	120.10	108.20
2	A	1750	C	P-O3'-C3'	14.66	137.29	119.70
2	A	396	U	P-O3'-C3'	14.62	137.24	119.70
2	A	66	G	P-O3'-C3'	14.49	137.09	119.70
2	A	876	G	P-O3'-C3'	14.45	137.03	119.70
2	A	141	A	P-O3'-C3'	14.43	137.02	119.70
2	A	170	A	N1-C6-N6	14.26	127.15	118.60
2	A	997	A	N1-C6-N6	14.19	127.11	118.60
2	A	1573	U	P-O3'-C3'	14.18	136.72	119.70
2	A	1517	A	N1-C6-N6	14.17	127.10	118.60
2	A	141	A	N1-C6-N6	14.16	127.10	118.60
2	A	1210	A	N1-C6-N6	14.07	127.04	118.60
2	A	68	A	N1-C6-N6	14.04	127.03	118.60
2	A	483	A	N1-C6-N6	14.04	127.03	118.60
2	A	790	A	N1-C6-N6	14.03	127.02	118.60
2	A	1824	U	P-O3'-C3'	13.98	136.48	119.70
2	A	133	C	P-O3'-C3'	13.98	136.48	119.70
2	A	1141	A	N1-C6-N6	13.89	126.94	118.60
2	A	288	A	N1-C6-N6	13.79	126.87	118.60
2	A	638	A	N1-C6-N6	13.76	126.86	118.60
2	A	225	C	P-O3'-C3'	13.74	136.19	119.70
2	A	958	A	N1-C6-N6	13.65	126.79	118.60
2	A	1200	A	N1-C6-N6	13.59	126.76	118.60
2	A	1397	A	P-O3'-C3'	13.50	135.90	119.70
1	N	71	U	P-O3'-C3'	13.46	135.85	119.70
2	A	1490	U	P-O3'-C3'	13.43	135.81	119.70
2	A	1574	A	N1-C6-N6	13.41	126.64	118.60
2	A	64	A	N1-C6-N6	13.40	126.64	118.60
2	A	606	A	N1-C6-N6	13.35	126.61	118.60
2	A	1710	A	N1-C6-N6	13.35	126.61	118.60
1	N	6	A	N1-C6-N6	13.33	126.60	118.60
2	A	339	A	N1-C6-N6	13.28	126.57	118.60
2	A	1289	A	N1-C6-N6	13.28	126.57	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1434	A	N1-C6-N6	13.26	126.56	118.60
2	A	227	A	N1-C6-N6	13.25	126.55	118.60
2	A	1646	A	N1-C6-N6	13.19	126.52	118.60
2	A	1146	A	N1-C6-N6	13.12	126.47	118.60
2	A	1451	A	N1-C6-N6	13.11	126.47	118.60
2	A	1825	A	N1-C6-N6	13.11	126.47	118.60
2	A	1730	A	N1-C6-N6	13.11	126.46	118.60
2	A	545	A	N1-C6-N6	13.09	126.45	118.60
2	A	1384	A	N1-C6-N6	13.08	126.45	118.60
2	A	589	A	N1-C6-N6	13.06	126.44	118.60
2	A	843	A	N1-C6-N6	13.06	126.44	118.60
2	A	510	A	N1-C6-N6	13.06	126.43	118.60
2	A	25	A	N1-C6-N6	13.05	126.43	118.60
2	A	1027	A	N1-C6-N6	13.05	126.43	118.60
2	A	445	A	N1-C6-N6	13.03	126.42	118.60
2	A	463	A	N1-C6-N6	13.03	126.42	118.60
2	A	1353	A	N1-C6-N6	13.02	126.41	118.60
2	A	882	A	N1-C6-N6	13.02	126.41	118.60
2	A	173	A	N1-C6-N6	12.99	126.39	118.60
2	A	1615	A	N1-C6-N6	12.97	126.38	118.60
2	A	538	C	P-O3'-C3'	12.97	135.26	119.70
2	A	554	A	N1-C6-N6	12.96	126.38	118.60
2	A	1853	A	N1-C6-N6	12.94	126.36	118.60
2	A	1066	A	N1-C6-N6	12.93	126.36	118.60
2	A	1809	A	N1-C6-N6	12.91	126.35	118.60
2	A	594	A	P-O3'-C3'	12.90	135.19	119.70
1	N	37	A	N1-C6-N6	12.89	126.34	118.60
2	A	1826	A	N1-C6-N6	12.89	126.33	118.60
2	A	1242	A	N1-C6-N6	12.86	126.31	118.60
2	A	519	A	N1-C6-N6	12.82	126.30	118.60
2	A	1279	C	P-O3'-C3'	12.82	135.08	119.70
2	A	1670	A	N1-C6-N6	12.81	126.29	118.60
2	A	1328	A	N1-C6-N6	12.79	126.27	118.60
2	A	164	A	N1-C6-N6	12.77	126.27	118.60
2	A	1532	A	N1-C6-N6	12.77	126.26	118.60
2	A	1609	A	N1-C6-N6	12.77	126.26	118.60
2	A	490	A	N1-C6-N6	12.77	126.26	118.60
2	A	1378	A	N1-C6-N6	12.75	126.25	118.60
2	A	1414	C	P-O3'-C3'	12.75	135.00	119.70
2	A	871	A	N1-C6-N6	12.75	126.25	118.60
2	A	91	A	N1-C6-N6	12.74	126.25	118.60
2	A	1178	A	N1-C6-N6	12.74	126.24	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	53	A	N1-C6-N6	12.73	126.24	118.60
2	A	858	A	N1-C6-N6	12.73	126.24	118.60
2	A	1026	A	N1-C6-N6	12.72	126.23	118.60
2	A	523	A	N1-C6-N6	12.72	126.23	118.60
2	A	1472	A	N1-C6-N6	12.71	126.23	118.60
2	A	22	A	N1-C6-N6	12.71	126.23	118.60
1	N	41	A	N1-C6-N6	12.71	126.22	118.60
2	A	233	A	N1-C6-N6	12.69	126.21	118.60
2	A	1140	A	N1-C6-N6	12.69	126.21	118.60
2	A	1635	A	N1-C6-N6	12.67	126.20	118.60
2	A	848	G	P-O3'-C3'	12.66	134.89	119.70
2	A	1280	A	N1-C6-N6	12.65	126.19	118.60
2	A	1008	A	N1-C6-N6	12.65	126.19	118.60
2	A	584	A	N1-C6-N6	12.64	126.19	118.60
2	A	951	A	N1-C6-N6	12.64	126.19	118.60
2	A	798	A	N1-C6-N6	12.64	126.18	118.60
2	A	1860	A	N1-C6-N6	12.64	126.18	118.60
2	A	624	A	N1-C6-N6	12.63	126.18	118.60
2	A	31	U	P-O3'-C3'	12.63	134.85	119.70
2	A	1819	A	P-O3'-C3'	12.63	134.85	119.70
2	A	619	A	N1-C6-N6	12.62	126.17	118.60
2	A	1628	A	N1-C6-N6	12.62	126.17	118.60
1	N	49	A	N1-C6-N6	12.61	126.16	118.60
2	A	976	A	N1-C6-N6	12.60	126.16	118.60
2	A	1080	A	N1-C6-N6	12.58	126.15	118.60
2	A	992	A	N1-C6-N6	12.55	126.13	118.60
2	A	1340	A	N1-C6-N6	12.55	126.13	118.60
2	A	1379	A	N1-C6-N6	12.54	126.13	118.60
2	A	609	A	N1-C6-N6	12.54	126.12	118.60
2	A	805	A	N1-C6-N6	12.53	126.12	118.60
2	A	551	A	N1-C6-N6	12.53	126.12	118.60
2	A	573	A	N1-C6-N6	12.52	126.11	118.60
2	A	807	A	N1-C6-N6	12.51	126.11	118.60
2	A	1784	A	N1-C6-N6	12.50	126.10	118.60
2	A	329	A	N1-C6-N6	12.50	126.10	118.60
2	A	1169	A	N1-C6-N6	12.50	126.10	118.60
2	A	1374	A	N1-C6-N6	12.49	126.09	118.60
2	A	1179	A	N1-C6-N6	12.49	126.09	118.60
1	N	4	A	N1-C6-N6	12.48	126.09	118.60
2	A	388	A	N1-C6-N6	12.47	126.08	118.60
2	A	1007	A	N1-C6-N6	12.47	126.08	118.60
2	A	808	A	N1-C6-N6	12.46	126.07	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	111	A	N1-C6-N6	12.45	126.07	118.60
2	A	241	A	N1-C6-N6	12.45	126.07	118.60
2	A	60	A	N1-C6-N6	12.44	126.06	118.60
2	A	404	A	N1-C6-N6	12.43	126.06	118.60
2	A	809	A	N1-C6-N6	12.43	126.06	118.60
2	A	1272	A	N1-C6-N6	12.42	126.05	118.60
2	A	11	A	N1-C6-N6	12.42	126.05	118.60
2	A	46	A	N1-C6-N6	12.41	126.05	118.60
2	A	1714	A	N1-C6-N6	12.41	126.05	118.60
2	A	565	A	N1-C6-N6	12.41	126.05	118.60
2	A	382	A	N1-C6-N6	12.41	126.04	118.60
2	A	27	A	N1-C6-N6	12.39	126.03	118.60
2	A	1019	A	N1-C6-N6	12.38	126.03	118.60
2	A	640	A	N1-C6-N6	12.38	126.03	118.60
2	A	1656	A	N1-C6-N6	12.37	126.03	118.60
2	A	912	A	N1-C6-N6	12.37	126.02	118.60
2	A	1803	A	N1-C6-N6	12.37	126.02	118.60
2	A	1185	A	N1-C6-N6	12.36	126.02	118.60
2	A	595	A	N1-C6-N6	12.36	126.01	118.60
2	A	994	A	N1-C6-N6	12.35	126.01	118.60
2	A	425	A	N1-C6-N6	12.35	126.01	118.60
2	A	1526	A	N1-C6-N6	12.34	126.00	118.60
2	A	1584	A	N1-C6-N6	12.33	126.00	118.60
2	A	1690	A	N1-C6-N6	12.33	126.00	118.60
2	A	1038	A	N1-C6-N6	12.33	126.00	118.60
2	A	1813	A	N1-C6-N6	12.33	126.00	118.60
2	A	659	A	N1-C6-N6	12.31	125.99	118.60
2	A	1224	A	N1-C6-N6	12.31	125.99	118.60
2	A	1016	A	N1-C6-N6	12.31	125.98	118.60
2	A	309	A	N1-C6-N6	12.30	125.98	118.60
2	A	1032	A	N1-C6-N6	12.30	125.98	118.60
2	A	1410	A	N1-C6-N6	12.29	125.98	118.60
2	A	1659	A	P-O3'-C3'	12.29	134.45	119.70
2	A	398	A	N1-C6-N6	12.29	125.97	118.60
2	A	214	A	N1-C6-N6	12.29	125.97	118.60
2	A	476	A	N1-C6-N6	12.28	125.97	118.60
2	A	438	A	N1-C6-N6	12.27	125.96	118.60
2	A	103	A	N1-C6-N6	12.26	125.96	118.60
2	A	1854	A	N1-C6-N6	12.26	125.96	118.60
2	A	61	A	N1-C6-N6	12.26	125.95	118.60
2	A	1190	A	N1-C6-N6	12.25	125.95	118.60
2	A	232	A	N1-C6-N6	12.24	125.95	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	643	A	N1-C6-N6	12.24	125.95	118.60
2	A	1719	A	N1-C6-N6	12.24	125.94	118.60
2	A	448	A	N1-C6-N6	12.24	125.94	118.60
2	A	631	A	N1-C6-N6	12.24	125.94	118.60
2	A	454	A	N1-C6-N6	12.22	125.93	118.60
2	A	577	A	N1-C6-N6	12.22	125.93	118.60
1	N	20	A	N1-C6-N6	12.21	125.93	118.60
2	A	829	C	P-O3'-C3'	12.21	134.35	119.70
2	A	915	A	N1-C6-N6	12.21	125.93	118.60
1	N	20	A	P-O3'-C3'	12.20	134.34	119.70
2	A	977	A	N1-C6-N6	12.20	125.92	118.60
2	A	1629	A	N1-C6-N6	12.19	125.92	118.60
2	A	1817	A	N1-C6-N6	12.19	125.91	118.60
3	F	11	A	N1-C6-N6	12.19	125.91	118.60
2	A	960	A	N1-C6-N6	12.19	125.91	118.60
2	A	1828	A	N1-C6-N6	12.19	125.91	118.60
2	A	99	A	N1-C6-N6	12.18	125.91	118.60
2	A	222	G	P-O3'-C3'	12.17	134.31	119.70
2	A	1249	A	N1-C6-N6	12.17	125.90	118.60
2	A	1274	A	N1-C6-N6	12.17	125.90	118.60
2	A	1096	A	N1-C6-N6	12.17	125.90	118.60
2	A	1392	A	N1-C6-N6	12.17	125.90	118.60
2	A	1465	A	N1-C6-N6	12.16	125.90	118.60
2	A	1078	A	N1-C6-N6	12.16	125.89	118.60
2	A	1844	A	N1-C6-N6	12.16	125.89	118.60
1	N	1	A	N1-C6-N6	12.15	125.89	118.60
2	A	1448	A	N1-C6-N6	12.15	125.89	118.60
2	A	206	A	N1-C6-N6	12.15	125.89	118.60
2	A	660	A	N1-C6-N6	12.15	125.89	118.60
2	A	904	A	N1-C6-N6	12.15	125.89	118.60
2	A	807	A	P-O3'-C3'	12.14	134.27	119.70
2	A	2	A	N1-C6-N6	12.14	125.89	118.60
2	A	1129	A	N1-C6-N6	12.14	125.88	118.60
2	A	1246	A	N1-C6-N6	12.14	125.88	118.60
2	A	988	A	N1-C6-N6	12.14	125.88	118.60
2	A	1196	A	N1-C6-N6	12.13	125.88	118.60
2	A	594	A	N1-C6-N6	12.13	125.88	118.60
2	A	1219	A	N1-C6-N6	12.13	125.88	118.60
1	N	43	A	N1-C6-N6	12.12	125.87	118.60
1	N	58	A	N1-C6-N6	12.12	125.87	118.60
2	A	455	A	N1-C6-N6	12.12	125.87	118.60
2	A	535	A	N1-C6-N6	12.12	125.87	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1812	A	N1-C6-N6	12.11	125.87	118.60
2	A	102	A	N1-C6-N6	12.11	125.86	118.60
2	A	509	A	N1-C6-N6	12.11	125.86	118.60
2	A	550	A	N1-C6-N6	12.11	125.87	118.60
2	A	1618	A	N1-C6-N6	12.11	125.86	118.60
2	A	850	A	N1-C6-N6	12.10	125.86	118.60
2	A	1716	U	P-O3'-C3'	12.10	134.22	119.70
2	A	511	A	N1-C6-N6	12.10	125.86	118.60
2	A	1349	A	N1-C6-N6	12.09	125.86	118.60
2	A	860	A	N1-C6-N6	12.09	125.85	118.60
2	A	1482	A	N1-C6-N6	12.09	125.85	118.60
2	A	1023	A	N1-C6-N6	12.08	125.85	118.60
2	A	1366	A	N1-C6-N6	12.07	125.84	118.60
2	A	1020	A	N1-C6-N6	12.06	125.84	118.60
2	A	1295	A	N1-C6-N6	12.06	125.84	118.60
2	A	1502	A	N1-C6-N6	12.06	125.84	118.60
2	A	85	A	N1-C6-N6	12.06	125.83	118.60
2	A	959	A	N1-C6-N6	12.06	125.83	118.60
2	A	1184	A	N1-C6-N6	12.06	125.83	118.60
2	A	1564	A	N1-C6-N6	12.06	125.83	118.60
2	A	940	A	N1-C6-N6	12.05	125.83	118.60
2	A	983	A	N1-C6-N6	12.05	125.83	118.60
2	A	171	A	N1-C6-N6	12.05	125.83	118.60
2	A	228	A	N1-C6-N6	12.04	125.83	118.60
2	A	993	A	N1-C6-N6	12.04	125.83	118.60
2	A	1283	A	N1-C6-N6	12.04	125.82	118.60
2	A	1589	A	N1-C6-N6	12.04	125.82	118.60
2	A	1144	A	N1-C6-N6	12.03	125.82	118.60
2	A	1596	A	N1-C6-N6	12.03	125.82	118.60
2	A	833	A	N1-C6-N6	12.03	125.82	118.60
2	A	1375	A	N1-C6-N6	12.02	125.81	118.60
2	A	559	A	N1-C6-N6	12.01	125.81	118.60
2	A	1045	A	N1-C6-N6	12.01	125.81	118.60
2	A	1237	A	N1-C6-N6	12.01	125.81	118.60
2	A	1717	G	N1-C6-O6	12.01	127.11	119.90
2	A	1839	A	N1-C6-N6	12.01	125.81	118.60
2	A	1470	A	N1-C6-N6	12.01	125.80	118.60
2	A	423	A	N1-C6-N6	12.00	125.80	118.60
2	A	746	C	P-O3'-C3'	12.00	134.10	119.70
2	A	1216	A	N1-C6-N6	12.00	125.80	118.60
2	A	107	A	N1-C6-N6	11.99	125.80	118.60
2	A	159	A	N1-C6-N6	11.99	125.80	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1417	A	N1-C6-N6	11.99	125.79	118.60
2	A	1636	A	N1-C6-N6	11.99	125.79	118.60
2	A	42	A	N1-C6-N6	11.99	125.79	118.60
2	A	293	A	N1-C6-N6	11.99	125.79	118.60
2	A	1213	A	N1-C6-N6	11.98	125.79	118.60
2	A	366	A	N1-C6-N6	11.98	125.79	118.60
2	A	845	A	N1-C6-N6	11.98	125.79	118.60
2	A	1397	A	N1-C6-N6	11.98	125.79	118.60
2	A	1673	A	N1-C6-N6	11.98	125.79	118.60
2	A	684	A	N1-C6-N6	11.98	125.79	118.60
2	A	1247	A	N1-C6-N6	11.97	125.78	118.60
2	A	574	A	N1-C6-N6	11.97	125.78	118.60
2	A	918	A	N1-C6-N6	11.96	125.78	118.60
2	A	1382	A	N1-C6-N6	11.96	125.78	118.60
2	A	54	A	N1-C6-N6	11.96	125.78	118.60
2	A	580	A	N1-C6-N6	11.96	125.77	118.60
2	A	518	A	N1-C6-N6	11.95	125.77	118.60
1	N	34	A	N1-C6-N6	11.95	125.77	118.60
1	N	72	A	N1-C6-N6	11.95	125.77	118.60
2	A	826	A	N1-C6-N6	11.95	125.77	118.60
2	A	1674	A	N1-C6-N6	11.95	125.77	118.60
2	A	50	A	N1-C6-N6	11.94	125.76	118.60
2	A	158	A	N1-C6-N6	11.94	125.76	118.60
2	A	190	A	N1-C6-N6	11.94	125.76	118.60
2	A	24	C	O4'-C1'-N1	11.94	117.75	108.20
2	A	1863	A	N1-C6-N6	11.93	125.76	118.60
2	A	338	A	N1-C6-N6	11.93	125.76	118.60
2	A	353	A	N1-C6-N6	11.93	125.76	118.60
2	A	1442	A	N1-C6-N6	11.93	125.76	118.60
3	F	23	A	N1-C6-N6	11.93	125.76	118.60
2	A	502	A	N1-C6-N6	11.93	125.75	118.60
2	A	1726	A	N1-C6-N6	11.92	125.75	118.60
2	A	645	A	N1-C6-N6	11.92	125.75	118.60
2	A	1485	A	N1-C6-N6	11.91	125.75	118.60
2	A	1089	A	N1-C6-N6	11.91	125.75	118.60
2	A	40	A	N1-C6-N6	11.91	125.75	118.60
2	A	868	A	N1-C6-N6	11.90	125.74	118.60
2	A	83	A	N1-C6-N6	11.90	125.74	118.60
2	A	1494	A	N1-C6-N6	11.90	125.74	118.60
2	A	1291	A	N1-C6-N6	11.89	125.74	118.60
2	A	1819	A	N1-C6-N6	11.89	125.74	118.60
2	A	1048	A	N1-C6-N6	11.89	125.73	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	429	A	N1-C6-N6	11.88	125.73	118.60
2	A	221	A	N1-C6-N6	11.88	125.73	118.60
2	A	1236	A	N1-C6-N6	11.88	125.72	118.60
2	A	968	A	N1-C6-N6	11.87	125.72	118.60
2	A	1775	A	N1-C6-N6	11.87	125.72	118.60
2	A	521	A	N1-C6-N6	11.86	125.72	118.60
2	A	1476	A	N1-C6-N6	11.87	125.72	118.60
2	A	283	A	N1-C6-N6	11.86	125.72	118.60
2	A	361	A	N1-C6-N6	11.86	125.72	118.60
2	A	354	A	N1-C6-N6	11.85	125.71	118.60
2	A	564	A	N1-C6-N6	11.85	125.71	118.60
2	A	1787	A	N1-C6-N6	11.85	125.71	118.60
2	A	644	A	N1-C6-N6	11.84	125.71	118.60
2	A	166	A	N1-C6-N6	11.84	125.70	118.60
2	A	181	A	N1-C6-N6	11.84	125.70	118.60
3	F	8	A	N1-C6-N6	11.84	125.70	118.60
1	N	75	A	N1-C6-N6	11.84	125.70	118.60
2	A	437	A	N1-C6-N6	11.83	125.70	118.60
2	A	986	A	N1-C6-N6	11.83	125.70	118.60
2	A	1845	A	N1-C6-N6	11.83	125.70	118.60
2	A	391	A	N1-C6-N6	11.83	125.70	118.60
2	A	512	A	N1-C6-N6	11.83	125.70	118.60
2	A	1405	A	N1-C6-N6	11.83	125.70	118.60
1	N	36	A	N1-C6-N6	11.82	125.69	118.60
2	A	19	A	N1-C6-N6	11.82	125.69	118.60
2	A	479	A	N1-C6-N6	11.82	125.69	118.60
2	A	104	A	N1-C6-N6	11.82	125.69	118.60
2	A	566	A	N1-C6-N6	11.81	125.69	118.60
2	A	922	A	N1-C6-N6	11.81	125.69	118.60
2	A	1109	A	N1-C6-N6	11.81	125.69	118.60
2	A	416	A	N1-C6-N6	11.81	125.69	118.60
2	A	1707	A	N1-C6-N6	11.81	125.69	118.60
2	A	292	A	N1-C6-N6	11.81	125.69	118.60
2	A	806	A	N1-C6-N6	11.81	125.69	118.60
2	A	1602	A	N1-C6-N6	11.81	125.68	118.60
2	A	435	A	N1-C6-N6	11.80	125.68	118.60
2	A	1625	A	N1-C6-N6	11.79	125.68	118.60
2	A	405	A	N1-C6-N6	11.79	125.67	118.60
2	A	1632	A	P-O3'-C3'	11.78	133.84	119.70
2	A	1632	A	N1-C6-N6	11.78	125.67	118.60
2	A	77	A	N1-C6-N6	11.78	125.67	118.60
2	A	408	A	N1-C6-N6	11.78	125.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1054	A	N1-C6-N6	11.78	125.67	118.60
2	A	1365	A	N1-C6-N6	11.78	125.67	118.60
1	N	7	G	N1-C6-O6	11.77	126.97	119.90
2	A	1079	A	N1-C6-N6	11.77	125.66	118.60
2	A	1795	A	N1-C6-N6	11.77	125.66	118.60
2	A	127	C	P-O3'-C3'	11.76	133.82	119.70
2	A	662	A	N1-C6-N6	11.76	125.66	118.60
2	A	1083	A	N1-C6-N6	11.76	125.66	118.60
2	A	1004	A	N1-C6-N6	11.76	125.65	118.60
2	A	1450	A	N1-C6-N6	11.76	125.65	118.60
2	A	147	A	N1-C6-N6	11.75	125.65	118.60
2	A	869	G	P-O3'-C3'	11.75	133.80	119.70
2	A	1583	A	N1-C6-N6	11.75	125.65	118.60
2	A	1614	A	N1-C6-N6	11.75	125.65	118.60
2	A	759	A	N1-C6-N6	11.74	125.65	118.60
2	A	223	A	N1-C6-N6	11.74	125.64	118.60
2	A	1694	A	N1-C6-N6	11.74	125.64	118.60
2	A	854	A	N1-C6-N6	11.74	125.64	118.60
2	A	1005	A	N1-C6-N6	11.74	125.64	118.60
2	A	1166	A	N1-C6-N6	11.74	125.64	118.60
2	A	1551	A	N1-C6-N6	11.74	125.64	118.60
2	A	1659	A	N1-C6-N6	11.73	125.64	118.60
2	A	814	A	N1-C6-N6	11.73	125.64	118.60
2	A	1287	A	N1-C6-N6	11.73	125.64	118.60
2	A	526	A	N1-C6-N6	11.72	125.64	118.60
2	A	630	A	N1-C6-N6	11.72	125.63	118.60
2	A	953	A	N1-C6-N6	11.72	125.63	118.60
2	A	1740	A	N1-C6-N6	11.71	125.63	118.60
2	A	861	A	N1-C6-N6	11.71	125.63	118.60
2	A	1479	A	N1-C6-N6	11.71	125.63	118.60
2	A	633	A	N1-C6-N6	11.71	125.62	118.60
2	A	1254	A	N1-C6-N6	11.71	125.62	118.60
2	A	290	A	N1-C6-N6	11.70	125.62	118.60
2	A	675	A	N1-C6-N6	11.69	125.61	118.60
3	F	30	A	N1-C6-N6	11.69	125.61	118.60
2	A	1444	A	N1-C6-N6	11.69	125.61	118.60
2	A	333	A	N1-C6-N6	11.69	125.61	118.60
2	A	1031	A	N1-C6-N6	11.68	125.61	118.60
2	A	1073	A	N1-C6-N6	11.67	125.60	118.60
2	A	654	A	N1-C6-N6	11.67	125.60	118.60
2	A	900	A	N1-C6-N6	11.67	125.60	118.60
2	A	38	A	N1-C6-N6	11.66	125.60	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1683	C	P-O3'-C3'	-11.66	105.71	119.70
2	A	812	A	N1-C6-N6	11.66	125.59	118.60
2	A	45	A	N1-C6-N6	11.65	125.59	118.60
2	A	934	A	N1-C6-N6	11.65	125.59	118.60
2	A	128	U	O4'-C1'-N1	11.65	117.52	108.20
2	A	661	A	N1-C6-N6	11.65	125.59	118.60
2	A	899	A	N1-C6-N6	11.64	125.59	118.60
2	A	979	A	N1-C6-N6	11.64	125.59	118.60
1	N	19	A	N1-C6-N6	11.64	125.58	118.60
2	A	1186	A	N1-C6-N6	11.64	125.58	118.60
2	A	1309	A	N1-C6-N6	11.64	125.58	118.60
2	A	1800	A	N1-C6-N6	11.64	125.58	118.60
2	A	1118	A	N1-C6-N6	11.62	125.57	118.60
2	A	1051	A	N1-C6-N6	11.62	125.57	118.60
2	A	866	A	N1-C6-N6	11.62	125.57	118.60
1	N	48	G	N1-C6-O6	11.61	126.86	119.90
3	F	4	A	N1-C6-N6	11.60	125.56	118.60
3	F	18	A	N1-C6-N6	11.60	125.56	118.60
2	A	658	A	N1-C6-N6	11.60	125.56	118.60
2	A	459	A	N1-C6-N6	11.59	125.55	118.60
2	A	1076	A	N1-C6-N6	11.58	125.55	118.60
2	A	1408	C	O4'-C1'-N1	11.58	117.47	108.20
2	A	1596	A	P-O3'-C3'	11.58	133.60	119.70
2	A	92	A	N1-C6-N6	11.58	125.55	118.60
2	A	1056	A	N1-C6-N6	11.58	125.55	118.60
2	A	1818	A	N1-C6-N6	11.58	125.55	118.60
2	A	823	A	N1-C6-N6	11.57	125.55	118.60
2	A	865	A	N1-C6-N6	11.57	125.55	118.60
2	A	1177	A	N1-C6-N6	11.57	125.54	118.60
2	A	1435	A	N1-C6-N6	11.56	125.54	118.60
2	A	175	A	N1-C6-N6	11.56	125.54	118.60
2	A	513	A	N1-C6-N6	11.56	125.54	118.60
2	A	857	A	N1-C6-N6	11.56	125.53	118.60
2	A	821	A	N1-C6-N6	11.55	125.53	118.60
2	A	1139	A	N1-C6-N6	11.55	125.53	118.60
2	A	384	G	N1-C6-O6	11.55	126.83	119.90
2	A	229	A	N1-C6-N6	11.54	125.53	118.60
2	A	450	A	N1-C6-N6	11.54	125.52	118.60
2	A	1210	A	P-O3'-C3'	11.53	133.54	119.70
2	A	1111	U	P-O3'-C3'	11.53	133.53	119.70
2	A	1575	A	N1-C6-N6	11.53	125.52	118.60
2	A	1261	A	N1-C6-N6	11.52	125.51	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1642	A	N1-C6-N6	11.51	125.50	118.60
2	A	1372	A	N1-C6-N6	11.50	125.50	118.60
2	A	1540	A	N1-C6-N6	11.50	125.50	118.60
2	A	1807	A	N1-C6-N6	11.50	125.50	118.60
2	A	1461	A	N1-C6-N6	11.49	125.50	118.60
2	A	138	C	P-O3'-C3'	11.49	133.49	119.70
2	A	84	A	N1-C6-N6	11.48	125.49	118.60
2	A	1398	A	N1-C6-N6	11.48	125.49	118.60
2	A	326	A	N1-C6-N6	11.48	125.49	118.60
2	A	1692	A	N1-C6-N6	11.47	125.48	118.60
3	F	6	A	N1-C6-N6	11.46	125.48	118.60
2	A	909	A	N1-C6-N6	11.46	125.47	118.60
2	A	1829	A	N1-C6-N6	11.45	125.47	118.60
2	A	458	A	N1-C6-N6	11.44	125.47	118.60
2	A	1857	A	N1-C6-N6	11.44	125.46	118.60
2	A	506	A	N1-C6-N6	11.44	125.46	118.60
2	A	474	A	N1-C6-N6	11.43	125.46	118.60
2	A	1204	A	N1-C6-N6	11.42	125.45	118.60
2	A	1483	A	N1-C6-N6	11.42	125.45	118.60
2	A	475	A	N1-C6-N6	11.41	125.45	118.60
2	A	149	A	N1-C6-N6	11.41	125.44	118.60
2	A	1098	G	N1-C6-O6	11.40	126.74	119.90
2	A	1205	A	N1-C6-N6	11.39	125.44	118.60
1	N	21	G	N1-C6-O6	11.38	126.73	119.90
2	A	218	A	N1-C6-N6	11.38	125.43	118.60
2	A	1104	G	P-O3'-C3'	11.35	133.32	119.70
2	A	1195	A	N1-C6-N6	11.35	125.41	118.60
2	A	1528	A	N1-C6-N6	11.35	125.41	118.60
2	A	80	G	N1-C6-O6	11.33	126.70	119.90
2	A	1782	A	N1-C6-N6	11.32	125.39	118.60
1	N	73	C	P-O3'-C3'	11.31	133.27	119.70
2	A	804	A	N1-C6-N6	11.29	125.37	118.60
2	A	882	A	P-O3'-C3'	11.28	133.24	119.70
2	A	786	C	P-O3'-C3'	11.26	133.22	119.70
1	N	14	A	N1-C6-N6	11.26	125.36	118.60
2	A	208	G	N1-C6-O6	11.25	126.65	119.90
2	A	1658	A	N1-C6-N6	11.25	125.35	118.60
2	A	1762	A	N1-C6-N6	11.24	125.34	118.60
2	A	1255	A	N1-C6-N6	11.23	125.34	118.60
2	A	916	A	N1-C6-N6	11.22	125.33	118.60
2	A	1024	A	N1-C6-N6	11.22	125.33	118.60
2	A	1030	A	N1-C6-N6	11.22	125.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	150	A	N1-C6-N6	11.20	125.32	118.60
2	A	515	A	N1-C6-N6	11.20	125.32	118.60
1	N	10	G	N1-C6-O6	11.20	126.62	119.90
2	A	1504	A	N1-C6-N6	11.20	125.32	118.60
2	A	1191	A	N1-C6-N6	11.16	125.30	118.60
2	A	1145	A	N1-C6-N6	11.16	125.30	118.60
2	A	544	A	N1-C6-N6	11.14	125.28	118.60
2	A	1816	A	N1-C6-N6	11.11	125.27	118.60
2	A	442	G	N1-C6-O6	11.08	126.55	119.90
2	A	542	G	N1-C6-O6	11.08	126.55	119.90
2	A	1115	A	N1-C6-N6	11.07	125.24	118.60
2	A	581	U	O4'-C1'-N1	11.07	117.05	108.20
2	A	379	A	N1-C6-N6	11.06	125.24	118.60
2	A	516	A	N1-C6-N6	11.05	125.23	118.60
2	A	79	A	N1-C6-N6	11.01	125.21	118.60
2	A	1556	A	N1-C6-N6	11.00	125.20	118.60
2	A	237	G	P-O3'-C3'	10.99	132.89	119.70
2	A	1058	A	N1-C6-N6	10.99	125.19	118.60
2	A	1496	G	N1-C6-O6	10.97	126.48	119.90
2	A	1785	A	N1-C6-N6	10.96	125.18	118.60
2	A	1645	A	N1-C6-N6	10.95	125.17	118.60
2	A	1425	G	P-O3'-C3'	10.95	132.84	119.70
2	A	185	C	C2-N3-C4	-10.94	114.43	119.90
2	A	39	A	N1-C6-N6	10.92	125.15	118.60
2	A	409	G	N1-C6-O6	10.92	126.45	119.90
2	A	1303	U	P-O3'-C3'	10.92	132.80	119.70
2	A	131	C	P-O3'-C3'	10.90	132.79	119.70
2	A	1480	A	N1-C6-N6	10.88	125.13	118.60
2	A	273	G	N1-C6-O6	10.88	126.43	119.90
2	A	1183	G	N1-C6-O6	10.88	126.43	119.90
2	A	1414	C	C2-N1-C1'	10.88	130.76	118.80
2	A	618	A	N1-C6-N6	10.87	125.12	118.60
2	A	1794	A	N1-C6-N6	10.86	125.12	118.60
1	N	59	A	N1-C6-N6	10.86	125.12	118.60
2	A	791	A	N1-C6-N6	10.85	125.11	118.60
2	A	1046	A	N1-C6-N6	10.85	125.11	118.60
2	A	1297	A	N1-C6-N6	10.84	125.10	118.60
2	A	1256	A	N1-C6-N6	10.84	125.10	118.60
2	A	1137	G	N1-C6-O6	10.80	126.38	119.90
2	A	1192	A	N1-C6-N6	10.78	125.07	118.60
2	A	203	G	N1-C6-O6	10.77	126.36	119.90
2	A	686	G	N1-C6-O6	10.76	126.36	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	278	U	P-O3'-C3'	10.75	132.60	119.70
2	A	478	U	P-O3'-C3'	10.75	132.60	119.70
2	A	1278	A	N1-C6-N6	10.72	125.03	118.60
2	A	1006	G	N1-C6-O6	10.71	126.33	119.90
2	A	1106	G	N1-C6-O6	10.66	126.30	119.90
2	A	1418	G	N1-C6-O6	10.66	126.30	119.90
2	A	601	G	N1-C6-O6	10.66	126.30	119.90
1	N	62	A	N1-C6-N6	10.64	124.98	118.60
2	A	835	C	O4'-C1'-N1	10.62	116.70	108.20
2	A	1311	U	O4'-C1'-N1	10.62	116.70	108.20
2	A	907	C	P-O5'-C5'	10.62	137.88	120.90
2	A	1535	G	N1-C6-O6	10.58	126.25	119.90
2	A	1486	G	N1-C6-O6	10.58	126.25	119.90
1	N	52	G	N1-C6-O6	10.54	126.22	119.90
2	A	273	G	C5-C6-O6	-10.53	122.28	128.60
2	A	578	G	N1-C6-O6	10.51	126.20	119.90
2	A	421	G	N1-C6-O6	10.49	126.19	119.90
2	A	1127	G	N1-C6-O6	10.49	126.20	119.90
1	N	5	G	N1-C6-O6	10.48	126.19	119.90
2	A	1061	G	N1-C6-O6	10.47	126.18	119.90
2	A	1683	C	O4'-C1'-N1	10.47	116.58	108.20
2	A	1323	G	N1-C6-O6	10.47	126.18	119.90
2	A	1241	G	N1-C6-O6	10.46	126.17	119.90
2	A	1361	G	N1-C6-O6	10.45	126.17	119.90
2	A	320	G	N1-C6-O6	10.45	126.17	119.90
2	A	201	G	N1-C6-O6	10.43	126.16	119.90
2	A	304	A	N1-C6-N6	10.39	124.83	118.60
2	A	1688	G	N1-C6-O6	10.34	126.10	119.90
2	A	1171	G	N1-C6-O6	10.34	126.10	119.90
2	A	1402	G	P-O3'-C3'	10.33	132.10	119.70
2	A	1855	G	N1-C6-O6	10.33	126.10	119.90
2	A	319	G	N1-C6-O6	10.33	126.10	119.90
2	A	1033	G	N1-C6-O6	10.32	126.09	119.90
2	A	1371	G	N1-C6-O6	10.26	126.06	119.90
2	A	185	C	C6-N1-C2	-10.25	116.20	120.30
2	A	1072	G	N1-C6-O6	10.24	126.05	119.90
2	A	1225	G	N1-C6-O6	10.24	126.04	119.90
2	A	1598	G	N1-C6-O6	10.24	126.04	119.90
2	A	784	G	N1-C6-O6	10.23	126.04	119.90
2	A	869	G	N1-C6-O6	10.23	126.04	119.90
2	A	156	G	N1-C6-O6	10.23	126.04	119.90
2	A	1750	C	O4'-C1'-N1	10.22	116.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	360	G	N1-C6-O6	10.21	126.03	119.90
2	A	546	U	P-O5'-C5'	10.21	137.23	120.90
1	N	42	G	N1-C6-O6	10.20	126.02	119.90
2	A	6	G	N1-C6-O6	10.17	126.00	119.90
2	A	1817	A	P-O3'-C3'	10.16	131.89	119.70
2	A	1566	G	N1-C6-O6	10.13	125.98	119.90
2	A	10	G	N1-C6-O6	10.12	125.97	119.90
2	A	65	C	P-O3'-C3'	10.12	131.85	119.70
2	A	208	G	C5-C6-O6	-10.12	122.53	128.60
2	A	393	G	N1-C6-O6	10.12	125.97	119.90
2	A	1570	G	N1-C6-O6	10.10	125.96	119.90
2	A	457	G	N1-C6-O6	10.09	125.95	119.90
2	A	625	G	N1-C6-O6	10.08	125.95	119.90
2	A	1331	G	N1-C6-O6	10.08	125.95	119.90
1	N	28	G	N1-C6-O6	10.07	125.94	119.90
2	A	995	G	N1-C6-O6	10.07	125.94	119.90
2	A	1067	G	N1-C6-O6	10.07	125.94	119.90
2	A	102	A	P-O3'-C3'	10.07	131.78	119.70
2	A	274	G	N1-C6-O6	10.07	125.94	119.90
2	A	212	G	N1-C6-O6	10.07	125.94	119.90
2	A	822	A	N1-C6-N6	10.07	124.64	118.60
2	A	300	G	N1-C6-O6	10.06	125.94	119.90
2	A	466	A	N1-C6-N6	10.06	124.64	118.60
2	A	1401	A	N1-C6-N6	10.05	124.63	118.60
2	A	439	A	N1-C6-N6	10.04	124.63	118.60
2	A	1460	C	O4'-C1'-N1	10.04	116.23	108.20
2	A	1722	G	N1-C6-O6	10.04	125.93	119.90
2	A	1100	G	N1-C6-O6	10.04	125.92	119.90
2	A	897	G	N1-C6-O6	10.04	125.92	119.90
2	A	424	G	N1-C6-O6	10.03	125.92	119.90
2	A	345	G	N1-C6-O6	10.02	125.91	119.90
1	N	48	G	C5-C6-O6	-10.02	122.59	128.60
1	N	51	G	N1-C6-O6	10.00	125.90	119.90
2	A	1770	G	N1-C6-O6	9.99	125.90	119.90
2	A	1037	G	N1-C6-O6	9.99	125.89	119.90
1	N	25	G	N1-C6-O6	9.98	125.89	119.90
2	A	783	G	N1-C6-O6	9.98	125.89	119.90
2	A	1561	G	N1-C6-O6	9.98	125.89	119.90
2	A	1050	G	N1-C6-O6	9.97	125.88	119.90
2	A	62	G	N1-C6-O6	9.96	125.88	119.90
2	A	1208	G	N1-C6-O6	9.96	125.88	119.90
2	A	891	G	N1-C6-O6	9.95	125.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	2	G	N1-C6-O6	9.94	125.86	119.90
2	A	1851	G	N1-C6-O6	9.94	125.86	119.90
2	A	989	G	N1-C6-O6	9.94	125.86	119.90
2	A	1220	G	N1-C6-O6	9.91	125.85	119.90
2	A	1345	G	N1-C6-O6	9.91	125.85	119.90
2	A	66	G	N1-C6-O6	9.90	125.84	119.90
2	A	1765	G	N1-C6-O6	9.89	125.84	119.90
2	A	367	G	N1-C6-O6	9.89	125.83	119.90
2	A	525	G	N1-C6-O6	9.88	125.83	119.90
2	A	1558	G	N1-C6-O6	9.88	125.83	119.90
1	N	7	G	C5-C6-O6	-9.86	122.68	128.60
2	A	906	G	N1-C6-O6	9.86	125.82	119.90
2	A	1605	G	N1-C6-O6	9.86	125.82	119.90
2	A	461	G	N1-C6-O6	9.85	125.81	119.90
2	A	80	G	C5-C6-O6	-9.83	122.70	128.60
2	A	1126	G	N1-C6-O6	9.83	125.80	119.90
2	A	400	G	N1-C6-O6	9.82	125.79	119.90
2	A	952	G	N1-C6-O6	9.82	125.79	119.90
2	A	1452	G	N1-C6-O6	9.82	125.79	119.90
2	A	1669	G	N1-C6-O6	9.82	125.79	119.90
2	A	1515	G	N1-C6-O6	9.81	125.79	119.90
2	A	929	G	O4'-C1'-N9	9.81	116.05	108.20
2	A	1849	G	N1-C6-O6	9.81	125.78	119.90
2	A	7	G	N1-C6-O6	9.81	125.78	119.90
2	A	753	C	O4'-C1'-N1	9.80	116.04	108.20
2	A	1277	G	N1-C6-O6	9.79	125.77	119.90
2	A	1545	G	N1-C6-O6	9.78	125.77	119.90
2	A	981	G	N1-C6-O6	9.78	125.77	119.90
2	A	1347	G	N1-C6-O6	9.76	125.76	119.90
2	A	883	U	O4'-C1'-N1	9.76	116.01	108.20
2	A	1085	G	N1-C6-O6	9.76	125.75	119.90
2	A	1044	G	N1-C6-O6	9.76	125.75	119.90
2	A	1487	G	N1-C6-O6	9.76	125.75	119.90
2	A	591	G	N1-C6-O6	9.75	125.75	119.90
2	A	1414	C	P-O5'-C5'	9.75	136.50	120.90
1	N	30	G	N1-C6-O6	9.74	125.75	119.90
2	A	29	G	N1-C6-O6	9.74	125.74	119.90
2	A	1217	G	N1-C6-O6	9.74	125.74	119.90
2	A	267	G	N1-C6-O6	9.73	125.74	119.90
2	A	555	G	N1-C6-O6	9.73	125.74	119.90
2	A	1568	G	N1-C6-O6	9.73	125.74	119.90
2	A	1745	C	O4'-C1'-N1	9.73	115.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1430	C	P-O3'-C3'	9.72	131.37	119.70
2	A	47	G	N1-C6-O6	9.70	125.72	119.90
1	N	31	C	O4'-C1'-N1	9.70	115.96	108.20
2	A	1270	G	N1-C6-O6	9.70	125.72	119.90
2	A	1506	G	N1-C6-O6	9.70	125.72	119.90
2	A	167	G	N1-C6-O6	9.69	125.72	119.90
2	A	341	G	N1-C6-O6	9.70	125.72	119.90
2	A	1304	U	O4'-C1'-N1	9.69	115.95	108.20
2	A	1717	G	C5-C6-O6	-9.69	122.78	128.60
2	A	88	G	N1-C6-O6	9.68	125.71	119.90
2	A	890	G	N1-C6-O6	9.68	125.71	119.90
2	A	920	G	N1-C6-O6	9.67	125.70	119.90
2	A	494	G	N1-C6-O6	9.66	125.70	119.90
2	A	1653	G	N1-C6-O6	9.66	125.70	119.90
2	A	186	G	N1-C6-O6	9.66	125.70	119.90
2	A	1647	G	N1-C6-O6	9.65	125.69	119.90
2	A	1698	C	O4'-C1'-N1	9.65	115.92	108.20
4	P	116	ALA	N-CA-CB	9.65	123.62	110.10
2	A	536	G	N1-C6-O6	9.65	125.69	119.90
1	N	12	G	N1-C6-O6	9.64	125.69	119.90
2	A	748	G	N1-C6-O6	9.64	125.69	119.90
2	A	1468	C	O4'-C1'-N1	9.63	115.91	108.20
2	A	95	G	N1-C6-O6	9.63	125.68	119.90
2	A	1443	G	N1-C6-O6	9.62	125.67	119.90
2	A	311	C	P-O5'-C5'	9.62	136.29	120.90
2	A	877	G	N1-C6-O6	9.61	125.67	119.90
2	A	1823	G	N1-C6-O6	9.61	125.67	119.90
2	A	1683	C	C4'-C3'-C2'	-9.60	93.00	102.60
2	A	1651	G	N1-C6-O6	9.60	125.66	119.90
2	A	828	G	N1-C6-O6	9.59	125.65	119.90
2	A	498	A	N1-C6-N6	9.57	124.34	118.60
2	A	1125	G	N1-C6-O6	9.57	125.64	119.90
2	A	1098	G	C5-C6-O6	-9.57	122.86	128.60
2	A	1790	G	N1-C6-O6	9.56	125.64	119.90
2	A	52	G	N1-C6-O6	9.56	125.64	119.90
2	A	646	G	N1-C6-O6	9.56	125.64	119.90
2	A	1675	G	N1-C6-O6	9.55	125.63	119.90
2	A	1202	G	N1-C6-O6	9.54	125.62	119.90
2	A	1036	G	N1-C6-O6	9.54	125.62	119.90
2	A	1229	G	N1-C6-O6	9.54	125.62	119.90
2	A	1752	G	N1-C6-O6	9.53	125.62	119.90
2	A	1359	C	O4'-C1'-N1	9.53	115.82	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	29	G	N1-C6-O6	9.50	125.60	119.90
2	A	774	U	O4'-C1'-N1	9.50	115.80	108.20
2	A	1521	G	N1-C6-O6	9.50	125.60	119.90
1	N	23	G	N1-C6-O6	9.50	125.60	119.90
2	A	468	G	N1-C6-O6	9.49	125.60	119.90
2	A	758	G	N1-C6-O6	9.49	125.59	119.90
2	A	1799	G	N1-C6-O6	9.49	125.59	119.90
2	A	395	G	N1-C6-O6	9.48	125.59	119.90
2	A	1344	G	N1-C6-O6	9.48	125.59	119.90
2	A	542	G	C5-C6-O6	-9.48	122.91	128.60
2	A	1744	G	N1-C6-O6	9.47	125.58	119.90
1	N	21	G	C5-C6-O6	-9.46	122.92	128.60
2	A	279	G	N1-C6-O6	9.46	125.58	119.90
2	A	930	G	N1-C6-O6	9.46	125.58	119.90
2	A	1334	G	N1-C6-O6	9.46	125.58	119.90
2	A	1455	G	N1-C6-O6	9.45	125.57	119.90
2	A	1194	G	N1-C6-O6	9.45	125.57	119.90
2	A	938	G	N1-C6-O6	9.43	125.56	119.90
2	A	1523	G	N1-C6-O6	9.43	125.56	119.90
2	A	1006	G	C5-C6-O6	-9.43	122.94	128.60
2	A	280	G	O4'-C1'-N9	9.43	115.74	108.20
2	A	634	G	N1-C6-O6	9.43	125.56	119.90
2	A	925	G	N1-C6-O6	9.41	125.55	119.90
2	A	1047	G	N1-C6-O6	9.41	125.55	119.90
2	A	1727	G	N1-C6-O6	9.41	125.55	119.90
2	A	587	G	N1-C6-O6	9.39	125.54	119.90
2	A	1172	G	N1-C6-O6	9.39	125.53	119.90
2	A	1324	G	N1-C6-O6	9.39	125.53	119.90
2	A	1207	G	N1-C6-O6	9.38	125.53	119.90
2	A	317	G	N1-C6-O6	9.38	125.53	119.90
2	A	544	A	O4'-C1'-N9	9.38	115.70	108.20
2	A	1316	G	N1-C6-O6	9.38	125.53	119.90
2	A	785	G	N1-C6-O6	9.37	125.52	119.90
2	A	955	G	N1-C6-O6	9.37	125.52	119.90
2	A	23	G	N1-C6-O6	9.36	125.52	119.90
2	A	1154	G	N1-C6-O6	9.36	125.52	119.90
2	A	1218	G	N1-C6-O6	9.36	125.52	119.90
2	A	1414	C	C6-N1-C1'	-9.36	109.57	120.80
2	A	1814	G	N1-C6-O6	9.36	125.51	119.90
2	A	1421	G	N1-C6-O6	9.35	125.51	119.90
2	A	1136	G	N1-C6-O6	9.35	125.51	119.90
2	A	1511	G	N1-C6-O6	9.34	125.50	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	22	C	O4'-C1'-N1	9.34	115.67	108.20
2	A	1206	G	N1-C6-O6	9.34	125.50	119.90
2	A	1840	G	N1-C6-O6	9.33	125.50	119.90
2	A	1147	G	N1-C6-O6	9.33	125.50	119.90
2	A	1330	G	N1-C6-O6	9.33	125.50	119.90
2	A	1454	G	N1-C6-O6	9.33	125.50	119.90
2	A	384	G	C5-C6-O6	-9.32	123.01	128.60
2	A	434	G	N1-C6-O6	9.32	125.49	119.90
2	A	403	G	N1-C6-O6	9.31	125.49	119.90
2	A	495	G	N1-C6-O6	9.31	125.49	119.90
2	A	394	G	N1-C6-O6	9.31	125.48	119.90
2	A	1517	A	O4'-C1'-N9	9.31	115.64	108.20
2	A	967	G	N1-C6-O6	9.30	125.48	119.90
2	A	1392	A	O4'-C1'-N9	9.30	115.64	108.20
2	A	978	G	N1-C6-O6	9.30	125.48	119.90
2	A	827	G	N1-C6-O6	9.29	125.47	119.90
3	F	8	A	P-O3'-C3'	9.29	130.84	119.70
2	A	1608	G	N1-C6-O6	9.28	125.47	119.90
1	N	52	G	C5-C6-O6	-9.27	123.04	128.60
2	A	1810	G	N1-C6-O6	9.27	125.47	119.90
2	A	146	G	N1-C6-O6	9.27	125.46	119.90
2	A	534	G	N1-C6-O6	9.27	125.46	119.90
2	A	238	G	N1-C6-O6	9.26	125.46	119.90
2	A	1391	C	O4'-C1'-N1	9.26	115.61	108.20
2	A	1394	G	N1-C6-O6	9.26	125.45	119.90
2	A	456	G	N1-C6-O6	9.26	125.45	119.90
2	A	686	G	C5-C6-O6	-9.25	123.05	128.60
2	A	856	G	N1-C6-O6	9.25	125.45	119.90
2	A	1546	U	O4'-C1'-N1	9.25	115.60	108.20
2	A	285	U	P-O3'-C3'	9.24	130.79	119.70
2	A	1820	G	N1-C6-O6	9.24	125.45	119.90
2	A	350	A	N1-C6-N6	9.24	124.14	118.60
2	A	1290	G	N1-C6-O6	9.24	125.44	119.90
2	A	613	G	N1-C6-O6	9.24	125.44	119.90
2	A	1786	G	N1-C6-O6	9.23	125.44	119.90
2	A	1321	G	N1-C6-O6	9.23	125.44	119.90
2	A	1536	G	N1-C6-O6	9.22	125.44	119.90
2	A	1193	G	N1-C6-O6	9.22	125.43	119.90
2	A	1161	G	N1-C6-O6	9.22	125.43	119.90
2	A	1362	G	N1-C6-O6	9.22	125.43	119.90
2	A	971	G	N1-C6-O6	9.21	125.43	119.90
2	A	271	G	N1-C6-O6	9.20	125.42	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1276	G	N1-C6-O6	9.20	125.42	119.90
2	A	1381	G	N1-C6-O6	9.20	125.42	119.90
2	A	1164	G	N1-C6-O6	9.20	125.42	119.90
2	A	20	G	N1-C6-O6	9.20	125.42	119.90
1	N	56	G	N1-C6-O6	9.19	125.41	119.90
2	A	401	G	N1-C6-O6	9.19	125.41	119.90
2	A	865	A	P-O3'-C3'	9.19	130.73	119.70
2	A	314	U	O4'-C1'-N1	9.19	115.55	108.20
2	A	1475	G	N1-C6-O6	9.19	125.41	119.90
2	A	1360	U	O4'-C1'-N1	9.19	115.55	108.20
2	A	1753	G	N1-C6-O6	9.19	125.41	119.90
2	A	1697	G	N1-C6-O6	9.18	125.41	119.90
2	A	553	G	N1-C6-O6	9.18	125.41	119.90
2	A	803	G	N1-C6-O6	9.18	125.41	119.90
2	A	1748	G	N1-C6-O6	9.18	125.41	119.90
2	A	1429	C	O4'-C1'-N1	9.17	115.54	108.20
2	A	885	U	O4'-C1'-N1	9.16	115.53	108.20
2	A	1649	G	N1-C6-O6	9.16	125.40	119.90
2	A	441	G	N1-C6-O6	9.16	125.40	119.90
2	A	855	G	N1-C6-O6	9.16	125.40	119.90
3	F	29	G	N1-C6-O6	9.15	125.39	119.90
2	A	1191	A	O4'-C1'-N9	9.15	115.52	108.20
2	A	817	G	N1-C6-O6	9.15	125.39	119.90
2	A	1416	G	N1-C6-O6	9.15	125.39	119.90
2	A	1774	G	N1-C6-O6	9.14	125.39	119.90
2	A	1582	G	N1-C6-O6	9.14	125.38	119.90
2	A	1314	G	N1-C6-O6	9.12	125.37	119.90
2	A	945	G	N1-C6-O6	9.12	125.37	119.90
2	A	114	G	N1-C6-O6	9.11	125.37	119.90
2	A	1180	G	N1-C6-O6	9.11	125.36	119.90
2	A	1509	G	N1-C6-O6	9.10	125.36	119.90
2	A	1001	G	N1-C6-O6	9.10	125.36	119.90
2	A	426	G	N1-C6-O6	9.10	125.36	119.90
2	A	1732	G	N1-C6-O6	9.10	125.36	119.90
2	A	370	G	N1-C6-O6	9.09	125.36	119.90
2	A	874	G	N1-C6-O6	9.09	125.35	119.90
2	A	931	G	N1-C6-O6	9.09	125.36	119.90
2	A	1841	G	N1-C6-O6	9.09	125.36	119.90
2	A	1606	G	N1-C6-O6	9.09	125.35	119.90
2	A	1420	G	N1-C6-O6	9.08	125.35	119.90
2	A	607	G	N1-C6-O6	9.08	125.34	119.90
2	A	1607	G	N1-C6-O6	9.06	125.33	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1831	G	N1-C6-O6	9.06	125.33	119.90
2	A	86	C	O4'-C1'-N1	9.06	115.45	108.20
2	A	1510	G	N1-C6-O6	9.05	125.33	119.90
2	A	1579	G	N1-C6-O6	9.05	125.33	119.90
2	A	957	G	N1-C6-O6	9.05	125.33	119.90
2	A	1383	G	N1-C6-O6	9.05	125.33	119.90
2	A	604	G	N1-C6-O6	9.05	125.33	119.90
2	A	1425	G	N1-C6-O6	9.05	125.33	119.90
2	A	442	G	C5-C6-O6	-9.05	123.17	128.60
2	A	1122	G	N1-C6-O6	9.04	125.33	119.90
2	A	1162	G	N1-C6-O6	9.04	125.33	119.90
2	A	1025	G	N1-C6-O6	9.04	125.32	119.90
2	A	289	G	N1-C6-O6	9.04	125.32	119.90
2	A	1294	G	N1-C6-O6	9.03	125.32	119.90
2	A	1503	G	O4'-C1'-N9	9.03	115.42	108.20
2	A	972	G	N1-C6-O6	9.03	125.32	119.90
2	A	1163	G	N1-C6-O6	9.03	125.32	119.90
2	A	1811	G	N1-C6-O6	9.03	125.32	119.90
2	A	830	C	O4'-C1'-N1	9.02	115.42	108.20
2	A	130	G	N1-C6-O6	9.02	125.31	119.90
2	A	1541	G	N1-C6-O6	9.02	125.31	119.90
2	A	588	G	N1-C6-O6	9.02	125.31	119.90
2	A	307	G	N1-C6-O6	9.02	125.31	119.90
2	A	1348	G	N1-C6-O6	9.02	125.31	119.90
2	A	1402	G	N1-C6-O6	9.02	125.31	119.90
2	A	1664	G	N1-C6-O6	9.01	125.31	119.90
2	A	411	G	N1-C6-O6	9.00	125.30	119.90
2	A	70	G	N1-C6-O6	9.00	125.30	119.90
2	A	375	G	N1-C6-O6	9.00	125.30	119.90
2	A	1612	G	N1-C6-O6	8.99	125.30	119.90
2	A	203	G	C5-C6-O6	-8.99	123.21	128.60
2	A	663	G	N1-C6-O6	8.99	125.29	119.90
2	A	165	G	N1-C6-O6	8.98	125.29	119.90
2	A	1281	G	N1-C6-O6	8.98	125.29	119.90
2	A	1341	G	N1-C6-O6	8.98	125.29	119.90
2	A	240	C	O4'-C1'-N1	8.97	115.38	108.20
2	A	1117	G	N1-C6-O6	8.97	125.28	119.90
2	A	1160	G	N1-C6-O6	8.97	125.28	119.90
1	N	18	G	N1-C6-O6	8.97	125.28	119.90
2	A	123	G	N1-C6-O6	8.97	125.28	119.90
2	A	402	G	N1-C6-O6	8.97	125.28	119.90
2	A	497	G	N1-C6-O6	8.97	125.28	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	13	G	N1-C6-O6	8.97	125.28	119.90
2	A	1548	C	O4'-C1'-N1	8.96	115.37	108.20
2	A	1183	G	C5-C6-O6	-8.96	123.22	128.60
2	A	1771	G	N1-C6-O6	8.96	125.28	119.90
2	A	325	G	N1-C6-O6	8.96	125.28	119.90
2	A	1029	G	N1-C6-O6	8.96	125.27	119.90
2	A	842	G	N1-C6-O6	8.95	125.27	119.90
2	A	1701	G	N1-C6-O6	8.95	125.27	119.90
2	A	430	G	N1-C6-O6	8.94	125.27	119.90
2	A	1155	G	N1-C6-O6	8.94	125.27	119.90
2	A	464	G	N1-C6-O6	8.94	125.26	119.90
2	A	1231	G	N1-C6-O6	8.94	125.26	119.90
2	A	1232	G	N1-C6-O6	8.93	125.26	119.90
2	A	204	G	N1-C6-O6	8.92	125.25	119.90
2	A	733	G	N1-C6-O6	8.92	125.25	119.90
2	A	45	A	O4'-C1'-N9	8.92	115.34	108.20
2	A	1153	G	N1-C6-O6	8.92	125.25	119.90
2	A	1361	G	C5-C6-O6	-8.92	123.25	128.60
2	A	1660	G	N1-C6-O6	8.92	125.25	119.90
2	A	460	G	N1-C6-O6	8.92	125.25	119.90
2	A	210	G	N1-C6-O6	8.92	125.25	119.90
2	A	974	G	N1-C6-O6	8.91	125.25	119.90
2	A	685	G	N1-C6-O6	8.91	125.25	119.90
2	A	1444	A	P-O3'-C3'	8.91	130.39	119.70
2	A	145	G	N1-C6-O6	8.91	125.25	119.90
2	A	1010	G	N1-C6-O6	8.91	125.25	119.90
2	A	1565	G	N1-C6-O6	8.90	125.24	119.90
2	A	1776	G	O4'-C1'-N9	8.90	115.32	108.20
2	A	1662	U	O4'-C1'-N1	8.90	115.32	108.20
2	A	177	G	N1-C6-O6	8.90	125.24	119.90
2	A	747	G	N1-C6-O6	8.90	125.24	119.90
2	A	1059	C	O4'-C1'-N1	8.90	115.32	108.20
2	A	1856	G	N1-C6-O6	8.90	125.24	119.90
2	A	320	G	C5-C6-O6	-8.89	123.26	128.60
2	A	1789	G	N1-C6-O6	8.89	125.24	119.90
2	A	1512	G	N1-C6-O6	8.89	125.24	119.90
2	A	683	G	N1-C6-O6	8.89	125.23	119.90
2	A	1594	U	O4'-C1'-N1	8.89	115.31	108.20
2	A	1093	G	N1-C6-O6	8.88	125.23	119.90
2	A	1137	G	C5-C6-O6	-8.87	123.28	128.60
2	A	1593	G	N1-C6-O6	8.87	125.22	119.90
2	A	667	G	N1-C6-O6	8.87	125.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1852	G	N1-C6-O6	8.87	125.22	119.90
2	A	582	C	C2-N1-C1'	8.87	128.55	118.80
2	A	1266	G	N1-C6-O6	8.87	125.22	119.90
2	A	1718	G	N1-C6-O6	8.87	125.22	119.90
2	A	422	G	N1-C6-O6	8.86	125.22	119.90
2	A	440	C	O4'-C1'-N1	8.86	115.29	108.20
2	A	815	G	N1-C6-O6	8.86	125.22	119.90
2	A	1757	G	N1-C6-O6	8.86	125.22	119.90
2	A	1113	C	O4'-C1'-N1	8.86	115.28	108.20
2	A	1055	G	N1-C6-O6	8.85	125.21	119.90
2	A	126	G	N1-C6-O6	8.85	125.21	119.90
2	A	1165	G	N1-C6-O6	8.85	125.21	119.90
2	A	90	G	N1-C6-O6	8.84	125.21	119.90
2	A	1742	C	O4'-C1'-N1	8.84	115.28	108.20
2	A	56	G	N1-C6-O6	8.84	125.20	119.90
2	A	1223	G	N1-C6-O6	8.84	125.20	119.90
2	A	409	G	C5-C6-O6	-8.83	123.30	128.60
2	A	427	G	N1-C6-O6	8.83	125.20	119.90
3	F	5	G	N1-C6-O6	8.83	125.20	119.90
2	A	71	G	N1-C6-O6	8.83	125.20	119.90
2	A	1427	G	N1-C6-O6	8.83	125.20	119.90
2	A	1731	G	N1-C6-O6	8.82	125.19	119.90
2	A	1773	G	N1-C6-O6	8.82	125.19	119.90
2	A	1477	G	N1-C6-O6	8.82	125.19	119.90
2	A	636	G	N1-C6-O6	8.82	125.19	119.90
2	A	1040	G	N1-C6-O6	8.81	125.19	119.90
2	A	274	G	C5-C6-O6	-8.81	123.32	128.60
2	A	1104	G	N1-C6-O6	8.80	125.18	119.90
2	A	1768	C	O4'-C1'-N1	8.80	115.24	108.20
1	N	9	G	N1-C6-O6	8.80	125.18	119.90
2	A	4	C	O4'-C1'-N1	8.79	115.23	108.20
2	A	165	G	O4'-C1'-N9	8.79	115.24	108.20
2	A	1227	C	O4'-C1'-N1	8.79	115.23	108.20
2	A	503	G	N1-C6-O6	8.79	125.17	119.90
2	A	582	C	O4'-C1'-N1	8.79	115.23	108.20
3	F	32	G	N1-C6-O6	8.79	125.17	119.90
2	A	1631	G	N1-C6-O6	8.79	125.17	119.90
2	A	1751	G	N1-C6-O6	8.79	125.17	119.90
3	F	14	G	N1-C6-O6	8.78	125.17	119.90
1	N	5	G	C5-C6-O6	-8.78	123.33	128.60
2	A	789	G	N1-C6-O6	8.78	125.17	119.90
2	A	1138	G	N1-C6-O6	8.78	125.17	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	156	G	C5-C6-O6	-8.78	123.33	128.60
2	A	649	G	N1-C6-O6	8.78	125.17	119.90
2	A	734	C	O4'-C1'-N1	8.77	115.22	108.20
2	A	1619	U	O4'-C1'-N1	8.77	115.22	108.20
2	A	1251	G	N1-C6-O6	8.77	125.16	119.90
2	A	1600	G	N1-C6-O6	8.77	125.16	119.90
2	A	1781	G	N1-C6-O6	8.77	125.16	119.90
2	A	898	G	N1-C6-O6	8.76	125.16	119.90
2	A	919	G	N1-C6-O6	8.76	125.16	119.90
2	A	1793	G	N1-C6-O6	8.76	125.16	119.90
2	A	1496	G	C5-C6-O6	-8.76	123.34	128.60
2	A	387	G	N1-C6-O6	8.76	125.15	119.90
2	A	948	G	N1-C6-O6	8.76	125.15	119.90
2	A	1471	G	N1-C6-O6	8.76	125.16	119.90
2	A	834	G	N1-C6-O6	8.76	125.15	119.90
2	A	385	G	N1-C6-O6	8.75	125.15	119.90
2	A	1099	C	O4'-C1'-N1	8.75	115.20	108.20
2	A	1082	G	N1-C6-O6	8.75	125.15	119.90
2	A	1409	G	N1-C6-O6	8.75	125.15	119.90
2	A	1175	G	N1-C6-O6	8.75	125.15	119.90
2	A	180	G	N1-C6-O6	8.74	125.15	119.90
2	A	932	G	N1-C6-O6	8.74	125.14	119.90
2	A	113	G	N1-C6-O6	8.74	125.14	119.90
2	A	1627	G	N1-C6-O6	8.74	125.14	119.90
2	A	1633	G	N1-C6-O6	8.74	125.14	119.90
1	N	69	G	N1-C6-O6	8.74	125.14	119.90
2	A	943	G	N1-C6-O6	8.74	125.14	119.90
2	A	750	G	N1-C6-O6	8.74	125.14	119.90
2	A	880	C	O4'-C1'-N1	8.73	115.19	108.20
2	A	1203	G	N1-C6-O6	8.73	125.14	119.90
2	A	1357	G	N1-C6-O6	8.73	125.14	119.90
2	A	1837	G	N1-C6-O6	8.73	125.14	119.90
2	A	1320	G	N1-C6-O6	8.73	125.14	119.90
2	A	1095	G	N1-C6-O6	8.73	125.14	119.90
2	A	1469	G	N1-C6-O6	8.73	125.14	119.90
2	A	373	G	N1-C6-O6	8.72	125.14	119.90
2	A	505	G	N1-C6-O6	8.72	125.13	119.90
2	A	1407	G	N1-C6-O6	8.72	125.13	119.90
2	A	74	G	N1-C6-O6	8.72	125.13	119.90
2	A	270	G	N1-C6-O6	8.72	125.13	119.90
2	A	1390	G	N1-C6-O6	8.72	125.13	119.90
2	A	1670	A	O4'-C1'-N9	8.72	115.18	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1827	C	O4'-C1'-N1	8.72	115.18	108.20
2	A	1199	G	N1-C6-O6	8.72	125.13	119.90
2	A	122	G	N1-C6-O6	8.72	125.13	119.90
2	A	863	G	N1-C6-O6	8.71	125.13	119.90
2	A	832	G	N1-C6-O6	8.71	125.13	119.90
2	A	954	G	N1-C6-O6	8.71	125.13	119.90
2	A	794	G	N1-C6-O6	8.71	125.13	119.90
2	A	1571	G	N1-C6-O6	8.71	125.13	119.90
2	A	1721	G	N1-C6-O6	8.71	125.13	119.90
2	A	1729	G	N1-C6-O6	8.71	125.12	119.90
1	N	44	G	N1-C6-O6	8.71	125.12	119.90
2	A	870	G	N1-C6-O6	8.71	125.12	119.90
2	A	905	G	N1-C6-O6	8.71	125.12	119.90
2	A	41	G	N1-C6-O6	8.70	125.12	119.90
2	A	655	G	N1-C6-O6	8.70	125.12	119.90
2	A	578	G	C5-C6-O6	-8.70	123.38	128.60
2	A	1226	C	O4'-C1'-N1	8.70	115.16	108.20
2	A	1595	G	N1-C6-O6	8.70	125.12	119.90
2	A	1738	G	N1-C6-O6	8.70	125.12	119.90
2	A	1749	C	O4'-C1'-N1	8.70	115.16	108.20
2	A	610	G	N1-C6-O6	8.69	125.12	119.90
2	A	813	G	N1-C6-O6	8.69	125.12	119.90
2	A	1308	G	N1-C6-O6	8.69	125.12	119.90
2	A	841	G	N1-C6-O6	8.69	125.11	119.90
2	A	421	G	C5-C6-O6	-8.69	123.39	128.60
2	A	592	G	N1-C6-O6	8.69	125.11	119.90
2	A	1446	G	N1-C6-O6	8.69	125.11	119.90
2	A	775	G	N1-C6-O6	8.69	125.11	119.90
2	A	359	C	O4'-C1'-N1	8.68	115.15	108.20
2	A	670	G	N1-C6-O6	8.68	125.11	119.90
2	A	1209	C	O4'-C1'-N1	8.68	115.14	108.20
2	A	837	G	O4'-C1'-N9	8.67	115.14	108.20
2	A	906	G	C5-C6-O6	-8.67	123.40	128.60
2	A	222	G	N1-C6-O6	8.67	125.10	119.90
2	A	1562	G	N1-C6-O6	8.67	125.10	119.90
2	A	784	G	C5-C6-O6	-8.67	123.40	128.60
2	A	1377	G	N1-C6-O6	8.67	125.10	119.90
2	A	1704	G	N1-C6-O6	8.67	125.10	119.90
2	A	471	C	O4'-C1'-N1	8.66	115.13	108.20
2	A	242	G	N1-C6-O6	8.66	125.10	119.90
2	A	1088	G	N1-C6-O6	8.66	125.10	119.90
2	A	1159	C	O4'-C1'-N1	8.66	115.13	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	864	G	N1-C6-O6	8.66	125.10	119.90
2	A	760	U	O4'-C1'-N1	8.66	115.13	108.20
2	A	268	G	N1-C6-O6	8.65	125.09	119.90
2	A	360	G	C5-C6-O6	-8.65	123.41	128.60
2	A	178	C	O4'-C1'-N1	8.65	115.12	108.20
2	A	1106	G	C5-C6-O6	-8.65	123.41	128.60
2	A	1053	C	C2-N1-C1'	8.65	128.31	118.80
2	A	1426	C	O4'-C1'-N1	8.65	115.12	108.20
2	A	673	G	N1-C6-O6	8.64	125.09	119.90
2	A	415	G	N1-C6-O6	8.64	125.08	119.90
2	A	500	G	N1-C6-O6	8.64	125.08	119.90
1	N	39	C	O4'-C1'-N1	8.64	115.11	108.20
2	A	1513	C	O4'-C1'-N1	8.64	115.11	108.20
2	A	108	G	N1-C6-O6	8.63	125.08	119.90
2	A	1743	G	N1-C6-O6	8.63	125.08	119.90
2	A	1699	C	O4'-C1'-N1	8.63	115.10	108.20
2	A	337	G	N1-C6-O6	8.63	125.08	119.90
2	A	887	G	N1-C6-O6	8.63	125.08	119.90
2	A	153	G	N1-C6-O6	8.62	125.07	119.90
2	A	470	G	N1-C6-O6	8.62	125.07	119.90
2	A	537	G	N1-C6-O6	8.62	125.07	119.90
2	A	903	G	N1-C6-O6	8.62	125.07	119.90
2	A	948	G	O4'-C1'-N9	8.62	115.09	108.20
2	A	1318	G	N1-C6-O6	8.62	125.07	119.90
2	A	1103	G	N1-C6-O6	8.62	125.07	119.90
2	A	1808	G	N1-C6-O6	8.62	125.07	119.90
2	A	1418	G	C5-C6-O6	-8.61	123.43	128.60
2	A	616	G	N1-C6-O6	8.61	125.07	119.90
2	A	1282	G	N1-C6-O6	8.61	125.07	119.90
2	A	1713	G	N1-C6-O6	8.61	125.06	119.90
2	A	82	G	N1-C6-O6	8.60	125.06	119.90
2	A	579	G	N1-C6-O6	8.60	125.06	119.90
2	A	462	C	O4'-C1'-N1	8.60	115.08	108.20
2	A	1601	G	N1-C6-O6	8.60	125.06	119.90
2	A	319	G	C5-C6-O6	-8.60	123.44	128.60
2	A	424	G	C5-C6-O6	-8.60	123.44	128.60
2	A	1424	G	N1-C6-O6	8.60	125.06	119.90
2	A	1134	C	O4'-C1'-N1	8.60	115.08	108.20
2	A	1503	G	N1-C6-O6	8.60	125.06	119.90
2	A	924	G	N1-C6-O6	8.59	125.06	119.90
2	A	1457	G	N1-C6-O6	8.59	125.06	119.90
2	A	1389	G	N1-C6-O6	8.59	125.05	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1548	C	P-O3'-C3'	8.59	130.01	119.70
2	A	372	C	O4'-C1'-N1	8.59	115.07	108.20
2	A	590	G	N1-C6-O6	8.59	125.05	119.90
2	A	966	G	N1-C6-O6	8.59	125.05	119.90
2	A	1621	C	O4'-C1'-N1	8.58	115.07	108.20
2	A	1286	G	N1-C6-O6	8.58	125.05	119.90
2	A	869	G	C5-C6-O6	-8.58	123.45	128.60
2	A	237	G	N1-C6-O6	8.57	125.05	119.90
2	A	1783	G	N1-C6-O6	8.57	125.04	119.90
3	F	31	G	N1-C6-O6	8.57	125.05	119.90
2	A	1039	G	N1-C6-O6	8.57	125.04	119.90
2	A	1599	G	N1-C6-O6	8.57	125.04	119.90
2	A	669	A	N1-C6-N6	8.57	123.74	118.60
2	A	1739	G	N1-C6-O6	8.57	125.04	119.90
2	A	1405	A	P-O5'-C5'	8.56	134.60	120.90
2	A	782	G	N1-C6-O6	8.55	125.03	119.90
2	A	1830	G	N1-C6-O6	8.55	125.03	119.90
2	A	754	C	O4'-C1'-N1	8.55	115.04	108.20
2	A	16	G	N1-C6-O6	8.55	125.03	119.90
1	N	40	C	O4'-C1'-N1	8.55	115.04	108.20
2	A	183	G	N1-C6-O6	8.54	125.03	119.90
2	A	364	G	N1-C6-O6	8.55	125.03	119.90
2	A	1045	A	O4'-C1'-N9	8.54	115.03	108.20
2	A	824	G	N1-C6-O6	8.54	125.02	119.90
2	A	410	G	N1-C6-O6	8.53	125.02	119.90
2	A	1297	A	O4'-C1'-N9	8.53	115.03	108.20
2	A	1445	G	N1-C6-O6	8.53	125.02	119.90
2	A	987	G	N1-C6-O6	8.53	125.02	119.90
2	A	1253	G	N1-C6-O6	8.53	125.02	119.90
2	A	1676	U	O4'-C1'-N1	8.53	115.02	108.20
2	A	783	G	C5-C6-O6	-8.53	123.48	128.60
3	F	22	G	N1-C6-O6	8.53	125.02	119.90
2	A	966	G	P-O3'-C3'	8.52	129.93	119.70
2	A	94	G	N1-C6-O6	8.52	125.01	119.90
2	A	1258	C	O4'-C1'-N1	8.52	115.02	108.20
2	A	1553	C	O4'-C1'-N1	8.52	115.01	108.20
2	A	600	G	N1-C6-O6	8.52	125.01	119.90
2	A	749	C	O4'-C1'-N1	8.51	115.01	108.20
2	A	928	G	N1-C6-O6	8.51	125.01	119.90
2	A	939	U	O4'-C1'-N1	8.51	115.01	108.20
2	A	1414	C	O4'-C1'-N1	8.51	115.01	108.20
2	A	1716	U	O4'-C1'-N1	8.51	115.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	C	O4'-C1'-N1	8.50	115.00	108.20
2	A	323	G	N1-C6-O6	8.50	125.00	119.90
2	A	1167	G	N1-C6-O6	8.50	125.00	119.90
2	A	328	G	N1-C6-O6	8.50	125.00	119.90
2	A	792	G	N1-C6-O6	8.50	125.00	119.90
2	A	881	U	O4'-C1'-N1	8.49	115.00	108.20
2	A	280	G	N1-C6-O6	8.49	125.00	119.90
2	A	467	G	N1-C6-O6	8.49	125.00	119.90
2	A	517	C	O4'-C1'-N1	8.49	115.00	108.20
2	A	687	G	N1-C6-O6	8.49	125.00	119.90
2	A	225	C	O4'-C1'-N1	8.49	114.99	108.20
2	A	310	G	N1-C6-O6	8.49	124.99	119.90
2	A	1486	G	C5-C6-O6	-8.49	123.51	128.60
2	A	1754	G	N1-C6-O6	8.49	124.99	119.90
2	A	1447	G	N1-C6-O6	8.49	124.99	119.90
2	A	674	G	N1-C6-O6	8.48	124.99	119.90
2	A	436	G	N1-C6-O6	8.48	124.99	119.90
2	A	1317	G	N1-C6-O6	8.48	124.99	119.90
2	A	533	C	O4'-C1'-N1	8.47	114.98	108.20
2	A	472	G	N1-C6-O6	8.47	124.98	119.90
2	A	199	G	N1-C6-O6	8.47	124.98	119.90
2	A	545	A	P-O3'-C3'	8.47	129.86	119.70
2	A	1462	G	N1-C6-O6	8.47	124.98	119.90
2	A	1222	G	N1-C6-O6	8.46	124.98	119.90
1	N	25	G	C5-C6-O6	-8.46	123.52	128.60
2	A	875	C	O4'-C1'-N1	8.46	114.97	108.20
2	A	597	U	O4'-C1'-N1	8.46	114.97	108.20
2	A	626	C	O4'-C1'-N1	8.46	114.97	108.20
2	A	420	C	O4'-C1'-N1	8.45	114.96	108.20
2	A	625	G	C5-C6-O6	-8.45	123.53	128.60
2	A	1151	U	O4'-C1'-N1	8.45	114.96	108.20
2	A	1071	C	O4'-C1'-N1	8.45	114.96	108.20
2	A	926	C	O4'-C1'-N1	8.45	114.96	108.20
2	A	1666	G	N1-C6-O6	8.44	124.97	119.90
2	A	299	G	N1-C6-O6	8.44	124.97	119.90
2	A	848	G	N1-C6-O6	8.44	124.97	119.90
2	A	1092	G	N1-C6-O6	8.44	124.97	119.90
1	N	10	G	C5-C6-O6	-8.44	123.54	128.60
2	A	397	G	N1-C6-O6	8.44	124.96	119.90
2	A	487	C	O4'-C1'-N1	8.44	114.95	108.20
2	A	1778	G	N1-C6-O6	8.43	124.96	119.90
2	A	1531	G	N1-C6-O6	8.43	124.96	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	33	G	N1-C6-O6	8.43	124.95	119.90
2	A	1064	G	N1-C6-O6	8.43	124.96	119.90
2	A	481	C	O4'-C1'-N1	8.42	114.93	108.20
2	A	862	U	O4'-C1'-N1	8.42	114.94	108.20
2	A	1352	G	N1-C6-O6	8.42	124.95	119.90
2	A	1669	G	C5-C6-O6	-8.42	123.55	128.60
2	A	982	G	N1-C6-O6	8.41	124.95	119.90
2	A	1566	G	C5-C6-O6	-8.41	123.55	128.60
2	A	1615	A	O4'-C1'-N9	8.41	114.93	108.20
2	A	1310	U	O4'-C1'-N1	8.41	114.93	108.20
2	A	226	A	N1-C6-N6	8.41	123.64	118.60
2	A	1323	G	C5-C6-O6	-8.41	123.56	128.60
2	A	1585	C	O4'-C1'-N1	8.41	114.92	108.20
2	A	1770	G	C5-C6-O6	-8.40	123.56	128.60
2	A	1350	G	N1-C6-O6	8.40	124.94	119.90
2	A	1843	G	N1-C6-O6	8.40	124.94	119.90
2	A	72	C	P-O3'-C3'	8.40	129.78	119.70
2	A	332	C	O4'-C1'-N1	8.39	114.92	108.20
2	A	1028	C	O4'-C1'-N1	8.39	114.92	108.20
2	A	1516	C	O4'-C1'-N1	8.39	114.91	108.20
2	A	1063	C	O4'-C1'-N1	8.39	114.91	108.20
2	A	615	G	N1-C6-O6	8.38	124.93	119.90
2	A	1547	G	N1-C6-O6	8.38	124.93	119.90
2	A	1101	G	N1-C6-O6	8.38	124.93	119.90
2	A	343	C	O4'-C1'-N1	8.38	114.90	108.20
2	A	1033	G	C5-C6-O6	-8.38	123.57	128.60
2	A	300	G	C5-C6-O6	-8.38	123.58	128.60
2	A	414	C	O4'-C1'-N1	8.37	114.90	108.20
2	A	1472	A	O4'-C1'-N9	8.38	114.90	108.20
2	A	1105	C	O4'-C1'-N1	8.37	114.89	108.20
2	A	282	G	N1-C6-O6	8.37	124.92	119.90
2	A	1371	G	C5-C6-O6	-8.36	123.58	128.60
2	A	1265	G	N1-C6-O6	8.36	124.91	119.90
2	A	327	C	O4'-C1'-N1	8.36	114.88	108.20
2	A	455	A	P-O3'-C3'	8.36	129.73	119.70
2	A	169	U	P-O3'-C3'	8.35	129.72	119.70
2	A	1158	C	O4'-C1'-N1	8.35	114.88	108.20
2	A	1508	C	O4'-C1'-N1	8.35	114.88	108.20
2	A	325	G	O4'-C1'-N9	8.35	114.88	108.20
3	F	16	G	N1-C6-O6	8.35	124.91	119.90
2	A	469	C	O4'-C1'-N1	8.34	114.88	108.20
2	A	548	G	N1-C6-O6	8.34	124.91	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	189	G	N1-C6-O6	8.34	124.90	119.90
2	A	368	U	O4'-C1'-N1	8.34	114.87	108.20
2	A	492	C	O4'-C1'-N1	8.33	114.86	108.20
2	A	191	C	O4'-C1'-N1	8.33	114.86	108.20
2	A	539	C	O4'-C1'-N1	8.33	114.86	108.20
2	A	30	C	O4'-C1'-N1	8.32	114.85	108.20
2	A	201	G	C5-C6-O6	-8.32	123.61	128.60
2	A	489	G	N1-C6-O6	8.32	124.89	119.90
2	A	205	G	N1-C6-O6	8.31	124.89	119.90
2	A	1411	C	O4'-C1'-N1	8.31	114.85	108.20
2	A	1620	U	O4'-C1'-N1	8.31	114.85	108.20
2	A	1493	G	N1-C6-O6	8.31	124.89	119.90
2	A	1467	C	O4'-C1'-N1	8.31	114.85	108.20
2	A	1774	G	O4'-C1'-N9	8.31	114.85	108.20
2	A	1097	U	O4'-C1'-N1	8.31	114.85	108.20
2	A	628	C	O4'-C1'-N1	8.30	114.84	108.20
2	A	1041	U	O4'-C1'-N1	8.30	114.84	108.20
2	A	1241	G	C5-C6-O6	-8.30	123.62	128.60
2	A	1563	C	O4'-C1'-N1	8.30	114.84	108.20
2	A	1634	G	N1-C6-O6	8.30	124.88	119.90
2	A	1143	C	O4'-C1'-N1	8.29	114.83	108.20
2	A	1725	U	O4'-C1'-N1	8.29	114.83	108.20
2	A	1130	G	N1-C6-O6	8.28	124.87	119.90
2	A	1643	G	N1-C6-O6	8.28	124.87	119.90
2	A	991	G	N1-C6-O6	8.27	124.86	119.90
2	A	499	G	N1-C6-O6	8.27	124.86	119.90
2	A	303	G	N1-C6-O6	8.27	124.86	119.90
2	A	1592	C	O4'-C1'-N1	8.27	114.81	108.20
2	A	486	C	O4'-C1'-N1	8.26	114.81	108.20
2	A	911	G	O4'-C1'-N9	8.26	114.81	108.20
2	A	167	G	C5-C6-O6	-8.26	123.64	128.60
2	A	921	G	N1-C6-O6	8.26	124.86	119.90
2	A	1458	U	O4'-C1'-N1	8.26	114.81	108.20
2	A	1561	G	C5-C6-O6	-8.26	123.65	128.60
2	A	851	G	N1-C6-O6	8.25	124.85	119.90
2	A	555	G	C5-C6-O6	-8.24	123.65	128.60
2	A	933	C	O4'-C1'-N1	8.24	114.80	108.20
2	A	1022	C	O4'-C1'-N1	8.24	114.80	108.20
2	A	1214	C	O4'-C1'-N1	8.24	114.79	108.20
2	A	1570	G	C5-C6-O6	-8.23	123.66	128.60
2	A	1681	G	N1-C6-O6	8.22	124.83	119.90
2	A	884	U	P-O5'-C5'	8.22	134.05	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	212	G	C5-C6-O6	-8.22	123.67	128.60
2	A	1679	C	O4'-C1'-N1	8.21	114.77	108.20
2	A	496	G	N1-C6-O6	8.21	124.83	119.90
2	A	620	U	O4'-C1'-N1	8.21	114.77	108.20
2	A	182	C	O4'-C1'-N1	8.21	114.77	108.20
2	A	927	C	O4'-C1'-N1	8.21	114.77	108.20
2	A	1354	U	O4'-C1'-N1	8.21	114.77	108.20
2	A	155	G	N1-C6-O6	8.20	124.82	119.90
2	A	1208	G	C5-C6-O6	-8.20	123.68	128.60
2	A	1543	G	N1-C6-O6	8.20	124.82	119.90
2	A	524	G	N1-C6-O6	8.20	124.82	119.90
2	A	1559	C	O4'-C1'-N1	8.19	114.75	108.20
2	A	1326	G	N1-C6-O6	8.19	124.81	119.90
2	A	1689	U	O4'-C1'-N1	8.19	114.75	108.20
2	A	69	C	O4'-C1'-N1	8.19	114.75	108.20
2	A	785	G	C5-C6-O6	-8.19	123.69	128.60
2	A	1043	C	O4'-C1'-N1	8.19	114.75	108.20
2	A	1061	G	C5-C6-O6	-8.19	123.69	128.60
2	A	1370	C	O4'-C1'-N1	8.19	114.75	108.20
2	A	995	G	C5-C6-O6	-8.18	123.69	128.60
2	A	1515	G	C5-C6-O6	-8.18	123.69	128.60
2	A	538	C	O4'-C1'-N1	8.17	114.74	108.20
2	A	883	U	P-O5'-C5'	8.17	133.98	120.90
2	A	1562	G	O4'-C1'-N9	8.17	114.74	108.20
2	A	844	U	O4'-C1'-N1	8.17	114.74	108.20
2	A	118	C	O4'-C1'-N1	8.17	114.73	108.20
2	A	1572	G	N1-C6-O6	8.17	124.80	119.90
2	A	294	C	O4'-C1'-N1	8.17	114.73	108.20
2	A	917	G	N1-C6-O6	8.17	124.80	119.90
1	N	29	G	O4'-C1'-N9	8.17	114.73	108.20
2	A	1403	U	O4'-C1'-N1	8.16	114.73	108.20
1	N	28	G	C5-C6-O6	-8.16	123.70	128.60
2	A	1466	C	O4'-C1'-N1	8.16	114.73	108.20
2	A	6	G	C5-C6-O6	-8.16	123.70	128.60
2	A	75	G	N1-C6-O6	8.15	124.79	119.90
2	A	186	G	C5-C6-O6	-8.15	123.71	128.60
2	A	460	G	O4'-C1'-N9	8.15	114.72	108.20
2	A	298	G	N1-C6-O6	8.15	124.79	119.90
2	A	891	G	C5-C6-O6	-8.15	123.71	128.60
2	A	1648	U	O4'-C1'-N1	8.15	114.72	108.20
1	N	2	G	C5-C6-O6	-8.14	123.71	128.60
3	F	17	C	O4'-C1'-N1	8.14	114.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	62	G	C5-C6-O6	-8.14	123.72	128.60
1	N	38	C	O4'-C1'-N1	8.14	114.71	108.20
2	A	963	C	O4'-C1'-N1	8.14	114.71	108.20
2	A	521	A	O4'-C1'-N9	8.13	114.71	108.20
2	A	601	G	C5-C6-O6	-8.13	123.72	128.60
2	A	1358	U	O4'-C1'-N1	8.13	114.70	108.20
2	A	1846	C	O4'-C1'-N1	8.13	114.70	108.20
2	A	1072	G	C5-C6-O6	-8.13	123.72	128.60
3	F	26	C	O4'-C1'-N1	8.12	114.70	108.20
2	A	1136	G	O4'-C1'-N9	8.12	114.70	108.20
2	A	868	A	P-O3'-C3'	8.12	129.44	119.70
2	A	1652	G	N1-C6-O6	8.11	124.77	119.90
2	A	981	G	C5-C6-O6	-8.11	123.73	128.60
2	A	556	U	O4'-C1'-N1	8.11	114.69	108.20
2	A	1573	U	O4'-C1'-N1	8.11	114.69	108.20
2	A	78	C	P-O3'-C3'	8.11	129.43	119.70
2	A	1568	G	C5-C6-O6	-8.11	123.74	128.60
2	A	1298	G	N1-C6-O6	8.10	124.76	119.90
2	A	1514	U	O4'-C1'-N1	8.10	114.68	108.20
2	A	1034	U	O4'-C1'-N1	8.10	114.68	108.20
2	A	1345	G	C5-C6-O6	-8.10	123.74	128.60
2	A	1578	C	O4'-C1'-N1	8.10	114.68	108.20
2	A	1741	U	O4'-C1'-N1	8.10	114.68	108.20
2	A	88	G	C5-C6-O6	-8.10	123.74	128.60
2	A	168	C	O4'-C1'-N1	8.09	114.67	108.20
2	A	1598	G	C5-C6-O6	-8.09	123.74	128.60
2	A	508	G	N1-C6-O6	8.09	124.75	119.90
2	A	876	G	O4'-C1'-N9	8.09	114.67	108.20
2	A	1586	C	O4'-C1'-N1	8.09	114.67	108.20
2	A	1708	C	O4'-C1'-N1	8.09	114.67	108.20
2	A	529	C	O4'-C1'-N1	8.08	114.67	108.20
2	A	345	G	C5-C6-O6	-8.08	123.75	128.60
2	A	1764	G	N1-C6-O6	8.08	124.75	119.90
1	N	15	G	N1-C6-O6	8.08	124.75	119.90
1	N	30	G	C5-C6-O6	-8.08	123.75	128.60
2	A	446	C	O4'-C1'-N1	8.07	114.66	108.20
2	A	1855	G	C5-C6-O6	-8.07	123.76	128.60
2	A	1102	C	O4'-C1'-N1	8.05	114.64	108.20
2	A	1823	G	C5-C6-O6	-8.05	123.77	128.60
2	A	1557	C	O4'-C1'-N1	8.05	114.64	108.20
2	A	1250	C	O4'-C1'-N1	8.05	114.64	108.20
2	A	7	G	C5-C6-O6	-8.05	123.77	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	406	U	O4'-C1'-N1	8.05	114.64	108.20
2	A	627	U	O4'-C1'-N1	8.05	114.64	108.20
2	A	879	U	O4'-C1'-N1	8.05	114.64	108.20
2	A	1074	C	O4'-C1'-N1	8.05	114.64	108.20
2	A	301	C	O4'-C1'-N1	8.04	114.64	108.20
2	A	419	C	O4'-C1'-N1	8.04	114.64	108.20
2	A	732	C	O4'-C1'-N1	8.04	114.63	108.20
3	F	16	G	O4'-C1'-N9	8.04	114.63	108.20
2	A	1804	U	O4'-C1'-N1	8.04	114.63	108.20
2	A	1491	G	O4'-C1'-N9	8.03	114.63	108.20
2	A	780	G	N1-C6-O6	8.03	124.72	119.90
2	A	897	G	C5-C6-O6	-8.03	123.78	128.60
2	A	1650	C	O4'-C1'-N1	8.03	114.62	108.20
2	A	552	U	O4'-C1'-N1	8.03	114.62	108.20
2	A	1053	C	O4'-C1'-N1	8.03	114.62	108.20
2	A	374	U	O4'-C1'-N1	8.03	114.62	108.20
2	A	989	G	C5-C6-O6	-8.02	123.79	128.60
2	A	1206	G	P-O3'-C3'	-8.02	110.08	119.70
2	A	1801	C	O4'-C1'-N1	8.02	114.61	108.20
2	A	1806	U	O4'-C1'-N1	8.02	114.61	108.20
2	A	322	G	N1-C6-O6	8.02	124.71	119.90
2	A	1661	C	O4'-C1'-N1	8.02	114.61	108.20
2	A	536	G	P-O3'-C3'	8.01	129.32	119.70
2	A	980	C	O4'-C1'-N1	8.01	114.61	108.20
2	A	1127	G	C5-C6-O6	-8.01	123.79	128.60
2	A	1197	U	O4'-C1'-N1	8.01	114.61	108.20
2	A	1198	U	O4'-C1'-N1	8.01	114.61	108.20
2	A	853	U	O4'-C1'-N1	8.01	114.61	108.20
2	A	1128	C	O4'-C1'-N1	8.01	114.61	108.20
2	A	970	C	O4'-C1'-N1	8.01	114.61	108.20
2	A	1094	C	O4'-C1'-N1	8.01	114.61	108.20
2	A	1271	G	N1-C6-O6	8.01	124.70	119.90
2	A	10	G	C5-C6-O6	-8.01	123.80	128.60
2	A	72	C	O4'-C1'-N1	8.00	114.60	108.20
2	A	591	G	C5-C6-O6	-8.00	123.80	128.60
1	N	3	C	O4'-C1'-N1	8.00	114.60	108.20
2	A	457	G	C5-C6-O6	-8.00	123.80	128.60
2	A	549	G	N1-C6-O6	8.00	124.70	119.90
2	A	271	G	C5-C6-O6	-8.00	123.80	128.60
2	A	678	U	O4'-C1'-N1	8.00	114.60	108.20
2	A	1114	C	C2-N1-C1'	8.00	127.60	118.80
2	A	1675	G	C5-C6-O6	-8.00	123.80	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1835	C	O4'-C1'-N1	7.99	114.59	108.20
2	A	664	C	O4'-C1'-N1	7.99	114.59	108.20
2	A	1217	G	C5-C6-O6	-7.99	123.81	128.60
2	A	1385	C	O4'-C1'-N1	7.99	114.59	108.20
2	A	1171	G	C5-C6-O6	-7.99	123.81	128.60
2	A	1431	C	O4'-C1'-N1	7.99	114.59	108.20
2	A	1487	G	C5-C6-O6	-7.99	123.81	128.60
2	A	1558	G	C5-C6-O6	-7.99	123.81	128.60
2	A	1440	U	O4'-C1'-N1	7.98	114.59	108.20
2	A	400	G	C5-C6-O6	-7.98	123.81	128.60
2	A	1067	G	C5-C6-O6	-7.98	123.81	128.60
2	A	375	G	C5-C6-O6	-7.97	123.82	128.60
3	F	3	C	O4'-C1'-N1	7.97	114.58	108.20
2	A	1469	G	P-O3'-C3'	7.97	129.27	119.70
2	A	1639	C	O4'-C1'-N1	7.97	114.58	108.20
2	A	1497	C	O4'-C1'-N1	7.97	114.58	108.20
1	N	57	A	N1-C6-N6	7.97	123.38	118.60
2	A	639	U	O4'-C1'-N1	7.97	114.57	108.20
2	A	1442	A	O4'-C1'-N9	7.97	114.57	108.20
2	A	1591	U	O4'-C1'-N1	7.96	114.57	108.20
2	A	961	U	O4'-C1'-N1	7.96	114.57	108.20
2	A	1597	U	O4'-C1'-N1	7.96	114.57	108.20
2	A	348	C	O4'-C1'-N1	7.96	114.56	108.20
2	A	1805	C	O4'-C1'-N1	7.96	114.56	108.20
2	A	1712	C	O4'-C1'-N1	7.95	114.56	108.20
2	A	1851	G	C5-C6-O6	-7.95	123.83	128.60
2	A	1638	U	O4'-C1'-N1	7.95	114.56	108.20
2	A	1657	U	O4'-C1'-N1	7.95	114.56	108.20
2	A	911	G	N1-C6-O6	7.94	124.67	119.90
2	A	431	C	O4'-C1'-N1	7.94	114.56	108.20
2	A	1423	C	O4'-C1'-N1	7.94	114.55	108.20
2	A	187	C	O4'-C1'-N1	7.94	114.55	108.20
2	A	1637	U	O4'-C1'-N1	7.94	114.55	108.20
2	A	1225	G	C5-C6-O6	-7.94	123.84	128.60
2	A	629	C	O4'-C1'-N1	7.93	114.55	108.20
2	A	1665	C	O4'-C1'-N1	7.93	114.55	108.20
2	A	1758	G	N1-C6-O6	7.93	124.66	119.90
2	A	1814	G	C5-C6-O6	-7.93	123.84	128.60
3	F	21	U	O4'-C1'-N1	7.93	114.54	108.20
2	A	635	C	O4'-C1'-N1	7.93	114.54	108.20
2	A	235	C	O4'-C1'-N1	7.92	114.54	108.20
2	A	558	C	O4'-C1'-N1	7.92	114.54	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1114	C	O4'-C1'-N1	7.92	114.54	108.20
2	A	941	U	O4'-C1'-N1	7.92	114.53	108.20
1	N	7	G	O4'-C1'-N9	7.92	114.53	108.20
2	A	596	G	N1-C6-O6	7.92	124.65	119.90
2	A	385	G	O4'-C1'-N9	7.92	114.53	108.20
2	A	1296	U	O4'-C1'-N1	7.92	114.53	108.20
2	A	562	U	O4'-C1'-N1	7.91	114.53	108.20
2	A	882	A	O4'-C1'-N9	7.91	114.53	108.20
2	A	1520	C	O4'-C1'-N1	7.91	114.53	108.20
2	A	952	G	C5-C6-O6	-7.91	123.85	128.60
2	A	1687	U	O4'-C1'-N1	7.91	114.52	108.20
2	A	1387	C	O4'-C1'-N1	7.90	114.52	108.20
2	A	1439	C	O4'-C1'-N1	7.90	114.52	108.20
2	A	1859	C	O4'-C1'-N1	7.90	114.52	108.20
2	A	313	C	O4'-C1'-N1	7.90	114.52	108.20
2	A	1299	C	O4'-C1'-N1	7.90	114.52	108.20
2	A	1772	C	O4'-C1'-N1	7.90	114.52	108.20
2	A	29	G	C5-C6-O6	-7.89	123.86	128.60
2	A	1728	U	O4'-C1'-N1	7.89	114.52	108.20
1	N	17	G	N1-C6-O6	7.89	124.64	119.90
2	A	1776	G	N1-C6-O6	7.89	124.63	119.90
2	A	1100	G	C5-C6-O6	-7.89	123.87	128.60
2	A	1847	C	O4'-C1'-N1	7.88	114.51	108.20
2	A	31	U	O4'-C1'-N1	7.88	114.50	108.20
2	A	1678	C	O4'-C1'-N1	7.88	114.51	108.20
2	A	1126	G	C5-C6-O6	-7.88	123.87	128.60
2	A	1655	C	C2-N1-C1'	7.88	127.47	118.80
2	A	1688	G	C5-C6-O6	-7.88	123.87	128.60
2	A	581	U	P-O3'-C3'	7.88	129.15	119.70
2	A	892	U	O4'-C1'-N1	7.88	114.50	108.20
2	A	461	G	C5-C6-O6	-7.87	123.88	128.60
2	A	468	G	O4'-C1'-N9	7.87	114.50	108.20
2	A	828	G	C5-C6-O6	-7.87	123.88	128.60
1	N	51	G	C5-C6-O6	-7.87	123.88	128.60
2	A	954	G	O4'-C1'-N9	7.87	114.49	108.20
2	A	418	U	O4'-C1'-N1	7.86	114.49	108.20
2	A	1312	C	O4'-C1'-N1	7.86	114.49	108.20
2	A	1765	G	C5-C6-O6	-7.86	123.88	128.60
2	A	227	A	C4-C5-C6	7.86	120.93	117.00
2	A	231	C	O4'-C1'-N1	7.86	114.49	108.20
2	A	1111	U	O4'-C1'-N1	7.86	114.49	108.20
2	A	1334	G	C5-C6-O6	-7.86	123.89	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	111	A	O4'-C1'-N9	7.86	114.48	108.20
2	A	393	G	C5-C6-O6	-7.86	123.89	128.60
2	A	1252	G	N1-C6-O6	7.86	124.61	119.90
2	A	1820	G	C5-C6-O6	-7.86	123.89	128.60
2	A	1050	G	C5-C6-O6	-7.85	123.89	128.60
2	A	1519	G	N1-C6-O6	7.85	124.61	119.90
2	A	1522	C	O4'-C1'-N1	7.85	114.48	108.20
2	A	761	G	N1-C6-O6	7.85	124.61	119.90
1	N	23	G	C5-C6-O6	-7.85	123.89	128.60
2	A	478	U	O4'-C1'-N1	7.85	114.48	108.20
2	A	1705	C	O4'-C1'-N1	7.85	114.48	108.20
2	A	413	U	O4'-C1'-N1	7.84	114.48	108.20
2	A	1380	C	O4'-C1'-N1	7.84	114.47	108.20
2	A	800	U	O4'-C1'-N1	7.84	114.47	108.20
2	A	1655	C	O4'-C1'-N1	7.84	114.47	108.20
2	A	507	C	O4'-C1'-N1	7.84	114.47	108.20
2	A	560	C	O4'-C1'-N1	7.84	114.47	108.20
2	A	896	C	O4'-C1'-N1	7.83	114.47	108.20
2	A	576	G	N1-C6-O6	7.83	124.60	119.90
2	A	1790	G	C5-C6-O6	-7.83	123.90	128.60
2	A	401	G	C5-C6-O6	-7.82	123.91	128.60
2	A	279	G	C5-C6-O6	-7.82	123.91	128.60
2	A	650	C	O4'-C1'-N1	7.82	114.45	108.20
2	A	1464	C	O4'-C1'-N1	7.82	114.45	108.20
2	A	1759	C	O4'-C1'-N1	7.82	114.45	108.20
2	A	1267	C	O4'-C1'-N1	7.81	114.45	108.20
2	A	452	C	O4'-C1'-N1	7.80	114.44	108.20
2	A	1518	C	O4'-C1'-N1	7.80	114.44	108.20
2	A	563	U	O4'-C1'-N1	7.80	114.44	108.20
2	A	944	C	O4'-C1'-N1	7.80	114.44	108.20
2	A	1535	G	C5-C6-O6	-7.80	123.92	128.60
2	A	1551	A	P-O3'-C3'	7.80	129.06	119.70
2	A	838	C	O4'-C1'-N1	7.79	114.44	108.20
2	A	184	G	N1-C6-O6	7.79	124.57	119.90
2	A	376	C	O4'-C1'-N1	7.79	114.43	108.20
2	A	1433	C	O4'-C1'-N1	7.79	114.43	108.20
2	A	1533	C	O4'-C1'-N1	7.79	114.43	108.20
2	A	1545	G	C5-C6-O6	-7.79	123.93	128.60
2	A	849	C	C2-N1-C1'	7.78	127.36	118.80
2	A	1395	C	O4'-C1'-N1	7.78	114.43	108.20
2	A	317	G	C5-C6-O6	-7.78	123.93	128.60
2	A	1160	G	C5-C6-O6	-7.78	123.93	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1647	G	C5-C6-O6	-7.78	123.93	128.60
2	A	1836	C	O4'-C1'-N1	7.78	114.42	108.20
1	N	61	C	O4'-C1'-N1	7.77	114.42	108.20
2	A	1605	G	C5-C6-O6	-7.77	123.94	128.60
2	A	239	U	O4'-C1'-N1	7.76	114.41	108.20
2	A	306	C	O4'-C1'-N1	7.76	114.41	108.20
1	N	60	C	O4'-C1'-N1	7.76	114.41	108.20
2	A	492	C	C2-N1-C1'	7.76	127.33	118.80
2	A	525	G	C5-C6-O6	-7.76	123.95	128.60
2	A	949	C	O4'-C1'-N1	7.76	114.41	108.20
2	A	946	C	O4'-C1'-N1	7.75	114.40	108.20
2	A	747	G	O4'-C1'-N9	7.75	114.40	108.20
2	A	1037	G	C5-C6-O6	-7.75	123.95	128.60
2	A	1587	C	O4'-C1'-N1	7.75	114.40	108.20
2	A	1840	G	C5-C6-O6	-7.75	123.95	128.60
2	A	317	G	O4'-C1'-N9	7.74	114.39	108.20
1	N	29	G	C5-C6-O6	-7.74	123.96	128.60
2	A	1125	G	C5-C6-O6	-7.74	123.96	128.60
2	A	1154	G	C5-C6-O6	-7.73	123.96	128.60
2	A	1449	C	C2-N1-C1'	7.73	127.31	118.80
2	A	1792	C	O4'-C1'-N1	7.73	114.39	108.20
2	A	200	U	O4'-C1'-N1	7.73	114.38	108.20
2	A	1062	U	O4'-C1'-N1	7.73	114.38	108.20
1	N	24	U	O4'-C1'-N1	7.73	114.38	108.20
2	A	363	G	O4'-C1'-N9	7.73	114.38	108.20
2	A	1277	G	C5-C6-O6	-7.73	123.96	128.60
2	A	1722	G	C5-C6-O6	-7.73	123.96	128.60
2	A	1744	G	C5-C6-O6	-7.73	123.96	128.60
2	A	66	G	C5-C6-O6	-7.72	123.97	128.60
2	A	665	U	O4'-C1'-N1	7.71	114.37	108.20
2	A	923	C	O4'-C1'-N1	7.71	114.36	108.20
2	A	1275	C	O4'-C1'-N1	7.71	114.37	108.20
2	A	877	G	C5-C6-O6	-7.71	123.98	128.60
2	A	207	U	O4'-C1'-N1	7.70	114.36	108.20
2	A	1703	C	O4'-C1'-N1	7.70	114.36	108.20
2	A	1085	G	C5-C6-O6	-7.70	123.98	128.60
2	A	1201	C	O4'-C1'-N1	7.70	114.36	108.20
2	A	1542	C	O4'-C1'-N1	7.70	114.36	108.20
2	A	1123	C	O4'-C1'-N1	7.69	114.35	108.20
3	F	30	A	O4'-C1'-N9	7.69	114.35	108.20
2	A	634	G	C5-C6-O6	-7.69	123.99	128.60
2	A	367	G	C5-C6-O6	-7.69	123.99	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1142	C	O4'-C1'-N1	7.68	114.35	108.20
2	A	856	G	C5-C6-O6	-7.68	123.99	128.60
2	A	582	C	C6-N1-C1'	-7.68	111.59	120.80
2	A	960	A	O4'-C1'-N9	7.67	114.34	108.20
2	A	1343	U	O4'-C1'-N1	7.67	114.34	108.20
2	A	483	A	C5-C6-N6	-7.67	117.57	123.70
2	A	1301	C	O4'-C1'-N1	7.67	114.34	108.20
2	A	1767	C	O4'-C1'-N1	7.67	114.33	108.20
1	N	35	U	O4'-C1'-N1	7.66	114.33	108.20
2	A	531	U	O4'-C1'-N1	7.66	114.33	108.20
2	A	817	G	P-O3'-C3'	7.66	128.89	119.70
2	A	1249	A	P-O3'-C3'	7.66	128.89	119.70
2	A	330	C	O4'-C1'-N1	7.66	114.33	108.20
2	A	981	G	O4'-C1'-N9	7.66	114.33	108.20
2	A	1536	G	C5-C6-O6	-7.66	124.00	128.60
2	A	392	C	O4'-C1'-N1	7.66	114.32	108.20
2	A	1245	C	O4'-C1'-N1	7.66	114.32	108.20
2	A	1233	C	O4'-C1'-N1	7.65	114.32	108.20
2	A	461	G	O4'-C1'-N9	7.65	114.32	108.20
2	A	1733	C	O4'-C1'-N1	7.65	114.32	108.20
2	A	226	A	O4'-C1'-N9	7.65	114.32	108.20
2	A	787	C	O4'-C1'-N1	7.65	114.32	108.20
2	A	1455	G	C5-C6-O6	-7.65	124.01	128.60
2	A	1538	U	O4'-C1'-N1	7.64	114.31	108.20
2	A	96	C	O4'-C1'-N1	7.64	114.31	108.20
2	A	47	G	C5-C6-O6	-7.64	124.02	128.60
2	A	820	C	O4'-C1'-N1	7.64	114.31	108.20
3	F	31	G	O4'-C1'-N9	7.64	114.31	108.20
2	A	1070	C	O4'-C1'-N1	7.63	114.31	108.20
2	A	1332	C	O4'-C1'-N1	7.63	114.31	108.20
2	A	1752	G	C5-C6-O6	-7.63	124.02	128.60
3	F	19	C	O4'-C1'-N1	7.63	114.31	108.20
2	A	1543	G	O4'-C1'-N9	7.63	114.31	108.20
2	A	220	C	O4'-C1'-N1	7.63	114.30	108.20
2	A	1452	G	C5-C6-O6	-7.63	124.02	128.60
2	A	52	G	C5-C6-O6	-7.62	124.03	128.60
2	A	453	C	O4'-C1'-N1	7.62	114.30	108.20
2	A	312	C	O4'-C1'-N1	7.62	114.30	108.20
2	A	494	G	C5-C6-O6	-7.62	124.03	128.60
2	A	1425	G	C5-C6-O6	-7.62	124.03	128.60
2	A	583	C	O4'-C1'-N1	7.62	114.30	108.20
2	A	1001	G	O4'-C1'-N9	7.62	114.29	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1524	C	O4'-C1'-N1	7.62	114.30	108.20
2	A	1622	C	O4'-C1'-N1	7.62	114.30	108.20
2	A	371	C	O4'-C1'-N1	7.62	114.29	108.20
2	A	1512	G	C5-C6-O6	-7.62	124.03	128.60
2	A	1144	A	O4'-C1'-N9	7.62	114.29	108.20
2	A	1818	A	O4'-C1'-N9	7.61	114.29	108.20
2	A	377	C	O4'-C1'-N1	7.61	114.29	108.20
1	N	65	C	O4'-C1'-N1	7.61	114.29	108.20
2	A	287	U	O4'-C1'-N1	7.61	114.29	108.20
2	A	428	G	N1-C6-O6	7.61	124.47	119.90
2	A	1315	U	O4'-C1'-N1	7.61	114.29	108.20
2	A	1331	G	C5-C6-O6	-7.61	124.03	128.60
2	A	1463	C	O4'-C1'-N1	7.61	114.28	108.20
2	A	613	G	C5-C6-O6	-7.60	124.04	128.60
2	A	1711	C	O4'-C1'-N1	7.60	114.28	108.20
2	A	1208	G	O4'-C1'-N9	7.60	114.28	108.20
3	F	9	C	O4'-C1'-N1	7.60	114.28	108.20
2	A	352	C	O4'-C1'-N1	7.60	114.28	108.20
2	A	1773	G	P-O3'-C3'	7.60	128.81	119.70
2	A	355	C	O4'-C1'-N1	7.59	114.28	108.20
2	A	1644	U	O4'-C1'-N1	7.59	114.28	108.20
2	A	349	U	O4'-C1'-N1	7.59	114.28	108.20
2	A	456	G	C5-C6-O6	-7.59	124.04	128.60
2	A	1248	C	O4'-C1'-N1	7.59	114.27	108.20
2	A	1056	A	O4'-C1'-N9	7.59	114.27	108.20
2	A	978	G	O4'-C1'-N9	7.58	114.27	108.20
2	A	1539	C	O4'-C1'-N1	7.58	114.27	108.20
2	A	1673	A	O4'-C1'-N9	7.58	114.27	108.20
2	A	308	C	O4'-C1'-N1	7.58	114.26	108.20
2	A	527	C	O4'-C1'-N1	7.58	114.26	108.20
2	A	969	C	O4'-C1'-N1	7.58	114.26	108.20
2	A	1751	G	C5-C6-O6	-7.58	124.05	128.60
2	A	1212	C	O4'-C1'-N1	7.58	114.26	108.20
2	A	1555	U	O4'-C1'-N1	7.58	114.26	108.20
2	A	584	A	P-O3'-C3'	7.57	128.79	119.70
2	A	999	U	O4'-C1'-N1	7.57	114.26	108.20
2	A	1270	G	C5-C6-O6	-7.57	124.06	128.60
2	A	230	C	O4'-C1'-N1	7.57	114.25	108.20
2	A	28	U	O4'-C1'-N1	7.57	114.25	108.20
2	A	1172	G	C5-C6-O6	-7.57	124.06	128.60
2	A	1290	G	O4'-C1'-N9	7.57	114.25	108.20
2	A	817	G	C5-C6-O6	-7.56	124.06	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	299	G	O4'-C1'-N9	7.56	114.25	108.20
2	A	1217	G	O4'-C1'-N9	7.56	114.25	108.20
2	A	1488	U	O4'-C1'-N1	7.56	114.25	108.20
2	A	1324	G	C5-C6-O6	-7.56	124.07	128.60
2	A	324	C	O4'-C1'-N1	7.55	114.24	108.20
2	A	1706	U	O4'-C1'-N1	7.55	114.24	108.20
2	A	1815	U	O4'-C1'-N1	7.55	114.24	108.20
2	A	967	G	C5-C6-O6	-7.55	124.07	128.60
2	A	637	U	O4'-C1'-N1	7.54	114.24	108.20
2	A	68	A	C5-C6-N6	-7.54	117.67	123.70
2	A	608	C	O4'-C1'-N1	7.54	114.23	108.20
2	A	684	A	O4'-C1'-N9	7.54	114.23	108.20
2	A	832	G	O4'-C1'-N9	7.54	114.23	108.20
2	A	837	G	N1-C6-O6	7.54	124.42	119.90
2	A	1009	U	O4'-C1'-N1	7.54	114.23	108.20
2	A	1202	G	C5-C6-O6	-7.54	124.08	128.60
2	A	1117	G	C5-C6-O6	-7.54	124.08	128.60
2	A	1136	G	C5-C6-O6	-7.54	124.08	128.60
1	N	13	C	O4'-C1'-N1	7.54	114.23	108.20
2	A	1523	G	C5-C6-O6	-7.54	124.08	128.60
2	A	1135	C	O4'-C1'-N1	7.53	114.23	108.20
2	A	1430	C	O4'-C1'-N1	7.53	114.23	108.20
2	A	1292	U	O4'-C1'-N1	7.53	114.22	108.20
2	A	1753	G	O4'-C1'-N9	7.53	114.22	108.20
2	A	1087	C	O4'-C1'-N1	7.52	114.22	108.20
2	A	179	C	O4'-C1'-N1	7.52	114.21	108.20
2	A	1709	U	O4'-C1'-N1	7.52	114.21	108.20
2	A	495	G	C5-C6-O6	-7.51	124.09	128.60
2	A	1416	G	C5-C6-O6	-7.51	124.09	128.60
2	A	1141	A	C5-C6-N6	-7.51	117.69	123.70
2	A	1653	G	C5-C6-O6	-7.51	124.09	128.60
2	A	1811	G	C5-C6-O6	-7.51	124.09	128.60
2	A	1492	U	O4'-C1'-N1	7.51	114.21	108.20
3	F	7	C	O4'-C1'-N1	7.51	114.21	108.20
2	A	1122	G	O4'-C1'-N9	7.50	114.20	108.20
2	A	1849	G	C5-C6-O6	-7.50	124.10	128.60
1	N	14	A	C4-C5-C6	7.50	120.75	117.00
2	A	395	G	C5-C6-O6	-7.50	124.10	128.60
2	A	378	U	O4'-C1'-N1	7.50	114.20	108.20
2	A	1294	G	C5-C6-O6	-7.49	124.10	128.60
2	A	1506	G	C5-C6-O6	-7.49	124.11	128.60
2	A	213	C	O4'-C1'-N1	7.49	114.19	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	975	C	O4'-C1'-N1	7.49	114.19	108.20
2	A	568	C	O4'-C1'-N1	7.49	114.19	108.20
2	A	1607	G	C5-C6-O6	-7.49	124.11	128.60
2	A	561	U	O4'-C1'-N1	7.48	114.19	108.20
2	A	57	U	O4'-C1'-N1	7.48	114.19	108.20
2	A	334	U	O4'-C1'-N1	7.48	114.19	108.20
2	A	1774	G	C5-C6-O6	-7.48	124.11	128.60
2	A	1362	G	C5-C6-O6	-7.48	124.11	128.60
2	A	267	G	C5-C6-O6	-7.48	124.11	128.60
2	A	1047	G	C5-C6-O6	-7.48	124.11	128.60
2	A	1607	G	O4'-C1'-N9	7.48	114.18	108.20
2	A	752	C	O4'-C1'-N1	7.47	114.18	108.20
2	A	910	U	O4'-C1'-N1	7.47	114.18	108.20
1	N	67	C	O4'-C1'-N1	7.47	114.17	108.20
2	A	1517	A	C5-C6-N6	-7.47	117.73	123.70
2	A	163	U	O4'-C1'-N1	7.47	114.17	108.20
1	N	30	G	O4'-C1'-N9	7.46	114.17	108.20
2	A	653	C	O4'-C1'-N1	7.46	114.17	108.20
2	A	1131	C	O4'-C1'-N1	7.46	114.17	108.20
2	A	235	C	N3-C4-N4	7.46	123.22	118.00
2	A	846	C	O4'-C1'-N1	7.46	114.17	108.20
2	A	357	U	O4'-C1'-N1	7.46	114.17	108.20
1	N	33	C	O4'-C1'-N1	7.46	114.17	108.20
2	A	816	U	O4'-C1'-N1	7.46	114.17	108.20
2	A	895	U	O4'-C1'-N1	7.46	114.17	108.20
2	A	1220	G	C5-C6-O6	-7.46	124.13	128.60
2	A	192	U	O4'-C1'-N1	7.46	114.16	108.20
2	A	570	U	O4'-C1'-N1	7.45	114.16	108.20
2	A	1186	A	C4-C5-C6	7.45	120.73	117.00
2	A	296	U	O4'-C1'-N1	7.45	114.16	108.20
2	A	990	C	O4'-C1'-N1	7.45	114.16	108.20
2	A	1841	G	C5-C6-O6	-7.45	124.13	128.60
2	A	359	C	C2-N1-C1'	7.44	126.99	118.80
2	A	1850	C	O4'-C1'-N1	7.44	114.16	108.20
2	A	344	U	O4'-C1'-N1	7.44	114.15	108.20
2	A	1858	U	O4'-C1'-N1	7.44	114.15	108.20
2	A	1347	G	C5-C6-O6	-7.44	124.14	128.60
2	A	1394	G	C5-C6-O6	-7.44	124.14	128.60
2	A	434	G	C5-C6-O6	-7.43	124.14	128.60
2	A	542	G	O4'-C1'-N9	7.43	114.15	108.20
2	A	893	U	O4'-C1'-N1	7.43	114.15	108.20
2	A	1409	G	O4'-C1'-N9	7.43	114.15	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1697	G	C5-C6-O6	-7.43	124.14	128.60
2	A	795	U	O4'-C1'-N1	7.43	114.14	108.20
2	A	1112	C	O4'-C1'-N1	7.43	114.15	108.20
2	A	1643	G	O4'-C1'-N9	7.43	114.14	108.20
2	A	638	A	C5-C6-N6	-7.43	117.76	123.70
2	A	1232	G	C5-C6-O6	-7.43	124.14	128.60
2	A	815	G	C5-C6-O6	-7.42	124.15	128.60
2	A	1478	C	O4'-C1'-N1	7.42	114.14	108.20
2	A	412	U	O4'-C1'-N1	7.42	114.14	108.20
2	A	447	C	O4'-C1'-N1	7.42	114.14	108.20
2	A	298	G	O4'-C1'-N9	7.42	114.14	108.20
2	A	1454	G	C5-C6-O6	-7.42	124.15	128.60
2	A	95	G	C5-C6-O6	-7.41	124.15	128.60
2	A	516	A	O4'-C1'-N9	7.41	114.13	108.20
2	A	1060	C	O4'-C1'-N1	7.41	114.13	108.20
2	A	982	G	P-O3'-C3'	7.41	128.59	119.70
2	A	1441	U	O4'-C1'-N1	7.41	114.12	108.20
2	A	857	A	O4'-C1'-N9	7.40	114.12	108.20
1	N	19	A	O4'-C1'-N9	7.40	114.12	108.20
2	A	123	G	C5-C6-O6	-7.40	124.16	128.60
2	A	873	C	O4'-C1'-N1	7.40	114.12	108.20
1	N	70	C	O4'-C1'-N1	7.40	114.12	108.20
2	A	141	A	C5-C6-N6	-7.40	117.78	123.70
2	A	468	G	C5-C6-O6	-7.40	124.16	128.60
1	N	50	U	O4'-C1'-N1	7.40	114.12	108.20
2	A	144	U	O4'-C1'-N1	7.40	114.12	108.20
2	A	380	C	O4'-C1'-N1	7.40	114.12	108.20
2	A	291	U	O4'-C1'-N1	7.39	114.11	108.20
2	A	1330	G	C5-C6-O6	-7.39	124.16	128.60
2	A	1737	C	O4'-C1'-N1	7.39	114.12	108.20
1	N	32	C	O4'-C1'-N1	7.39	114.11	108.20
2	A	37	C	O4'-C1'-N1	7.39	114.11	108.20
2	A	683	G	O4'-C1'-N9	7.39	114.11	108.20
2	A	1068	U	O4'-C1'-N1	7.39	114.11	108.20
2	A	776	U	O4'-C1'-N1	7.39	114.11	108.20
2	A	1147	G	C5-C6-O6	-7.39	124.17	128.60
2	A	381	C	O4'-C1'-N1	7.39	114.11	108.20
2	A	534	G	C5-C6-O6	-7.39	124.17	128.60
2	A	103	A	O4'-C1'-N9	7.38	114.11	108.20
2	A	758	G	C5-C6-O6	-7.38	124.17	128.60
2	A	848	G	O4'-C1'-N9	7.38	114.10	108.20
2	A	305	U	O4'-C1'-N1	7.37	114.10	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	394	G	C5-C6-O6	-7.37	124.17	128.60
2	A	148	U	O4'-C1'-N1	7.37	114.10	108.20
2	A	532	U	O4'-C1'-N1	7.37	114.10	108.20
2	A	587	G	C5-C6-O6	-7.37	124.18	128.60
1	N	42	G	C5-C6-O6	-7.37	124.18	128.60
2	A	174	C	O4'-C1'-N1	7.37	114.09	108.20
2	A	1727	G	O4'-C1'-N9	7.37	114.09	108.20
2	A	51	U	O4'-C1'-N1	7.36	114.09	108.20
2	A	1386	U	O4'-C1'-N1	7.36	114.09	108.20
2	A	1036	G	C5-C6-O6	-7.36	124.18	128.60
2	A	1161	G	C5-C6-O6	-7.36	124.18	128.60
2	A	1684	C	C6-N1-C2	-7.36	117.36	120.30
2	A	1230	C	O4'-C1'-N1	7.36	114.09	108.20
3	F	29	G	O4'-C1'-N9	7.35	114.08	108.20
2	A	646	G	C5-C6-O6	-7.35	124.19	128.60
2	A	1210	A	C5-C6-N6	-7.35	117.82	123.70
2	A	1288	C	O4'-C1'-N1	7.35	114.08	108.20
2	A	1000	U	O4'-C1'-N1	7.35	114.08	108.20
2	A	1235	U	O4'-C1'-N1	7.35	114.08	108.20
3	F	20	C	O4'-C1'-N1	7.35	114.08	108.20
2	A	289	G	C5-C6-O6	-7.35	124.19	128.60
3	F	13	G	C5-C6-O6	-7.34	124.19	128.60
2	A	1376	C	O4'-C1'-N1	7.34	114.07	108.20
2	A	1608	G	C5-C6-O6	-7.34	124.19	128.60
2	A	1168	U	O4'-C1'-N1	7.34	114.07	108.20
2	A	1748	G	C5-C6-O6	-7.34	124.20	128.60
2	A	935	U	O4'-C1'-N1	7.34	114.07	108.20
2	A	411	G	C5-C6-O6	-7.33	124.20	128.60
2	A	484	C	O4'-C1'-N1	7.33	114.07	108.20
2	A	641	U	O4'-C1'-N1	7.33	114.06	108.20
1	N	18	G	O4'-C1'-N9	7.33	114.06	108.20
2	A	70	G	C5-C6-O6	-7.33	124.20	128.60
2	A	929	G	N1-C6-O6	7.33	124.30	119.90
2	A	1701	G	C5-C6-O6	-7.33	124.20	128.60
2	A	1108	U	O4'-C1'-N1	7.33	114.06	108.20
1	N	68	U	O4'-C1'-N1	7.32	114.06	108.20
2	A	1727	G	C5-C6-O6	-7.32	124.21	128.60
1	N	12	G	C5-C6-O6	-7.32	124.21	128.60
2	A	1181	C	O4'-C1'-N1	7.32	114.06	108.20
2	A	1263	C	O4'-C1'-N1	7.32	114.06	108.20
2	A	1588	C	O4'-C1'-N1	7.32	114.06	108.20
2	A	1257	C	O4'-C1'-N1	7.32	114.06	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	973	C	O4'-C1'-N1	7.32	114.05	108.20
2	A	1086	C	O4'-C1'-N1	7.32	114.05	108.20
2	A	920	G	C5-C6-O6	-7.32	124.21	128.60
2	A	1121	C	O4'-C1'-N1	7.32	114.05	108.20
2	A	1802	U	O4'-C1'-N1	7.32	114.05	108.20
2	A	1649	G	C5-C6-O6	-7.31	124.21	128.60
2	A	1157	U	O4'-C1'-N1	7.31	114.05	108.20
2	A	1822	C	O4'-C1'-N1	7.31	114.05	108.20
2	A	1021	U	O4'-C1'-N1	7.31	114.05	108.20
2	A	840	U	O4'-C1'-N1	7.31	114.05	108.20
2	A	1244	U	O4'-C1'-N1	7.31	114.05	108.20
2	A	1582	G	C5-C6-O6	-7.31	124.22	128.60
2	A	12	U	O4'-C1'-N1	7.31	114.05	108.20
2	A	1388	U	O4'-C1'-N1	7.31	114.05	108.20
2	A	1408	C	P-O5'-C5'	7.31	132.59	120.90
1	N	45	G	N1-C6-O6	7.30	124.28	119.90
2	A	212	G	O4'-C1'-N9	7.30	114.04	108.20
2	A	520	U	P-O3'-C3'	7.30	128.46	119.70
2	A	839	C	O4'-C1'-N1	7.30	114.04	108.20
2	A	1050	G	O4'-C1'-N9	7.30	114.04	108.20
2	A	746	C	O4'-C1'-N1	7.30	114.04	108.20
2	A	1005	A	O4'-C1'-N9	7.30	114.04	108.20
2	A	1229	G	C5-C6-O6	-7.29	124.22	128.60
2	A	1651	G	C5-C6-O6	-7.29	124.22	128.60
2	A	1424	G	C5-C6-O6	-7.29	124.23	128.60
2	A	1747	C	O4'-C1'-N1	7.29	114.03	108.20
2	A	238	G	C5-C6-O6	-7.29	124.23	128.60
2	A	971	G	C5-C6-O6	-7.29	124.23	128.60
2	A	1273	C	O4'-C1'-N1	7.28	114.03	108.20
2	A	1810	G	C5-C6-O6	-7.28	124.23	128.60
2	A	1732	G	C5-C6-O6	-7.28	124.23	128.60
2	A	1053	C	C6-N1-C1'	-7.28	112.07	120.80
2	A	1348	G	O4'-C1'-N9	7.28	114.02	108.20
2	A	528	U	O4'-C1'-N1	7.27	114.02	108.20
2	A	744	C	P-O3'-C3'	7.27	128.42	119.70
2	A	1164	G	C5-C6-O6	-7.27	124.24	128.60
2	A	1667	U	O4'-C1'-N1	7.27	114.02	108.20
2	A	162	C	O4'-C1'-N1	7.27	114.01	108.20
2	A	1001	G	C5-C6-O6	-7.27	124.24	128.60
2	A	1044	G	C5-C6-O6	-7.27	124.24	128.60
2	A	1753	G	C5-C6-O6	-7.27	124.24	128.60
2	A	209	C	O4'-C1'-N1	7.26	114.01	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	602	U	O4'-C1'-N1	7.26	114.01	108.20
2	A	1613	C	O4'-C1'-N1	7.26	114.01	108.20
2	A	117	C	O4'-C1'-N1	7.26	114.01	108.20
2	A	938	G	C5-C6-O6	-7.25	124.25	128.60
2	A	1014	U	O4'-C1'-N1	7.25	114.00	108.20
2	A	668	U	O4'-C1'-N1	7.25	114.00	108.20
2	A	501	U	O4'-C1'-N1	7.25	114.00	108.20
2	A	750	G	C5-C6-O6	-7.25	124.25	128.60
2	A	1342	U	O4'-C1'-N1	7.25	114.00	108.20
2	A	130	G	C5-C6-O6	-7.24	124.26	128.60
2	A	957	G	C5-C6-O6	-7.24	124.26	128.60
2	A	1294	G	O4'-C1'-N9	7.24	113.99	108.20
1	N	27	U	O4'-C1'-N1	7.24	113.99	108.20
2	A	341	G	O4'-C1'-N9	7.24	113.99	108.20
2	A	889	U	O4'-C1'-N1	7.24	113.99	108.20
2	A	890	G	C5-C6-O6	-7.23	124.26	128.60
2	A	105	U	O4'-C1'-N1	7.23	113.99	108.20
2	A	803	G	C5-C6-O6	-7.23	124.26	128.60
2	A	1419	C	O4'-C1'-N1	7.23	113.98	108.20
2	A	1540	A	O4'-C1'-N9	7.22	113.98	108.20
2	A	1174	U	O4'-C1'-N1	7.22	113.98	108.20
3	F	29	G	C5-C6-O6	-7.22	124.27	128.60
2	A	114	G	C5-C6-O6	-7.22	124.27	128.60
2	A	1142	C	N3-C4-N4	7.22	123.05	118.00
2	A	1548	C	C2-N1-C1'	7.22	126.74	118.80
2	A	331	C	O4'-C1'-N1	7.21	113.97	108.20
2	A	925	G	C5-C6-O6	-7.21	124.27	128.60
2	A	1663	U	O4'-C1'-N1	7.21	113.97	108.20
3	F	23	A	O4'-C1'-N9	7.21	113.97	108.20
2	A	571	U	O4'-C1'-N1	7.21	113.97	108.20
2	A	1281	G	C5-C6-O6	-7.21	124.27	128.60
2	A	536	G	C5-C6-O6	-7.21	124.28	128.60
2	A	25	A	C5-C6-N1	-7.21	114.10	117.70
2	A	1044	G	O4'-C1'-N9	7.20	113.96	108.20
1	N	60	C	N3-C4-N4	7.20	123.04	118.00
2	A	449	C	O4'-C1'-N1	7.20	113.96	108.20
2	A	1443	G	C5-C6-O6	-7.20	124.28	128.60
2	A	1311	U	C2-N1-C1'	7.20	126.34	117.70
1	N	67	C	N3-C4-N4	7.20	123.04	118.00
2	A	288	A	C5-C6-N6	-7.20	117.94	123.70
2	A	1355	U	O4'-C1'-N1	7.20	113.96	108.20
2	A	876	G	N1-C6-O6	7.19	124.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1377	G	O4'-C1'-N9	7.19	113.95	108.20
2	A	1799	G	C5-C6-O6	-7.19	124.29	128.60
2	A	1015	C	O4'-C1'-N1	7.18	113.94	108.20
2	A	930	G	C5-C6-O6	-7.18	124.29	128.60
2	A	1659	A	C4-C5-C6	7.18	120.59	117.00
2	A	1702	U	O4'-C1'-N1	7.17	113.94	108.20
2	A	307	G	C5-C6-O6	-7.17	124.30	128.60
2	A	997	A	C5-C6-N6	-7.17	117.96	123.70
2	A	1035	C	O4'-C1'-N1	7.17	113.94	108.20
2	A	126	G	O4'-C1'-N9	7.17	113.94	108.20
2	A	26	U	O4'-C1'-N1	7.17	113.94	108.20
2	A	441	G	C5-C6-O6	-7.17	124.30	128.60
2	A	1793	G	C5-C6-O6	-7.17	124.30	128.60
2	A	370	G	C5-C6-O6	-7.16	124.30	128.60
2	A	428	G	O4'-C1'-N9	7.16	113.93	108.20
2	A	652	G	N1-C6-O6	7.16	124.19	119.90
2	A	1624	C	O4'-C1'-N1	7.16	113.93	108.20
2	A	1574	A	C5-C6-N6	-7.16	117.97	123.70
2	A	557	C	O4'-C1'-N1	7.16	113.92	108.20
2	A	1229	G	O4'-C1'-N9	7.16	113.92	108.20
2	A	1406	C	O4'-C1'-N1	7.16	113.92	108.20
2	A	1565	G	C5-C6-O6	-7.16	124.31	128.60
2	A	140	U	O4'-C1'-N1	7.15	113.92	108.20
2	A	146	G	C5-C6-O6	-7.15	124.31	128.60
2	A	530	U	O4'-C1'-N1	7.15	113.92	108.20
2	A	1789	G	C5-C6-O6	-7.15	124.31	128.60
2	A	744	C	C5'-C4'-C3'	7.15	127.43	116.00
2	A	341	G	C5-C6-O6	-7.14	124.31	128.60
2	A	1755	U	O4'-C1'-N1	7.14	113.92	108.20
2	A	1150	U	O4'-C1'-N1	7.14	113.91	108.20
2	A	549	G	C5-C6-O6	-7.14	124.31	128.60
2	A	20	G	C5-C6-O6	-7.14	124.32	128.60
2	A	1421	G	C5-C6-O6	-7.14	124.32	128.60
2	A	1606	G	C5-C6-O6	-7.14	124.32	128.60
2	A	1018	U	C2-N1-C1'	7.14	126.27	117.70
2	A	1187	C	O4'-C1'-N1	7.14	113.91	108.20
2	A	115	U	O4'-C1'-N1	7.13	113.91	108.20
2	A	402	G	C5-C6-O6	-7.13	124.32	128.60
2	A	426	G	C5-C6-O6	-7.13	124.32	128.60
2	A	1290	G	C5-C6-O6	-7.13	124.32	128.60
2	A	1462	G	O4'-C1'-N9	7.13	113.91	108.20
1	N	54	U	O4'-C1'-N1	7.13	113.90	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1276	G	O4'-C1'-N9	7.13	113.90	108.20
2	A	1734	C	O4'-C1'-N1	7.13	113.90	108.20
2	A	135	U	O4'-C1'-N1	7.13	113.90	108.20
2	A	569	C	O4'-C1'-N1	7.13	113.90	108.20
2	A	845	A	O4'-C1'-N9	7.12	113.90	108.20
2	A	796	U	O4'-C1'-N1	7.12	113.90	108.20
2	A	1470	A	O4'-C1'-N9	7.12	113.90	108.20
2	A	666	C	O4'-C1'-N1	7.12	113.90	108.20
2	A	97	U	O4'-C1'-N1	7.12	113.90	108.20
2	A	5	U	O4'-C1'-N1	7.12	113.89	108.20
2	A	1333	C	O4'-C1'-N1	7.12	113.89	108.20
2	A	1788	C	O4'-C1'-N1	7.12	113.89	108.20
2	A	614	C	O4'-C1'-N1	7.11	113.89	108.20
2	A	756	U	O4'-C1'-N1	7.11	113.89	108.20
2	A	194	C	O4'-C1'-N1	7.11	113.89	108.20
2	A	1443	G	O4'-C1'-N9	7.11	113.89	108.20
14	R	48	TYR	CB-CG-CD2	-7.11	116.73	121.00
1	N	9	G	C5-C6-O6	-7.11	124.33	128.60
2	A	1155	G	C5-C6-O6	-7.11	124.33	128.60
2	A	1381	G	C5-C6-O6	-7.11	124.33	128.60
2	A	1604	C	O4'-C1'-N1	7.11	113.88	108.20
2	A	23	G	C5-C6-O6	-7.10	124.34	128.60
2	A	93	U	O4'-C1'-N1	7.10	113.88	108.20
2	A	996	C	O4'-C1'-N1	7.10	113.88	108.20
2	A	1286	G	C5-C6-O6	-7.10	124.34	128.60
2	A	1200	A	C5-C6-N6	-7.10	118.02	123.70
2	A	216	U	O4'-C1'-N1	7.09	113.88	108.20
2	A	403	G	C5-C6-O6	-7.09	124.34	128.60
2	A	649	G	C5-C6-O6	-7.09	124.34	128.60
2	A	685	G	C5-C6-O6	-7.09	124.34	128.60
2	A	1196	A	O4'-C1'-N9	7.09	113.88	108.20
2	A	1341	G	C5-C6-O6	-7.09	124.34	128.60
2	A	1500	U	O4'-C1'-N1	7.09	113.88	108.20
2	A	1004	A	O4'-C1'-N9	7.09	113.88	108.20
2	A	955	G	C5-C6-O6	-7.09	124.35	128.60
2	A	1543	G	C5-C6-O6	-7.09	124.34	128.60
2	A	1841	G	O4'-C1'-N9	7.09	113.87	108.20
2	A	1383	G	C5-C6-O6	-7.09	124.35	128.60
2	A	363	G	N1-C6-O6	7.09	124.15	119.90
2	A	849	C	O4'-C1'-N1	7.09	113.87	108.20
2	A	1314	G	C5-C6-O6	-7.09	124.35	128.60
2	A	919	G	C5-C6-O6	-7.08	124.35	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	747	G	C5-C6-O6	-7.08	124.35	128.60
2	A	1207	G	C5-C6-O6	-7.08	124.35	128.60
2	A	1446	G	O4'-C1'-N9	7.08	113.87	108.20
2	A	1660	G	C5-C6-O6	-7.08	124.35	128.60
3	F	22	G	O4'-C1'-N9	7.08	113.86	108.20
2	A	1339	U	O4'-C1'-N1	7.08	113.86	108.20
2	A	663	G	C5-C6-O6	-7.08	124.35	128.60
2	A	1122	G	C5-C6-O6	-7.08	124.35	128.60
2	A	995	G	O4'-C1'-N9	7.07	113.86	108.20
2	A	1218	G	C5-C6-O6	-7.07	124.36	128.60
2	A	1325	U	O4'-C1'-N1	7.07	113.86	108.20
2	A	799	C	O4'-C1'-N1	7.07	113.86	108.20
2	A	1153	G	C5-C6-O6	-7.07	124.36	128.60
2	A	1475	G	C5-C6-O6	-7.07	124.36	128.60
1	N	17	G	O4'-C1'-N9	7.07	113.86	108.20
2	A	1042	U	O4'-C1'-N1	7.07	113.86	108.20
3	F	15	U	O4'-C1'-N1	7.07	113.85	108.20
1	N	64	C	N3-C4-N4	7.06	122.94	118.00
2	A	1567	C	O4'-C1'-N1	7.06	113.85	108.20
2	A	1615	A	P-O3'-C3'	7.06	128.18	119.70
2	A	430	G	C5-C6-O6	-7.06	124.36	128.60
2	A	504	U	O4'-C1'-N1	7.06	113.85	108.20
2	A	607	G	C5-C6-O6	-7.06	124.36	128.60
2	A	1407	G	C5-C6-O6	-7.05	124.37	128.60
2	A	1569	C	O4'-C1'-N1	7.05	113.84	108.20
2	A	1796	C	O4'-C1'-N1	7.05	113.84	108.20
2	A	480	C	O4'-C1'-N1	7.05	113.84	108.20
2	A	515	A	P-O3'-C3'	7.05	128.16	119.70
2	A	1114	C	C6-N1-C1'	-7.05	112.34	120.80
2	A	572	U	O4'-C1'-N1	7.05	113.84	108.20
2	A	1577	C	O4'-C1'-N1	7.05	113.84	108.20
2	A	399	C	O4'-C1'-N1	7.05	113.84	108.20
2	A	1610	U	O4'-C1'-N1	7.05	113.84	108.20
2	A	672	U	O4'-C1'-N1	7.05	113.84	108.20
2	A	1786	G	C5-C6-O6	-7.04	124.37	128.60
2	A	1842	U	O4'-C1'-N1	7.04	113.83	108.20
2	A	1276	G	C5-C6-O6	-7.04	124.38	128.60
2	A	1499	C	O4'-C1'-N1	7.04	113.83	108.20
2	A	364	G	O4'-C1'-N9	7.04	113.83	108.20
2	A	1115	A	O4'-C1'-N9	7.04	113.83	108.20
2	A	1769	U	O4'-C1'-N1	7.04	113.83	108.20
2	A	1834	U	O4'-C1'-N1	7.04	113.83	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	829	C	O4'-C1'-N1	7.04	113.83	108.20
2	A	891	G	O4'-C1'-N9	7.04	113.83	108.20
2	A	467	G	O4'-C1'-N9	7.04	113.83	108.20
2	A	553	G	C5-C6-O6	-7.03	124.38	128.60
2	A	749	C	O5'-C5'-C4'	7.03	125.06	111.70
2	A	1247	A	O4'-C1'-N9	7.03	113.82	108.20
2	A	1446	G	C5-C6-O6	-7.03	124.38	128.60
2	A	53	C	O4'-C1'-N1	7.03	113.82	108.20
2	A	790	A	C5-C6-N6	-7.03	118.08	123.70
2	A	1527	C	O4'-C1'-N1	7.03	113.82	108.20
2	A	937	C	O4'-C1'-N1	7.02	113.82	108.20
2	A	1603	U	O4'-C1'-N1	7.02	113.82	108.20
2	A	1521	G	C5-C6-O6	-7.02	124.39	128.60
2	A	554	A	C4-C5-C6	7.02	120.51	117.00
2	A	596	G	O4'-C1'-N9	7.02	113.81	108.20
2	A	1664	G	C5-C6-O6	-7.02	124.39	128.60
3	F	32	G	C5-C6-O6	-7.02	124.39	128.60
2	A	907	C	O4'-C1'-N1	7.02	113.81	108.20
2	A	864	G	C5-C6-O6	-7.01	124.39	128.60
2	A	1771	G	O4'-C1'-N9	7.01	113.81	108.20
2	A	1781	G	C5-C6-O6	-7.01	124.39	128.60
2	A	79	A	O4'-C1'-N9	7.01	113.81	108.20
2	A	1405	A	O4'-C1'-N9	7.01	113.81	108.20
2	A	1185	A	C4-C5-C6	7.00	120.50	117.00
2	A	1052	U	O4'-C1'-N1	7.00	113.80	108.20
2	A	788	C	O4'-C1'-N1	7.00	113.80	108.20
2	A	1560	C	O4'-C1'-N1	7.00	113.80	108.20
2	A	1283	A	C4-C5-C6	7.00	120.50	117.00
2	A	1498	C	O4'-C1'-N1	7.00	113.80	108.20
1	N	64	C	O4'-C1'-N1	7.00	113.80	108.20
2	A	1641	C	N3-C4-N4	7.00	122.90	118.00
2	A	1771	G	C5-C6-O6	-7.00	124.40	128.60
2	A	90	G	C5-C6-O6	-7.00	124.40	128.60
2	A	588	G	C5-C6-O6	-7.00	124.40	128.60
2	A	1424	G	O4'-C1'-N9	7.00	113.80	108.20
2	A	1631	G	C5-C6-O6	-7.00	124.40	128.60
2	A	1554	C	O4'-C1'-N1	6.99	113.79	108.20
2	A	1415	C	O4'-C1'-N1	6.99	113.79	108.20
2	A	945	G	C5-C6-O6	-6.98	124.41	128.60
2	A	1135	C	C2-N1-C1'	6.98	126.48	118.80
2	A	152	U	O4'-C1'-N1	6.98	113.78	108.20
2	A	522	C	N3-C4-N4	6.98	122.88	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	851	G	O4'-C1'-N9	6.98	113.78	108.20
2	A	1633	G	C5-C6-O6	-6.98	124.41	128.60
2	A	1194	G	C5-C6-O6	-6.97	124.42	128.60
2	A	1735	C	O4'-C1'-N1	6.97	113.78	108.20
2	A	236	C	O4'-C1'-N1	6.97	113.77	108.20
2	A	1724	U	O4'-C1'-N1	6.97	113.77	108.20
2	A	1798	U	O4'-C1'-N1	6.96	113.77	108.20
2	A	1148	U	O4'-C1'-N1	6.96	113.77	108.20
2	A	971	G	O4'-C1'-N9	6.96	113.77	108.20
2	A	1040	G	C5-C6-O6	-6.96	124.42	128.60
2	A	1180	G	C5-C6-O6	-6.96	124.42	128.60
2	A	387	G	C5-C6-O6	-6.96	124.42	128.60
2	A	407	C	O4'-C1'-N1	6.96	113.77	108.20
2	A	1435	A	O4'-C1'-N9	6.96	113.77	108.20
1	N	26	C	O4'-C1'-N1	6.96	113.77	108.20
1	N	56	G	C5-C6-O6	-6.96	124.43	128.60
2	A	106	C	O4'-C1'-N1	6.96	113.76	108.20
2	A	1259	U	O4'-C1'-N1	6.96	113.77	108.20
2	A	1513	C	C2-N1-C1'	6.96	126.45	118.80
2	A	1550	U	O4'-C1'-N1	6.96	113.76	108.20
2	A	124	U	O4'-C1'-N1	6.95	113.76	108.20
2	A	1357	G	C5-C6-O6	-6.95	124.43	128.60
2	A	1732	G	O4'-C1'-N9	6.95	113.76	108.20
2	A	610	G	C5-C6-O6	-6.95	124.43	128.60
2	A	1420	G	C5-C6-O6	-6.95	124.43	128.60
2	A	364	G	C5-C6-O6	-6.95	124.43	128.60
2	A	1751	G	O4'-C1'-N9	6.95	113.76	108.20
2	A	422	G	C5-C6-O6	-6.95	124.43	128.60
2	A	1451	A	C5-C6-N6	-6.95	118.14	123.70
2	A	1231	G	O4'-C1'-N9	6.95	113.76	108.20
2	A	112	U	O4'-C1'-N1	6.94	113.75	108.20
2	A	786	C	O4'-C1'-N1	6.94	113.75	108.20
2	A	890	G	O4'-C1'-N9	6.94	113.75	108.20
2	A	972	G	C5-C6-O6	-6.94	124.44	128.60
3	F	5	G	C5-C6-O6	-6.94	124.44	128.60
2	A	1011	U	O4'-C1'-N1	6.94	113.75	108.20
2	A	1284	U	O4'-C1'-N1	6.94	113.75	108.20
10	L	92	ASP	N-CA-CB	6.94	123.09	110.60
2	A	1851	G	O4'-C1'-N9	6.94	113.75	108.20
2	A	356	U	O4'-C1'-N1	6.93	113.75	108.20
2	A	1077	U	O4'-C1'-N1	6.93	113.75	108.20
1	N	11	C	N3-C4-N4	6.93	122.85	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	869	G	O4'-C1'-N9	6.93	113.74	108.20
2	A	154	U	O4'-C1'-N1	6.93	113.74	108.20
2	A	185	C	N3-C4-N4	6.93	122.85	118.00
2	A	500	G	C5-C6-O6	-6.93	124.44	128.60
2	A	936	U	O4'-C1'-N1	6.93	113.74	108.20
2	A	655	G	C5-C6-O6	-6.93	124.44	128.60
2	A	733	G	C5-C6-O6	-6.93	124.44	128.60
2	A	1093	G	C5-C6-O6	-6.92	124.44	128.60
2	A	1373	U	O4'-C1'-N1	6.92	113.74	108.20
2	A	1401	A	O4'-C1'-N9	6.92	113.74	108.20
2	A	1549	C	O4'-C1'-N1	6.92	113.74	108.20
2	A	1773	G	C5-C6-O6	-6.92	124.44	128.60
2	A	1833	U	O4'-C1'-N1	6.92	113.74	108.20
2	A	1055	G	C5-C6-O6	-6.92	124.45	128.60
2	A	83	A	C4-C5-C6	6.92	120.46	117.00
2	A	427	G	C5-C6-O6	-6.92	124.45	128.60
2	A	1579	G	C5-C6-O6	-6.92	124.45	128.60
2	A	1589	A	C4-C5-C6	6.92	120.46	117.00
2	A	842	G	C5-C6-O6	-6.92	124.45	128.60
2	A	942	U	O4'-C1'-N1	6.92	113.73	108.20
2	A	1088	G	C5-C6-O6	-6.92	124.45	128.60
2	A	1105	C	C2-N1-C1'	6.91	126.41	118.80
2	A	198	U	O4'-C1'-N1	6.91	113.73	108.20
2	A	548	G	C5-C6-O6	-6.91	124.45	128.60
2	A	1501	U	O4'-C1'-N1	6.91	113.73	108.20
2	A	1785	A	C4-C5-C6	6.91	120.46	117.00
2	A	1838	U	O4'-C1'-N1	6.91	113.73	108.20
1	N	6	A	C5-C6-N1	-6.91	114.25	117.70
2	A	1790	G	O4'-C1'-N9	6.91	113.73	108.20
2	A	1630	C	O4'-C1'-N1	6.90	113.72	108.20
2	A	415	G	C5-C6-O6	-6.90	124.46	128.60
2	A	1427	G	C5-C6-O6	-6.90	124.46	128.60
2	A	818	U	O4'-C1'-N1	6.90	113.72	108.20
2	A	1305	C	O4'-C1'-N1	6.90	113.72	108.20
2	A	1541	G	C5-C6-O6	-6.90	124.46	128.60
2	A	1627	G	C5-C6-O6	-6.90	124.46	128.60
2	A	1165	G	N3-C2-N2	6.90	124.73	119.90
2	A	1459	U	O4'-C1'-N1	6.90	113.72	108.20
2	A	396	U	O4'-C1'-N1	6.89	113.72	108.20
2	A	1003	C	O4'-C1'-N1	6.89	113.71	108.20
2	A	1413	C	O4'-C1'-N1	6.89	113.71	108.20
2	A	448	A	O4'-C1'-N9	6.89	113.71	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	59	U	O4'-C1'-N1	6.89	113.71	108.20
2	A	109	U	O4'-C1'-N1	6.89	113.71	108.20
2	A	590	G	O4'-C1'-N9	6.89	113.71	108.20
2	A	954	G	C5-C6-O6	-6.89	124.47	128.60
2	A	1723	U	O4'-C1'-N1	6.89	113.71	108.20
2	A	543	U	O4'-C1'-N1	6.88	113.71	108.20
2	A	615	G	C5-C6-O6	-6.88	124.47	128.60
2	A	1137	G	O4'-C1'-N9	6.88	113.71	108.20
2	A	1182	U	O4'-C1'-N1	6.88	113.71	108.20
2	A	126	G	C5-C6-O6	-6.88	124.47	128.60
2	A	819	U	O4'-C1'-N1	6.88	113.71	108.20
2	A	567	U	O4'-C1'-N1	6.88	113.70	108.20
2	A	545	A	O4'-C1'-N9	6.88	113.70	108.20
2	A	849	C	C6-N1-C1'	-6.88	112.55	120.80
2	A	1100	G	O4'-C1'-N9	6.88	113.70	108.20
2	A	1491	G	N1-C6-O6	6.88	124.03	119.90
2	A	270	G	C5-C6-O6	-6.88	124.47	128.60
2	A	1113	C	C2-N1-C1'	6.88	126.36	118.80
2	A	48	C	O4'-C1'-N1	6.88	113.70	108.20
2	A	1206	G	C5-C6-O6	-6.88	124.47	128.60
2	A	342	U	O4'-C1'-N1	6.87	113.70	108.20
2	A	606	A	C5-C6-N6	-6.87	118.20	123.70
2	A	868	A	O4'-C1'-N9	6.87	113.70	108.20
2	A	870	G	C5-C6-O6	-6.87	124.48	128.60
2	A	417	U	O4'-C1'-N1	6.87	113.70	108.20
2	A	323	G	O4'-C1'-N9	6.87	113.70	108.20
2	A	817	G	O4'-C1'-N9	6.87	113.70	108.20
2	A	1721	G	C5-C6-O6	-6.87	124.48	128.60
2	A	1193	G	C5-C6-O6	-6.87	124.48	128.60
2	A	604	G	C5-C6-O6	-6.87	124.48	128.60
2	A	1544	U	O4'-C1'-N1	6.87	113.69	108.20
2	A	1730	A	C5-C6-N6	-6.87	118.21	123.70
2	A	616	G	C5-C6-O6	-6.86	124.48	128.60
2	A	1335	U	O4'-C1'-N1	6.86	113.69	108.20
3	F	14	G	C5-C6-O6	-6.86	124.48	128.60
2	A	621	U	O4'-C1'-N1	6.86	113.69	108.20
2	A	18	C	O4'-C1'-N1	6.86	113.69	108.20
2	A	874	G	C5-C6-O6	-6.86	124.48	128.60
2	A	1025	G	C5-C6-O6	-6.86	124.49	128.60
2	A	94	G	C5-C6-O6	-6.86	124.49	128.60
2	A	460	G	C5-C6-O6	-6.85	124.49	128.60
2	A	827	G	O4'-C1'-N9	6.85	113.68	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1285	U	O4'-C1'-N1	6.85	113.68	108.20
2	A	899	A	O4'-C1'-N9	6.85	113.68	108.20
2	A	1240	U	O4'-C1'-N1	6.85	113.68	108.20
2	A	1811	G	O4'-C1'-N9	6.85	113.68	108.20
2	A	1162	G	C5-C6-O6	-6.85	124.49	128.60
2	A	1282	G	C5-C6-O6	-6.85	124.49	128.60
2	A	1593	G	C5-C6-O6	-6.85	124.49	128.60
1	N	65	C	N3-C4-N4	6.84	122.79	118.00
2	A	590	G	C5-C6-O6	-6.84	124.49	128.60
2	A	878	U	O4'-C1'-N1	6.84	113.67	108.20
2	A	1076	A	O4'-C1'-N9	6.84	113.68	108.20
2	A	170	A	C5-C6-N6	-6.84	118.23	123.70
2	A	325	G	C5-C6-O6	-6.84	124.50	128.60
2	A	1239	U	O4'-C1'-N1	6.84	113.67	108.20
2	A	1054	A	O4'-C1'-N9	6.83	113.67	108.20
2	A	165	G	C5-C6-O6	-6.83	124.50	128.60
2	A	310	G	O4'-C1'-N9	6.83	113.66	108.20
2	A	1175	G	C5-C6-O6	-6.83	124.50	128.60
2	A	1203	G	C5-C6-O6	-6.83	124.50	128.60
1	N	4	A	C4-C5-C6	6.83	120.41	117.00
2	A	1786	G	O4'-C1'-N9	6.83	113.66	108.20
1	N	36	A	C4-C5-C6	6.83	120.41	117.00
2	A	673	G	C5-C6-O6	-6.83	124.50	128.60
2	A	905	G	C5-C6-O6	-6.83	124.50	128.60
2	A	1207	G	C5'-C4'-O4'	6.83	117.29	109.10
2	A	1313	U	O4'-C1'-N1	6.83	113.66	108.20
2	A	145	G	C5-C6-O6	-6.82	124.51	128.60
2	A	1761	C	O4'-C1'-N1	6.82	113.66	108.20
2	A	300	G	O4'-C1'-N9	6.82	113.66	108.20
2	A	1629	A	C4-C5-C6	6.82	120.41	117.00
2	A	64	A	C5-C6-N6	-6.82	118.24	123.70
2	A	322	G	O4'-C1'-N9	6.82	113.66	108.20
2	A	837	G	C5-C6-O6	-6.82	124.51	128.60
2	A	1817	A	O4'-C1'-N9	6.82	113.66	108.20
2	A	640	A	C4-C5-C6	6.82	120.41	117.00
2	A	662	A	O4'-C1'-N9	6.82	113.65	108.20
2	A	1402	G	C5-C6-O6	-6.82	124.51	128.60
2	A	340	C	O4'-C1'-N1	6.82	113.65	108.20
2	A	835	C	C2-N1-C1'	6.82	126.30	118.80
2	A	523	A	C4-C5-C6	6.81	120.41	117.00
2	A	1757	G	C5-C6-O6	-6.81	124.51	128.60
3	F	12	U	O4'-C1'-N1	6.81	113.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	56	G	C5-C6-O6	-6.81	124.51	128.60
2	A	966	G	C5-C6-O6	-6.81	124.51	128.60
35	m	101	PHE	CB-CG-CD2	6.81	125.57	120.80
2	A	994	A	C4-C5-C6	6.81	120.41	117.00
2	A	451	U	O4'-C1'-N1	6.81	113.65	108.20
2	A	1082	G	C5-C6-O6	-6.81	124.52	128.60
3	F	27	C	O4'-C1'-N1	6.81	113.64	108.20
2	A	71	G	C5-C6-O6	-6.80	124.52	128.60
2	A	268	G	C5-C6-O6	-6.80	124.52	128.60
2	A	98	C	O4'-C1'-N1	6.80	113.64	108.20
2	A	113	G	C5-C6-O6	-6.80	124.52	128.60
2	A	190	A	C4-C5-C6	6.80	120.40	117.00
2	A	410	G	C5-C6-O6	-6.80	124.52	128.60
2	A	928	G	O4'-C1'-N9	6.80	113.64	108.20
2	A	1090	C	O4'-C1'-N1	6.80	113.64	108.20
2	A	1504	A	C4-C5-C6	6.80	120.40	117.00
2	A	751	C	N3-C4-N4	6.80	122.76	118.00
2	A	908	C	O4'-C1'-N1	6.80	113.64	108.20
2	A	622	C	O4'-C1'-N1	6.80	113.64	108.20
2	A	1316	G	C5-C6-O6	-6.79	124.52	128.60
2	A	365	U	O4'-C1'-N1	6.79	113.63	108.20
2	A	437	A	C4-C5-C6	6.79	120.39	117.00
2	A	1316	G	O4'-C1'-N9	6.79	113.63	108.20
2	A	1107	U	O4'-C1'-N1	6.79	113.63	108.20
2	A	1713	G	C5-C6-O6	-6.79	124.53	128.60
2	A	1720	U	O4'-C1'-N1	6.79	113.63	108.20
2	A	432	C	O4'-C1'-N1	6.78	113.63	108.20
2	A	537	G	C5-C6-O6	-6.78	124.53	128.60
2	A	1436	C	O4'-C1'-N1	6.78	113.63	108.20
2	A	1606	G	O4'-C1'-N9	6.78	113.63	108.20
2	A	222	G	C5-C6-O6	-6.78	124.53	128.60
1	N	73	C	O4'-C1'-N1	6.78	113.62	108.20
2	A	735	C	O4'-C1'-N1	6.78	113.62	108.20
2	A	1595	G	C5-C6-O6	-6.78	124.53	128.60
2	A	1855	G	O4'-C1'-N9	6.78	113.62	108.20
2	A	1856	G	C5-C6-O6	-6.78	124.53	128.60
3	F	8	A	O4'-C1'-N9	6.78	113.62	108.20
2	A	505	G	C5-C6-O6	-6.78	124.53	128.60
2	A	1024	A	C4-C5-C6	6.78	120.39	117.00
2	A	1562	G	C5-C6-O6	-6.78	124.53	128.60
2	A	687	G	C5-C6-O6	-6.77	124.54	128.60
2	A	813	G	C5-C6-O6	-6.77	124.54	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	204	G	C5-C6-O6	-6.77	124.54	128.60
2	A	612	C	O4'-C1'-N1	6.77	113.62	108.20
2	A	1512	G	O4'-C1'-N9	6.77	113.62	108.20
2	A	1704	G	C5-C6-O6	-6.77	124.54	128.60
2	A	522	C	O4'-C1'-N1	6.77	113.62	108.20
2	A	1344	G	C5-C6-O6	-6.77	124.54	128.60
2	A	1489	C	N3-C4-N4	6.77	122.74	118.00
2	A	1684	C	N3-C4-C5	-6.77	119.19	121.90
2	A	1718	G	C5-C6-O6	-6.77	124.54	128.60
2	A	2	A	P-O3'-C3'	6.77	127.82	119.70
2	A	1469	G	C5-C6-O6	-6.77	124.54	128.60
2	A	280	G	C5-C6-O6	-6.77	124.54	128.60
2	A	34	U	O4'-C1'-N1	6.76	113.61	108.20
2	A	35	C	N3-C4-N4	6.76	122.73	118.00
2	A	671	U	O4'-C1'-N1	6.76	113.61	108.20
2	A	674	G	C5-C6-O6	-6.76	124.54	128.60
2	A	675	A	O4'-C1'-N9	6.76	113.61	108.20
2	A	1438	U	O4'-C1'-N1	6.76	113.61	108.20
2	A	1570	G	O4'-C1'-N9	6.76	113.61	108.20
39	q	28	TYR	CB-CG-CD2	-6.76	116.94	121.00
2	A	197	U	O4'-C1'-N1	6.76	113.61	108.20
2	A	1605	G	O4'-C1'-N9	6.76	113.61	108.20
2	A	1685	U	O4'-C1'-N1	6.76	113.61	108.20
2	A	1788	C	N3-C4-N4	6.76	122.73	118.00
2	A	1589	A	C5-C6-N1	-6.75	114.32	117.70
2	A	13	C	O4'-C1'-N1	6.75	113.60	108.20
2	A	958	A	C5-C6-N6	-6.75	118.30	123.70
2	A	1006	G	O4'-C1'-N9	6.75	113.60	108.20
2	A	1163	G	C5-C6-O6	-6.75	124.55	128.60
2	A	577	A	C4-C5-C6	6.75	120.37	117.00
2	A	619	A	C5-C6-N6	-6.75	118.30	123.70
2	A	827	G	C5-C6-O6	-6.75	124.55	128.60
2	A	1177	A	O4'-C1'-N9	6.75	113.60	108.20
2	A	1770	G	O4'-C1'-N9	6.75	113.60	108.20
2	A	206	A	C4-C5-C6	6.75	120.37	117.00
2	A	362	U	O4'-C1'-N1	6.75	113.60	108.20
2	A	1655	C	C6-N1-C1'	-6.75	112.70	120.80
2	A	841	G	C5-C6-O6	-6.75	124.55	128.60
2	A	927	C	N3-C4-N4	6.74	122.72	118.00
2	A	1473	U	O4'-C1'-N1	6.74	113.59	108.20
2	A	1616	U	O4'-C1'-N1	6.74	113.59	108.20
2	A	1623	C	O4'-C1'-N1	6.74	113.59	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1215	C	O4'-C1'-N1	6.74	113.59	108.20
2	A	1738	G	C5-C6-O6	-6.74	124.56	128.60
2	A	989	G	O4'-C1'-N9	6.73	113.59	108.20
2	A	1390	G	C5-C6-O6	-6.73	124.56	128.60
2	A	503	G	O4'-C1'-N9	6.73	113.59	108.20
2	A	1101	G	O4'-C1'-N9	6.73	113.59	108.20
2	A	596	G	C5-C6-O6	-6.73	124.56	128.60
2	A	1039	G	C5-C6-O6	-6.73	124.56	128.60
2	A	81	U	O4'-C1'-N1	6.73	113.58	108.20
2	A	683	G	C5-C6-O6	-6.73	124.56	128.60
2	A	1204	A	O4'-C1'-N9	6.73	113.58	108.20
2	A	1568	G	O4'-C1'-N9	6.73	113.58	108.20
2	A	1615	A	C5'-C4'-O4'	6.73	117.17	109.10
2	A	887	G	C5-C6-O6	-6.73	124.56	128.60
2	A	631	A	O4'-C1'-N9	6.72	113.58	108.20
2	A	794	G	C5-C6-O6	-6.72	124.56	128.60
2	A	824	G	C5-C6-O6	-6.72	124.56	128.60
2	A	786	C	N3-C4-N4	6.72	122.71	118.00
2	A	1626	U	O4'-C1'-N1	6.72	113.58	108.20
2	A	1251	G	C5-C6-O6	-6.72	124.57	128.60
2	A	336	C	N3-C4-N4	6.72	122.70	118.00
2	A	791	A	C4-C5-C6	6.72	120.36	117.00
2	A	670	G	C5-C6-O6	-6.72	124.57	128.60
2	A	985	C	O4'-C1'-N1	6.72	113.57	108.20
2	A	242	G	C5-C6-O6	-6.71	124.57	128.60
2	A	463	A	C5-C6-N6	-6.71	118.33	123.70
2	A	1138	G	C5-C6-O6	-6.71	124.57	128.60
2	A	151	C	O4'-C1'-N1	6.71	113.57	108.20
2	A	180	G	C5-C6-O6	-6.71	124.57	128.60
2	A	385	G	C5-C6-O6	-6.71	124.57	128.60
2	A	915	A	C4-C5-C6	6.71	120.36	117.00
2	A	1389	G	C5-C6-O6	-6.71	124.57	128.60
2	A	748	G	C5-C6-O6	-6.71	124.57	128.60
2	A	775	G	C5-C6-O6	-6.71	124.57	128.60
2	A	1534	U	O4'-C1'-N1	6.71	113.57	108.20
2	A	903	G	C5-C6-O6	-6.71	124.58	128.60
2	A	931	G	C5-C6-O6	-6.71	124.58	128.60
2	A	1369	C	O4'-C1'-N1	6.71	113.57	108.20
2	A	1715	U	O4'-C1'-N1	6.71	113.57	108.20
2	A	1220	G	O4'-C1'-N9	6.71	113.57	108.20
2	A	1507	U	O4'-C1'-N1	6.71	113.56	108.20
2	A	153	G	C5-C6-O6	-6.71	124.58	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	623	C	O4'-C1'-N1	6.71	113.56	108.20
2	A	863	G	C5-C6-O6	-6.71	124.58	128.60
2	A	1564	A	C4-C5-C6	6.71	120.35	117.00
1	N	18	G	C5-C6-O6	-6.70	124.58	128.60
1	N	28	G	O4'-C1'-N9	6.70	113.56	108.20
2	A	524	G	C5-C6-O6	-6.70	124.58	128.60
2	A	1615	A	C4-C5-C6	6.70	120.35	117.00
2	A	1681	G	C5-C6-O6	-6.70	124.58	128.60
2	A	843	A	C5-C6-N6	-6.70	118.34	123.70
2	A	1337	C	O4'-C1'-N1	6.70	113.56	108.20
2	A	1824	U	O4'-C1'-N1	6.70	113.56	108.20
2	A	982	G	C5-C6-O6	-6.70	124.58	128.60
2	A	1346	U	O4'-C1'-N1	6.70	113.56	108.20
2	A	1752	G	O4'-C1'-N9	6.70	113.56	108.20
2	A	1472	A	C4-C5-C6	6.69	120.35	117.00
2	A	1451	A	C4-C5-C6	6.69	120.35	117.00
2	A	1645	A	C4-C5-C6	6.69	120.35	117.00
2	A	1149	C	O4'-C1'-N1	6.69	113.55	108.20
2	A	1205	A	O4'-C1'-N9	6.68	113.55	108.20
2	A	497	G	C5-C6-O6	-6.68	124.59	128.60
2	A	1700	C	O4'-C1'-N1	6.68	113.55	108.20
2	A	503	G	C5-C6-O6	-6.68	124.59	128.60
2	A	575	C	O4'-C1'-N1	6.68	113.55	108.20
2	A	1511	G	C5-C6-O6	-6.68	124.59	128.60
2	A	1541	G	O4'-C1'-N9	6.68	113.54	108.20
2	A	1808	G	C5-C6-O6	-6.68	124.59	128.60
2	A	1010	G	O4'-C1'-N9	6.68	113.54	108.20
14	R	48	TYR	CB-CG-CD1	6.68	125.01	121.00
2	A	599	U	O4'-C1'-N1	6.67	113.54	108.20
2	A	1125	G	O4'-C1'-N9	6.67	113.54	108.20
2	A	1848	U	O4'-C1'-N1	6.67	113.54	108.20
2	A	11	A	O4'-C1'-N9	6.67	113.54	108.20
2	A	913	U	O4'-C1'-N1	6.67	113.54	108.20
2	A	1189	U	O4'-C1'-N1	6.67	113.54	108.20
2	A	1652	G	O4'-C1'-N9	6.67	113.54	108.20
2	A	1172	G	O4'-C1'-N9	6.67	113.53	108.20
16	T	125	PHE	CB-CG-CD1	6.67	125.47	120.80
1	N	37	A	O4'-C1'-N9	6.67	113.53	108.20
2	A	185	C	O4'-C1'-N1	6.67	113.53	108.20
2	A	1513	C	C6-N1-C1'	-6.67	112.80	120.80
2	A	1619	U	C2-N1-C1'	6.67	125.70	117.70
2	A	346	C	O4'-C1'-N1	6.67	113.53	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	74	G	C5-C6-O6	-6.66	124.60	128.60
2	A	802	U	O4'-C1'-N1	6.66	113.53	108.20
2	A	1525	U	O4'-C1'-N1	6.66	113.53	108.20
2	A	1729	G	C5-C6-O6	-6.66	124.60	128.60
2	A	202	U	O4'-C1'-N1	6.66	113.53	108.20
2	A	592	G	C5-C6-O6	-6.66	124.60	128.60
2	A	1707	A	O4'-C1'-N9	6.66	113.53	108.20
2	A	626	C	N3-C4-N4	6.66	122.66	118.00
2	A	1777	C	O4'-C1'-N1	6.66	113.53	108.20
2	A	898	G	C5-C6-O6	-6.66	124.61	128.60
3	F	22	G	C5-C6-O6	-6.66	124.61	128.60
2	A	1634	G	C5-C6-O6	-6.65	124.61	128.60
2	A	1056	A	C4-C5-C6	6.65	120.33	117.00
2	A	1272	A	C4-C5-C6	6.65	120.33	117.00
2	A	1101	G	C5-C6-O6	-6.65	124.61	128.60
2	A	1364	U	O4'-C1'-N1	6.65	113.52	108.20
2	A	888	U	O4'-C1'-N1	6.65	113.52	108.20
2	A	1477	G	C5-C6-O6	-6.65	124.61	128.60
2	A	32	U	O4'-C1'-N1	6.64	113.52	108.20
1	N	44	G	C5-C6-O6	-6.64	124.61	128.60
2	A	328	G	C5-C6-O6	-6.64	124.61	128.60
2	A	958	A	C4-C5-C6	6.64	120.32	117.00
2	A	676	U	O4'-C1'-N1	6.64	113.51	108.20
2	A	1794	A	C4-C5-C6	6.64	120.32	117.00
2	A	1809	A	C4-C5-C6	6.64	120.32	117.00
2	A	1470	A	C4-C5-C6	6.64	120.32	117.00
2	A	217	U	O4'-C1'-N1	6.64	113.51	108.20
2	A	828	G	O4'-C1'-N9	6.64	113.51	108.20
2	A	1126	G	O4'-C1'-N9	6.64	113.51	108.20
2	A	1447	G	C5-C6-O6	-6.64	124.62	128.60
2	A	33	G	C5-C6-O6	-6.63	124.62	128.60
2	A	858	A	C4-C5-C6	6.63	120.32	117.00
2	A	1268	C	O4'-C1'-N1	6.63	113.51	108.20
2	A	1509	G	O4'-C1'-N9	6.63	113.50	108.20
2	A	1743	G	C5-C6-O6	-6.63	124.62	128.60
2	A	1471	G	C5-C6-O6	-6.63	124.62	128.60
2	A	1773	G	O4'-C1'-N9	6.63	113.50	108.20
2	A	1817	A	C4-C5-C6	6.63	120.31	117.00
2	A	848	G	C5-C6-O6	-6.63	124.62	128.60
2	A	1214	C	N3-C4-N4	6.63	122.64	118.00
2	A	1797	U	O4'-C1'-N1	6.63	113.50	108.20
2	A	1392	A	C4-C5-C6	6.62	120.31	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1809	A	C5-C6-N6	-6.62	118.40	123.70
2	A	1299	C	C2-N1-C1'	6.62	126.08	118.80
2	A	1853	A	C5-C6-N6	-6.62	118.41	123.70
2	A	1307	C	O4'-C1'-N1	6.61	113.49	108.20
2	A	1348	G	C5-C6-O6	-6.61	124.63	128.60
2	A	1120	C	O4'-C1'-N1	6.61	113.49	108.20
2	A	227	A	C5-C6-N6	-6.61	118.41	123.70
2	A	978	G	C5-C6-O6	-6.61	124.64	128.60
2	A	1066	A	C5-C6-N6	-6.61	118.41	123.70
2	A	852	C	O4'-C1'-N1	6.61	113.49	108.20
2	A	1710	A	C4-C5-C6	6.61	120.30	117.00
2	A	932	G	C5-C6-O6	-6.61	124.64	128.60
2	A	1694	A	O4'-C1'-N9	6.61	113.48	108.20
2	A	1758	G	C5-C6-O6	-6.61	124.64	128.60
2	A	622	C	N3-C4-N4	6.60	122.62	118.00
1	N	40	C	N3-C4-N4	6.60	122.62	118.00
1	N	49	A	C5-C6-N1	-6.60	114.40	117.70
2	A	89	C	O4'-C1'-N1	6.60	113.48	108.20
2	A	347	C	O4'-C1'-N1	6.60	113.48	108.20
2	A	871	A	O4'-C1'-N9	6.60	113.48	108.20
2	A	1681	G	O4'-C1'-N9	6.60	113.48	108.20
2	A	1010	G	C5-C6-O6	-6.60	124.64	128.60
1	N	20	A	C5-C6-N1	-6.60	114.40	117.70
2	A	1030	A	O4'-C1'-N9	6.60	113.48	108.20
2	A	1308	G	C5-C6-O6	-6.60	124.64	128.60
2	A	948	G	C5-C6-O6	-6.60	124.64	128.60
2	A	1039	G	O4'-C1'-N9	6.60	113.48	108.20
2	A	1409	G	C5-C6-O6	-6.60	124.64	128.60
2	A	1599	G	C5-C6-O6	-6.60	124.64	128.60
2	A	1635	A	C4-C5-C6	6.60	120.30	117.00
2	A	122	G	C5-C6-O6	-6.60	124.64	128.60
2	A	1671	U	O4'-C1'-N1	6.59	113.48	108.20
2	A	1045	A	C4-C5-C6	6.59	120.30	117.00
2	A	1529	C	O4'-C1'-N1	6.59	113.47	108.20
2	A	75	G	C5-C6-O6	-6.59	124.64	128.60
2	A	515	A	O4'-C1'-N9	6.59	113.47	108.20
2	A	859	U	O4'-C1'-N1	6.59	113.47	108.20
2	A	1652	G	C5-C6-O6	-6.59	124.64	128.60
2	A	373	G	C5-C6-O6	-6.59	124.65	128.60
2	A	1178	A	C4-C5-C6	6.59	120.30	117.00
2	A	1404	U	O4'-C1'-N1	6.59	113.47	108.20
2	A	494	G	O4'-C1'-N9	6.59	113.47	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	667	G	C5-C6-O6	-6.59	124.65	128.60
2	A	968	A	C4-C5-C6	6.58	120.29	117.00
3	F	31	G	C5-C6-O6	-6.58	124.65	128.60
2	A	303	G	C5-C6-O6	-6.58	124.65	128.60
2	A	1118	A	C4-C5-C6	6.58	120.29	117.00
2	A	1787	A	C4-C5-C6	6.58	120.29	117.00
2	A	1454	G	O4'-C1'-N9	6.58	113.47	108.20
2	A	1318	G	C5-C6-O6	-6.58	124.65	128.60
2	A	793	C	O4'-C1'-N1	6.58	113.46	108.20
2	A	962	U	O4'-C1'-N1	6.58	113.46	108.20
2	A	1789	G	O4'-C1'-N9	6.58	113.46	108.20
2	A	814	A	O4'-C1'-N9	6.58	113.46	108.20
2	A	183	G	C5-C6-O6	-6.57	124.66	128.60
2	A	871	A	C4-C5-C6	6.57	120.29	117.00
2	A	1537	C	O4'-C1'-N1	6.57	113.46	108.20
2	A	1549	C	C2-N1-C1'	6.57	126.03	118.80
2	A	1656	A	C4-C5-C6	6.57	120.29	117.00
2	A	1831	G	C5-C6-O6	-6.57	124.66	128.60
2	A	615	G	O4'-C1'-N9	6.57	113.46	108.20
2	A	1234	U	O4'-C1'-N1	6.57	113.46	108.20
1	N	8	U	O4'-C1'-N1	6.57	113.45	108.20
2	A	102	A	C4-C5-C6	6.57	120.28	117.00
2	A	836	C	P-O3'-C3'	6.57	127.58	119.70
2	A	1828	A	C4-C5-C6	6.57	120.28	117.00
2	A	472	G	C5-C6-O6	-6.57	124.66	128.60
2	A	984	C	N3-C4-N4	6.57	122.59	118.00
2	A	1420	G	O4'-C1'-N9	6.57	113.45	108.20
2	A	16	G	C5-C6-O6	-6.56	124.66	128.60
2	A	792	G	C5-C6-O6	-6.56	124.66	128.60
2	A	914	U	O4'-C1'-N1	6.56	113.45	108.20
1	N	53	A	C4-C5-C6	6.56	120.28	117.00
2	A	318	U	O4'-C1'-N1	6.56	113.45	108.20
2	A	1601	G	C5-C6-O6	-6.56	124.66	128.60
2	A	35	C	O4'-C1'-N1	6.56	113.45	108.20
2	A	1321	G	C5-C6-O6	-6.56	124.66	128.60
2	A	464	G	C5-C6-O6	-6.56	124.67	128.60
2	A	210	G	C5-C6-O6	-6.55	124.67	128.60
2	A	1314	G	O4'-C1'-N9	6.55	113.44	108.20
2	A	790	A	C4-C5-C6	6.55	120.28	117.00
2	A	1091	U	O4'-C1'-N1	6.55	113.44	108.20
2	A	1548	C	C6-N1-C1'	-6.55	112.94	120.80
2	A	470	G	C5-C6-O6	-6.55	124.67	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1095	G	C5-C6-O6	-6.55	124.67	128.60
2	A	1169	A	C5-C6-N6	-6.55	118.46	123.70
2	A	339	A	C5-C6-N6	-6.55	118.46	123.70
2	A	1684	C	N3-C4-N4	6.55	122.58	118.00
1	N	52	G	O4'-C1'-N9	6.55	113.44	108.20
2	A	502	A	C5-C6-N1	-6.55	114.43	117.70
2	A	1672	U	O4'-C1'-N1	6.55	113.44	108.20
35	m	101	PHE	CB-CG-CD1	-6.55	116.22	120.80
2	A	337	G	C5-C6-O6	-6.54	124.67	128.60
2	A	884	U	O4'-C1'-N1	6.54	113.43	108.20
2	A	1231	G	C5-C6-O6	-6.54	124.68	128.60
2	A	1590	U	O4'-C1'-N1	6.54	113.43	108.20
2	A	1600	G	C5-C6-O6	-6.54	124.67	128.60
2	A	1766	C	O4'-C1'-N1	6.54	113.43	108.20
2	A	921	G	C5-C6-O6	-6.54	124.68	128.60
2	A	1432	C	O4'-C1'-N1	6.54	113.43	108.20
2	A	1007	A	C5-C6-N6	-6.54	118.47	123.70
2	A	1670	A	C4-C5-C6	6.54	120.27	117.00
2	A	1104	G	C5-C6-O6	-6.53	124.68	128.60
2	A	1795	A	O4'-C1'-N9	6.53	113.43	108.20
2	A	1303	U	O4'-C1'-N1	6.53	113.43	108.20
2	A	1643	G	C5-C6-O6	-6.53	124.68	128.60
2	A	1803	A	O4'-C1'-N9	6.53	113.43	108.20
2	A	443	C	O4'-C1'-N1	6.53	113.42	108.20
2	A	1222	G	N3-C2-N2	6.53	124.47	119.90
2	A	1279	C	O4'-C1'-N1	6.53	113.42	108.20
2	A	1509	G	C5-C6-O6	-6.53	124.68	128.60
2	A	1448	A	C4-C5-C6	6.53	120.26	117.00
2	A	237	G	C5-C6-O6	-6.53	124.69	128.60
2	A	943	G	C5-C6-O6	-6.53	124.69	128.60
2	A	594	A	C4-C5-C6	6.52	120.26	117.00
2	A	64	A	O4'-C1'-N9	6.52	113.42	108.20
2	A	1287	A	C4-C5-C6	6.52	120.26	117.00
2	A	1680	U	O4'-C1'-N1	6.52	113.42	108.20
2	A	1691	C	O4'-C1'-N1	6.52	113.42	108.20
2	A	1213	A	C4-C5-C6	6.52	120.26	117.00
2	A	527	C	N3-C4-N4	6.52	122.56	118.00
2	A	663	G	O4'-C1'-N9	6.52	113.42	108.20
2	A	886	U	O4'-C1'-N1	6.52	113.42	108.20
2	A	1192	A	C4-C5-C6	6.52	120.26	117.00
2	A	618	A	C4-C5-C6	6.52	120.26	117.00
2	A	674	G	O4'-C1'-N9	6.52	113.41	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	834	G	C5-C6-O6	-6.52	124.69	128.60
2	A	397	G	C5-C6-O6	-6.51	124.69	128.60
2	A	516	A	C5-C6-N6	-6.51	118.49	123.70
2	A	1384	A	C4-C5-C6	6.51	120.26	117.00
2	A	636	G	C5-C6-O6	-6.51	124.69	128.60
2	A	1682	C	N3-C4-N4	6.51	122.56	118.00
2	A	1721	G	O4'-C1'-N9	6.51	113.41	108.20
1	N	15	G	O4'-C1'-N9	6.51	113.41	108.20
2	A	585	U	O4'-C1'-N1	6.51	113.41	108.20
2	A	843	A	C4-C5-C6	6.51	120.25	117.00
2	A	991	G	C5-C6-O6	-6.51	124.70	128.60
2	A	1839	A	O4'-C1'-N9	6.50	113.40	108.20
2	A	550	A	O4'-C1'-N9	6.50	113.40	108.20
2	A	1722	G	O4'-C1'-N9	6.50	113.40	108.20
2	A	399	C	N3-C4-N4	6.50	122.55	118.00
2	A	924	G	C5-C6-O6	-6.50	124.70	128.60
2	A	1826	A	C5-C6-N6	-6.50	118.50	123.70
2	A	415	G	O4'-C1'-N9	6.50	113.40	108.20
2	A	550	A	C4-C5-C6	6.50	120.25	117.00
2	A	1471	G	P-O5'-C5'	6.50	131.29	120.90
2	A	1731	G	C5-C6-O6	-6.50	124.70	128.60
2	A	1778	G	C5-C6-O6	-6.50	124.70	128.60
2	A	1863	A	C4-C5-C6	6.50	120.25	117.00
2	A	566	A	C4-C5-C6	6.49	120.25	117.00
2	A	1322	U	O4'-C1'-N1	6.49	113.39	108.20
2	A	1572	G	C5-C6-O6	-6.49	124.70	128.60
2	A	1468	C	N3-C4-C5	-6.49	119.30	121.90
2	A	611	C	N3-C4-N4	6.49	122.54	118.00
2	A	298	G	C5-C6-O6	-6.49	124.71	128.60
2	A	1515	G	O4'-C1'-N9	6.49	113.39	108.20
2	A	1859	C	C2-N1-C1'	6.49	125.94	118.80
2	A	15	U	O4'-C1'-N1	6.49	113.39	108.20
2	A	959	A	C5-C6-N1	-6.49	114.46	117.70
2	A	1678	C	N3-C4-N4	6.49	122.54	118.00
2	A	1843	G	C5-C6-O6	-6.49	124.71	128.60
2	A	100	U	O4'-C1'-N1	6.48	113.39	108.20
2	A	870	G	O4'-C1'-N9	6.48	113.39	108.20
2	A	1503	G	C5-C6-O6	-6.48	124.71	128.60
2	A	811	U	O4'-C1'-N1	6.48	113.38	108.20
2	A	1837	G	C5-C6-O6	-6.48	124.71	128.60
2	A	38	A	O4'-C1'-N9	6.48	113.38	108.20
2	A	1547	G	C5-C6-O6	-6.47	124.72	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1352	G	C5-C6-O6	-6.47	124.72	128.60
2	A	1402	G	O4'-C1'-N9	6.47	113.38	108.20
2	A	104	A	C4-C5-C6	6.47	120.23	117.00
2	A	1474	U	O4'-C1'-N1	6.47	113.38	108.20
2	A	209	C	N3-C4-N4	6.47	122.53	118.00
2	A	1360	U	C2-N1-C1'	6.47	125.46	117.70
2	A	1612	G	C5-C6-O6	-6.47	124.72	128.60
2	A	146	G	O4'-C1'-N9	6.47	113.37	108.20
2	A	677	C	O4'-C1'-N1	6.46	113.37	108.20
2	A	858	A	C5-C6-N6	-6.46	118.53	123.70
2	A	9	U	O4'-C1'-N1	6.46	113.37	108.20
2	A	945	G	O4'-C1'-N9	6.46	113.37	108.20
2	A	1049	C	O4'-C1'-N1	6.46	113.37	108.20
2	A	1677	C	O4'-C1'-N1	6.46	113.37	108.20
2	A	234	C	O4'-C1'-N1	6.46	113.37	108.20
2	A	1456	C	O4'-C1'-N1	6.46	113.37	108.20
1	N	15	G	C5-C6-O6	-6.46	124.73	128.60
1	N	57	A	C4-C5-C6	6.46	120.23	117.00
2	A	1519	G	C5-C6-O6	-6.46	124.73	128.60
2	A	1484	C	O4'-C1'-N1	6.46	113.36	108.20
2	A	1552	C	C2'-C3'-O3'	6.46	124.03	113.70
1	N	70	C	N3-C4-N4	6.45	122.52	118.00
2	A	162	C	N3-C4-N4	6.45	122.52	118.00
2	A	1020	A	C4-C5-C6	6.45	120.23	117.00
2	A	1458	U	C2-N1-C1'	6.45	125.44	117.70
2	A	538	C	N3-C4-N4	6.45	122.52	118.00
2	A	1371	G	O4'-C1'-N9	6.45	113.36	108.20
2	A	1458	U	C5'-C4'-C3'	-6.45	105.68	116.00
2	A	564	A	C4-C5-C6	6.45	120.22	117.00
2	A	1078	A	C4-C5-C6	6.45	120.22	117.00
2	A	489	G	C5-C6-O6	-6.45	124.73	128.60
2	A	14	C	O4'-C1'-N1	6.45	113.36	108.20
2	A	513	A	O4'-C1'-N9	6.44	113.36	108.20
2	A	782	G	C5-C6-O6	-6.44	124.73	128.60
2	A	780	G	C5-C6-O6	-6.44	124.73	128.60
2	A	1199	G	C5-C6-O6	-6.44	124.73	128.60
2	A	1054	A	C4-C5-C6	6.44	120.22	117.00
2	A	1233	C	N3-C4-N4	6.44	122.51	118.00
2	A	1510	G	C5-C6-O6	-6.44	124.74	128.60
2	A	1726	A	O4'-C1'-N9	6.44	113.35	108.20
2	A	86	C	N3-C4-N4	6.43	122.50	118.00
2	A	1002	C	O4'-C1'-N1	6.43	113.35	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	292	A	O4'-C1'-N9	6.43	113.35	108.20
2	A	436	G	C5-C6-O6	-6.43	124.74	128.60
2	A	1206	G	O3'-P-O5'	-6.43	91.78	104.00
2	A	916	A	P-O3'-C3'	6.43	127.42	119.70
2	A	1165	G	C5-C6-O6	-6.43	124.74	128.60
2	A	647	U	O4'-C1'-N1	6.43	113.34	108.20
2	A	908	C	N3-C4-N4	6.43	122.50	118.00
2	A	1160	G	O4'-C1'-N9	6.43	113.34	108.20
2	A	506	A	C4-C5-C6	6.42	120.21	117.00
2	A	1167	G	C5-C6-O6	-6.42	124.75	128.60
2	A	1434	A	C5-C6-N6	-6.42	118.56	123.70
2	A	107	A	C4-C5-C6	6.42	120.21	117.00
2	A	455	A	C4-C5-C6	6.42	120.21	117.00
2	A	1467	C	N3-C4-N4	6.42	122.50	118.00
2	A	1584	A	O4'-C1'-N9	6.42	113.34	108.20
2	A	1595	G	O4'-C1'-N9	6.42	113.34	108.20
2	A	193	C	O4'-C1'-N1	6.42	113.33	108.20
2	A	223	A	C4-C5-C6	6.42	120.21	117.00
2	A	524	G	O3'-P-O5'	-6.42	91.80	104.00
2	A	912	A	C4-C5-C6	6.42	120.21	117.00
2	A	496	G	C5-C6-O6	-6.42	124.75	128.60
2	A	809	A	C4-C5-C6	6.42	120.21	117.00
2	A	1414	C	N3-C4-N4	6.42	122.49	118.00
2	A	1830	G	C5-C6-O6	-6.42	124.75	128.60
2	A	807	A	C5-C6-N6	-6.42	118.57	123.70
2	A	545	A	C5-C6-N1	-6.41	114.49	117.70
2	A	959	A	C4-C5-C6	6.41	120.21	117.00
16	T	124	PHE	CB-CG-CD2	-6.41	116.31	120.80
2	A	605	C	O4'-C1'-N1	6.41	113.33	108.20
2	A	1073	A	C4-C5-C6	6.41	120.21	117.00
2	A	366	A	O4'-C1'-N9	6.41	113.33	108.20
2	A	1048	A	C5-C6-N1	-6.41	114.49	117.70
2	A	1825	A	C5-C6-N6	-6.41	118.57	123.70
2	A	477	U	P-O3'-C3'	6.41	127.39	119.70
2	A	598	C	O4'-C1'-N1	6.41	113.33	108.20
2	A	966	G	O4'-C1'-N9	6.41	113.33	108.20
2	A	987	G	C5-C6-O6	-6.41	124.75	128.60
2	A	1083	A	C4-C5-C6	6.41	120.20	117.00
2	A	1646	A	C5-C6-N6	-6.41	118.58	123.70
2	A	282	G	C5-C6-O6	-6.41	124.76	128.60
2	A	1223	G	C5-C6-O6	-6.41	124.76	128.60
2	A	1344	G	O4'-C1'-N9	6.41	113.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	54	A	C4-C5-C6	6.40	120.20	117.00
2	A	173	A	C5-C6-N6	-6.40	118.58	123.70
1	N	69	G	C5-C6-O6	-6.40	124.76	128.60
2	A	1212	C	C2-N1-C1'	6.40	125.84	118.80
1	N	38	C	N3-C4-N4	6.40	122.48	118.00
2	A	752	C	N3-C4-N4	6.40	122.48	118.00
2	A	1261	A	C4-C5-C6	6.40	120.20	117.00
2	A	1074	C	N3-C4-N4	6.39	122.48	118.00
2	A	1266	G	C5-C6-O6	-6.39	124.76	128.60
3	F	11	A	O4'-C1'-N9	6.39	113.31	108.20
2	A	1714	A	C5-C6-N6	-6.39	118.59	123.70
2	A	857	A	C4-C5-C6	6.39	120.19	117.00
2	A	1089	A	C5-C6-N1	-6.39	114.50	117.70
2	A	1283	A	C5-C6-N1	-6.39	114.50	117.70
2	A	1819	A	C4-C5-C6	6.39	120.19	117.00
2	A	108	G	O4'-C1'-N9	6.39	113.31	108.20
2	A	1651	G	O4'-C1'-N9	6.39	113.31	108.20
2	A	1640	C	O4'-C1'-N1	6.39	113.31	108.20
2	A	141	A	C2'-C3'-O3'	6.39	123.92	113.70
2	A	1146	A	C5-C6-N6	-6.39	118.59	123.70
2	A	1793	G	O4'-C1'-N9	6.39	113.31	108.20
2	A	589	A	C5-C6-N6	-6.38	118.59	123.70
2	A	1356	U	O4'-C1'-N1	6.38	113.31	108.20
2	A	499	G	C5-C6-O6	-6.38	124.77	128.60
2	A	632	U	O4'-C1'-N1	6.38	113.31	108.20
2	A	898	G	O4'-C1'-N9	6.38	113.31	108.20
2	A	188	U	O4'-C1'-N1	6.38	113.30	108.20
2	A	482	C	N3-C4-N4	6.38	122.47	118.00
2	A	925	G	O4'-C1'-N9	6.38	113.30	108.20
2	A	1253	G	C5-C6-O6	-6.38	124.77	128.60
2	A	91	A	C4-C5-C6	6.38	120.19	117.00
2	A	333	A	C4-C5-C6	6.38	120.19	117.00
2	A	868	A	C4-C5-C6	6.38	120.19	117.00
2	A	974	G	C5-C6-O6	-6.38	124.78	128.60
2	A	1837	G	O4'-C1'-N9	6.38	113.30	108.20
2	A	789	G	C5-C6-O6	-6.37	124.78	128.60
2	A	855	G	C5-C6-O6	-6.37	124.78	128.60
2	A	1092	G	C5-C6-O6	-6.37	124.78	128.60
2	A	274	G	O4'-C1'-N9	6.37	113.30	108.20
2	A	323	G	C5-C6-O6	-6.37	124.78	128.60
2	A	526	A	C4-C5-C6	6.37	120.19	117.00
2	A	1836	C	N3-C4-N4	6.37	122.46	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	30	A	C4-C5-C6	6.37	120.19	117.00
2	A	832	G	C5-C6-O6	-6.37	124.78	128.60
2	A	1035	C	N3-C4-N4	6.37	122.46	118.00
2	A	52	G	O4'-C1'-N9	6.37	113.30	108.20
2	A	1119	C	O4'-C1'-N1	6.37	113.30	108.20
2	A	1169	A	O4'-C1'-N9	6.37	113.30	108.20
2	A	618	A	O4'-C1'-N9	6.37	113.29	108.20
2	A	1075	C	O4'-C1'-N1	6.36	113.29	108.20
1	N	53	A	C5-C6-N6	-6.36	118.61	123.70
2	A	185	C	N3-C4-C5	-6.36	119.36	121.90
2	A	310	G	C5-C6-O6	-6.36	124.78	128.60
2	A	1647	G	O4'-C1'-N9	6.36	113.29	108.20
2	A	1696	C	O4'-C1'-N1	6.36	113.29	108.20
2	A	1476	A	C4-C5-C6	6.36	120.18	117.00
2	A	241	A	C4-C5-C6	6.36	120.18	117.00
29	g	167	TYR	CB-CG-CD1	6.36	124.81	121.00
2	A	219	U	O4'-C1'-N1	6.36	113.28	108.20
2	A	947	C	O4'-C1'-N1	6.36	113.28	108.20
2	A	1066	A	C4-C5-C6	6.36	120.18	117.00
2	A	1320	G	C5-C6-O6	-6.36	124.79	128.60
2	A	1350	G	C5-C6-O6	-6.36	124.79	128.60
2	A	382	A	C4-C5-C6	6.35	120.18	117.00
2	A	894	U	O4'-C1'-N1	6.35	113.28	108.20
2	A	1565	G	O4'-C1'-N9	6.35	113.28	108.20
2	A	346	C	C2-N1-C1'	6.35	125.79	118.80
2	A	1256	A	C4-C5-C6	6.35	120.17	117.00
3	F	8	A	C4-C5-C6	6.35	120.18	117.00
2	A	648	U	O4'-C1'-N1	6.35	113.28	108.20
2	A	82	G	C5-C6-O6	-6.35	124.79	128.60
2	A	1481	U	O4'-C1'-N1	6.35	113.28	108.20
2	A	1571	G	C5-C6-O6	-6.35	124.79	128.60
2	A	951	A	O4'-C1'-N9	6.34	113.28	108.20
2	A	1317	G	C5-C6-O6	-6.34	124.79	128.60
2	A	215	U	O4'-C1'-N1	6.34	113.27	108.20
2	A	281	U	O4'-C1'-N1	6.34	113.27	108.20
2	A	1243	C	O4'-C1'-N1	6.34	113.27	108.20
2	A	1353	A	C5-C6-N6	-6.34	118.63	123.70
2	A	519	A	C5-C6-N1	-6.34	114.53	117.70
2	A	1103	G	C5-C6-O6	-6.34	124.80	128.60
2	A	940	A	C5-C6-N1	-6.34	114.53	117.70
2	A	1493	G	C5-C6-O6	-6.34	124.80	128.60
2	A	1532	A	C4-C5-C6	6.34	120.17	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1618	A	C4-C5-C6	6.34	120.17	117.00
2	A	1853	A	C4-C5-C6	6.34	120.17	117.00
2	A	1156	U	O4'-C1'-N1	6.33	113.27	108.20
2	A	106	C	N3-C4-N4	6.33	122.43	118.00
2	A	164	A	C5-C6-N6	-6.33	118.63	123.70
2	A	311	C	N3-C4-N4	6.33	122.43	118.00
2	A	781	C	O4'-C1'-C2'	-6.33	99.47	105.80
2	A	896	C	N3-C4-C5	-6.33	119.37	121.90
2	A	1783	G	C5-C6-O6	-6.33	124.80	128.60
2	A	902	U	O4'-C1'-N1	6.33	113.26	108.20
2	A	1133	U	O4'-C1'-N1	6.33	113.26	108.20
2	A	288	A	C4-C5-C6	6.33	120.16	117.00
2	A	645	A	C4-C5-C6	6.33	120.16	117.00
2	A	810	U	O4'-C1'-N1	6.33	113.26	108.20
2	A	1036	G	O4'-C1'-N9	6.33	113.26	108.20
2	A	1300	U	O4'-C1'-N1	6.33	113.26	108.20
2	A	1324	G	O4'-C1'-N9	6.33	113.26	108.20
2	A	1487	G	O4'-C1'-N9	6.33	113.26	108.20
2	A	1517	A	C4-C5-C6	6.33	120.16	117.00
1	N	41	A	O4'-C1'-N9	6.32	113.26	108.20
2	A	511	A	O4'-C1'-N9	6.32	113.26	108.20
2	A	559	A	C4-C5-C6	6.32	120.16	117.00
2	A	1216	A	C4-C5-C6	6.32	120.16	117.00
2	A	1246	A	C4-C5-C6	6.32	120.16	117.00
2	A	1359	C	N3-C4-N4	6.32	122.43	118.00
2	A	1432	C	N3-C4-N4	6.32	122.43	118.00
2	A	1494	A	C5-C6-N1	-6.32	114.54	117.70
2	A	147	A	C4-C5-C6	6.32	120.16	117.00
2	A	164	A	C4-C5-C6	6.32	120.16	117.00
2	A	408	A	C4-C5-C6	6.32	120.16	117.00
2	A	826	A	C4-C5-C6	6.32	120.16	117.00
2	A	983	A	C4-C5-C6	6.32	120.16	117.00
2	A	573	A	C5-C6-N6	-6.32	118.65	123.70
2	A	798	A	C4-C5-C6	6.32	120.16	117.00
2	A	1370	C	N3-C4-N4	6.32	122.42	118.00
2	A	1382	A	C4-C5-C6	6.32	120.16	117.00
2	A	992	A	C5-C6-N6	-6.31	118.65	123.70
2	A	119	U	O4'-C1'-N1	6.31	113.25	108.20
2	A	1027	A	C5-C6-N1	-6.31	114.54	117.70
2	A	1080	A	C4-C5-C6	6.31	120.16	117.00
2	A	1814	G	O4'-C1'-N9	6.31	113.25	108.20
2	A	508	G	C5-C6-O6	-6.31	124.81	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	917	G	C5-C6-O6	-6.31	124.81	128.60
2	A	488	C	N3-C4-N4	6.31	122.42	118.00
2	A	1081	C	O4'-C1'-N1	6.31	113.25	108.20
2	A	155	G	C5-C6-O6	-6.31	124.82	128.60
2	A	1380	C	N3-C4-N4	6.31	122.41	118.00
2	A	394	G	O4'-C1'-N9	6.30	113.24	108.20
2	A	430	G	O4'-C1'-N9	6.30	113.24	108.20
2	A	1457	G	C5-C6-O6	-6.30	124.82	128.60
2	A	1477	G	O4'-C1'-N9	6.30	113.24	108.20
2	A	1577	C	N3-C4-N4	6.30	122.41	118.00
2	A	1582	G	O4'-C1'-N9	6.30	113.24	108.20
2	A	1666	G	C5-C6-O6	-6.30	124.82	128.60
2	A	1739	G	C5-C6-O6	-6.30	124.82	128.60
16	T	118	TYR	CB-CG-CD1	-6.30	117.22	121.00
2	A	761	G	C5-C6-O6	-6.30	124.82	128.60
2	A	823	A	C4-C5-C6	6.30	120.15	117.00
2	A	36	U	O4'-C1'-N1	6.30	113.24	108.20
2	A	492	C	C6-N1-C1'	-6.30	113.25	120.80
2	A	748	G	O4'-C1'-N9	6.30	113.24	108.20
2	A	1428	U	O4'-C1'-N1	6.30	113.24	108.20
2	A	731	C	O4'-C1'-N1	6.29	113.23	108.20
2	A	1029	G	C5-C6-O6	-6.29	124.82	128.60
2	A	1273	C	N3-C4-C5	-6.29	119.38	121.90
2	A	1740	A	O4'-C1'-N9	6.29	113.23	108.20
40	r	114	TYR	CB-CG-CD1	-6.29	117.22	121.00
2	A	410	G	O4'-C1'-N9	6.29	113.23	108.20
2	A	183	G	O4'-C1'-N9	6.29	113.23	108.20
2	A	651	U	O4'-C1'-N1	6.29	113.23	108.20
2	A	173	A	C4-C5-C6	6.29	120.14	117.00
2	A	920	G	O4'-C1'-N9	6.29	113.23	108.20
2	A	299	G	C5-C6-O6	-6.28	124.83	128.60
2	A	899	A	C4-C5-C6	6.28	120.14	117.00
2	A	1389	G	O4'-C1'-N9	6.28	113.23	108.20
2	A	1367	U	O4'-C1'-N1	6.28	113.22	108.20
2	A	1710	A	C5-C6-N6	-6.28	118.67	123.70
2	A	1494	A	C4-C5-C6	6.28	120.14	117.00
2	A	1557	C	N3-C4-N4	6.28	122.40	118.00
2	A	1844	A	O4'-C1'-N9	6.28	113.22	108.20
2	A	938	G	O4'-C1'-N9	6.28	113.22	108.20
2	A	603	C	O4'-C1'-N1	6.28	113.22	108.20
2	A	1268	C	N3-C4-C5	-6.28	119.39	121.90
2	A	1775	A	C4-C5-C6	6.28	120.14	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	12	G	O4'-C1'-N9	6.28	113.22	108.20
2	A	392	C	N3-C4-N4	6.28	122.39	118.00
2	A	444	U	O4'-C1'-N1	6.28	113.22	108.20
2	A	1365	A	C4-C5-C6	6.28	120.14	117.00
2	A	1399	C	O4'-C1'-N1	6.28	113.22	108.20
2	A	799	C	N3-C4-N4	6.27	122.39	118.00
2	A	808	A	C5-C6-N6	-6.27	118.68	123.70
2	A	96	C	N3-C4-N4	6.27	122.39	118.00
2	A	1173	U	O4'-C1'-N1	6.27	113.22	108.20
2	A	1067	G	O4'-C1'-N9	6.27	113.22	108.20
2	A	1445	G	C5-C6-O6	-6.27	124.84	128.60
2	A	1452	G	O4'-C1'-N9	6.27	113.22	108.20
2	A	1482	A	O4'-C1'-N9	6.27	113.22	108.20
2	A	1686	U	O4'-C1'-N1	6.27	113.22	108.20
2	A	1740	A	C4-C5-C6	6.27	120.14	117.00
2	A	584	A	C4-C5-C6	6.27	120.13	117.00
2	A	1326	G	C5-C6-O6	-6.27	124.84	128.60
2	A	1415	C	N3-C4-N4	6.27	122.39	118.00
2	A	1531	G	C5-C6-O6	-6.26	124.84	128.60
2	A	1109	A	C4-C5-C6	6.26	120.13	117.00
2	A	540	C	O4'-C1'-N1	6.26	113.21	108.20
2	A	56	G	O4'-C1'-N9	6.26	113.21	108.20
2	A	171	A	C4-C5-C6	6.26	120.13	117.00
2	A	644	A	O4'-C1'-N9	6.26	113.21	108.20
2	A	650	C	N3-C4-N4	6.26	122.38	118.00
2	A	1444	A	C4-C5-C6	6.26	120.13	117.00
2	A	1733	C	N3-C4-N4	6.26	122.38	118.00
2	A	905	G	O4'-C1'-N9	6.26	113.20	108.20
2	A	872	C	O4'-C1'-N1	6.25	113.20	108.20
2	A	1279	C	N3-C4-N4	6.25	122.38	118.00
2	A	1593	G	O4'-C1'-N9	6.25	113.20	108.20
2	A	454	A	C4-C5-C6	6.25	120.13	117.00
2	A	511	A	C4-C5-C6	6.25	120.13	117.00
2	A	1615	A	C5-C6-N6	-6.25	118.70	123.70
2	A	1254	A	C4-C5-C6	6.25	120.13	117.00
2	A	1754	G	C5-C6-O6	-6.25	124.85	128.60
2	A	361	A	C4-C5-C6	6.25	120.12	117.00
2	A	1242	A	C5-C6-N6	-6.25	118.70	123.70
2	A	377	C	N3-C4-C5	-6.25	119.40	121.90
2	A	233	A	C4-C5-C6	6.25	120.12	117.00
1	N	16	C	O4'-C1'-N1	6.24	113.19	108.20
2	A	170	A	C5-C6-N1	-6.24	114.58	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	928	G	C5-C6-O6	-6.24	124.85	128.60
2	A	566	A	C5-C6-N1	-6.24	114.58	117.70
2	A	831	C	O4'-C1'-N1	6.24	113.19	108.20
2	A	1666	G	O4'-C1'-N9	6.24	113.19	108.20
2	A	321	C	O4'-C1'-N1	6.24	113.19	108.20
2	A	201	G	O4'-C1'-N9	6.24	113.19	108.20
2	A	1192	A	O4'-C1'-N9	6.24	113.19	108.20
2	A	871	A	C5-C6-N6	-6.23	118.71	123.70
2	A	1468	C	N3-C4-N4	6.23	122.36	118.00
2	A	213	C	P-O5'-C5'	6.23	130.87	120.90
2	A	804	A	C4-C5-C6	6.23	120.12	117.00
2	A	1199	G	O4'-C1'-N9	6.23	113.19	108.20
2	A	1439	C	N3-C4-N4	6.23	122.36	118.00
2	A	1184	A	C4-C5-C6	6.23	120.11	117.00
3	F	16	G	C5-C6-O6	-6.23	124.86	128.60
1	N	62	A	O4'-C1'-N9	6.23	113.18	108.20
2	A	1023	A	C4-C5-C6	6.23	120.11	117.00
2	A	11	A	C5-C6-N1	-6.23	114.59	117.70
2	A	121	U	O4'-C1'-N1	6.23	113.18	108.20
2	A	541	U	P-O3'-C3'	6.23	127.17	119.70
2	A	1170	U	O4'-C1'-N1	6.23	113.18	108.20
2	A	1210	A	C4-C5-C6	6.23	120.11	117.00
2	A	1232	G	O4'-C1'-N9	6.23	113.18	108.20
2	A	991	G	O4'-C1'-N9	6.23	113.18	108.20
2	A	1072	G	O4'-C1'-N9	6.23	113.18	108.20
2	A	90	G	O4'-C1'-N9	6.22	113.18	108.20
2	A	210	G	O4'-C1'-N9	6.22	113.18	108.20
2	A	1196	A	C4-C5-C6	6.22	120.11	117.00
2	A	1255	A	C4-C5-C6	6.22	120.11	117.00
2	A	1782	A	C4-C5-C6	6.22	120.11	117.00
2	A	546	U	O4'-C1'-N1	6.22	113.18	108.20
2	A	986	A	C5-C6-N1	-6.22	114.59	117.70
2	A	1378	A	C4-C5-C6	6.22	120.11	117.00
3	F	23	A	C4-C5-C6	6.22	120.11	117.00
2	A	1089	A	C4-C5-C6	6.22	120.11	117.00
2	A	1601	G	O4'-C1'-N9	6.22	113.18	108.20
25	c	175	SER	N-CA-CB	6.22	119.83	110.50
2	A	50	A	C4-C5-C6	6.22	120.11	117.00
2	A	459	A	C4-C5-C6	6.22	120.11	117.00
2	A	1766	C	N3-C4-C5	-6.22	119.41	121.90
2	A	1828	A	C5-C6-N1	-6.22	114.59	117.70
2	A	329	A	C4-C5-C6	6.22	120.11	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	469	C	N3-C4-N4	6.22	122.35	118.00
2	A	642	U	O4'-C1'-N1	6.22	113.17	108.20
2	A	861	A	C4-C5-C6	6.22	120.11	117.00
2	A	1038	A	C4-C5-C6	6.22	120.11	117.00
2	A	1291	A	C4-C5-C6	6.22	120.11	117.00
2	A	1329	U	O4'-C1'-N1	6.22	113.17	108.20
2	A	199	G	C5-C6-O6	-6.21	124.87	128.60
2	A	514	U	O4'-C1'-N1	6.21	113.17	108.20
2	A	960	A	C4-C5-C6	6.21	120.11	117.00
2	A	1642	A	O4'-C1'-N9	6.21	113.17	108.20
2	A	1694	A	C4-C5-C6	6.21	120.11	117.00
2	A	352	C	N3-C4-C5	-6.21	119.42	121.90
2	A	669	A	O4'-C1'-N9	6.21	113.17	108.20
2	A	1135	C	C6-N1-C1'	-6.21	113.35	120.80
2	A	1340	A	C4-C5-C6	6.21	120.11	117.00
2	A	1532	A	C5-C6-N6	-6.21	118.73	123.70
2	A	1668	U	O4'-C1'-N1	6.21	113.17	108.20
2	A	1682	C	O4'-C1'-N1	6.21	113.17	108.20
2	A	1719	A	O4'-C1'-N9	6.21	113.17	108.20
1	N	49	A	C4-C5-C6	6.21	120.11	117.00
2	A	1007	A	O4'-C1'-N9	6.21	113.17	108.20
2	A	383	U	O4'-C1'-N1	6.21	113.17	108.20
2	A	759	A	C4-C5-C6	6.21	120.11	117.00
2	A	851	G	C5-C6-O6	-6.21	124.88	128.60
2	A	998	U	O4'-C1'-N1	6.21	113.17	108.20
2	A	1060	C	N3-C4-N4	6.21	122.35	118.00
2	A	579	G	C5-C6-O6	-6.21	124.88	128.60
2	A	1635	A	C5-C6-N6	-6.21	118.73	123.70
2	A	1784	A	C5-C6-N6	-6.21	118.73	123.70
2	A	30	C	N3-C4-N4	6.21	122.34	118.00
2	A	189	G	C5-C6-O6	-6.20	124.88	128.60
2	A	586	U	O4'-C1'-N1	6.20	113.16	108.20
2	A	1273	C	N3-C4-N4	6.20	122.34	118.00
2	A	1485	A	P-O3'-C3'	6.20	127.14	119.70
2	A	1132	U	O4'-C1'-N1	6.20	113.16	108.20
2	A	369	C	O4'-C1'-N1	6.20	113.16	108.20
2	A	805	A	C4-C5-C6	6.20	120.10	117.00
2	A	1520	C	N3-C4-N4	6.20	122.34	118.00
2	A	241	A	O4'-C1'-N9	6.20	113.16	108.20
2	A	1128	C	N3-C4-N4	6.20	122.34	118.00
39	q	28	TYR	CB-CG-CD1	6.20	124.72	121.00
1	N	11	C	O4'-C1'-N1	6.20	113.16	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	20	G	O4'-C1'-N9	6.20	113.16	108.20
2	A	380	C	N3-C4-N4	6.20	122.34	118.00
2	A	423	A	C5-C6-N1	-6.20	114.60	117.70
2	A	546	U	P-O3'-C3'	6.20	127.13	119.70
2	A	638	A	O4'-C1'-N9	6.20	113.16	108.20
2	A	1026	A	C5-C6-N6	-6.20	118.74	123.70
2	A	1604	C	N3-C4-C5	-6.20	119.42	121.90
2	A	405	A	C4-C5-C6	6.19	120.10	117.00
2	A	1462	G	C5-C6-O6	-6.19	124.88	128.60
2	A	205	G	C5-C6-O6	-6.19	124.88	128.60
2	A	1347	G	O4'-C1'-N9	6.19	113.15	108.20
2	A	1377	G	C5-C6-O6	-6.19	124.89	128.60
2	A	1609	A	C5-C6-N6	-6.19	118.75	123.70
2	A	1384	A	C5-C6-N6	-6.19	118.75	123.70
2	A	490	A	C4-C5-C6	6.19	120.09	117.00
2	A	523	A	C5-C6-N6	-6.19	118.75	123.70
2	A	336	C	O4'-C1'-N1	6.19	113.15	108.20
2	A	401	G	O4'-C1'-N9	6.18	113.15	108.20
2	A	780	G	P-O3'-C3'	6.18	127.12	119.70
2	A	947	C	N3-C4-N4	6.18	122.33	118.00
2	A	1860	A	C5-C6-N6	-6.18	118.75	123.70
2	A	10	G	O4'-C1'-N9	6.18	113.14	108.20
2	A	228	A	C5-C6-N1	-6.18	114.61	117.70
2	A	1812	A	C5-C6-N1	-6.18	114.61	117.70
2	A	29	G	O4'-C1'-N9	6.18	113.14	108.20
1	N	62	A	C5-C6-N1	-6.18	114.61	117.70
2	A	438	A	C5-C6-N6	-6.18	118.76	123.70
2	A	520	U	O4'-C1'-N1	6.18	113.14	108.20
2	A	1412	C	O4'-C1'-N1	6.18	113.14	108.20
2	A	1746	C	O4'-C1'-N1	6.18	113.14	108.20
2	A	1690	A	C4-C5-C6	6.18	120.09	117.00
2	A	631	A	C5-C6-N1	-6.18	114.61	117.70
2	A	545	A	C4-C5-C6	6.17	120.09	117.00
2	A	1095	G	O4'-C1'-N9	6.17	113.14	108.20
3	F	32	G	O4'-C1'-N9	6.17	113.14	108.20
2	A	79	A	P-O3'-C3'	6.17	127.11	119.70
2	A	315	C	O4'-C1'-N1	6.17	113.14	108.20
2	A	551	A	C5-C6-N6	-6.17	118.76	123.70
2	A	1105	C	C6-N1-C1'	-6.17	113.39	120.80
2	A	1261	A	O4'-C1'-N9	6.17	113.14	108.20
2	A	1280	A	C5-C6-N6	-6.17	118.76	123.70
2	A	1413	C	N3-C4-N4	6.17	122.32	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	60	A	C4-C5-C6	6.17	120.08	117.00
2	A	1636	A	C5-C6-N1	-6.17	114.61	117.70
1	N	20	A	C4-C5-C6	6.17	120.08	117.00
1	N	25	G	O4'-C1'-N9	6.17	113.14	108.20
2	A	195	C	O4'-C1'-N1	6.17	113.14	108.20
2	A	103	A	C4-C5-C6	6.17	120.08	117.00
2	A	1673	A	C4-C5-C6	6.17	120.08	117.00
2	A	1066	A	O4'-C1'-N9	6.17	113.13	108.20
2	A	1295	A	C4-C5-C6	6.17	120.08	117.00
2	A	1807	A	O4'-C1'-N9	6.17	113.13	108.20
2	A	824	G	O4'-C1'-N9	6.16	113.13	108.20
2	A	1750	C	N3-C4-N4	6.16	122.31	118.00
37	o	142	SER	C-N-CA	6.16	137.11	121.70
2	A	479	A	C4-C5-C6	6.16	120.08	117.00
2	A	1730	A	C4-C5-C6	6.16	120.08	117.00
2	A	153	G	O4'-C1'-N9	6.16	113.13	108.20
2	A	783	G	O4'-C1'-N9	6.16	113.13	108.20
2	A	293	A	O4'-C1'-N9	6.16	113.13	108.20
2	A	1130	G	C5-C6-O6	-6.16	124.91	128.60
2	A	1153	G	O4'-C1'-N9	6.16	113.13	108.20
1	N	19	A	C4-C5-C6	6.16	120.08	117.00
2	A	1363	U	O4'-C1'-N1	6.16	113.13	108.20
2	A	1145	A	C4-C5-C6	6.16	120.08	117.00
2	A	1659	A	C5-C6-N1	-6.16	114.62	117.70
2	A	25	A	O4'-C1'-N9	6.15	113.12	108.20
2	A	778	C	N3-C4-N4	6.15	122.31	118.00
2	A	1195	A	O4'-C1'-N9	6.15	113.12	108.20
2	A	1461	A	C4-C5-C6	6.15	120.08	117.00
1	N	1	A	C5-C6-N6	-6.15	118.78	123.70
1	N	61	C	N3-C4-N4	6.15	122.31	118.00
2	A	445	A	C5-C6-N1	-6.15	114.62	117.70
2	A	629	C	N3-C4-N4	6.15	122.31	118.00
2	A	782	G	O4'-C1'-N9	6.15	113.12	108.20
2	A	986	A	C4-C5-C6	6.15	120.08	117.00
2	A	1566	G	O4'-C1'-N9	6.15	113.12	108.20
2	A	1821	U	O4'-C1'-N1	6.15	113.12	108.20
2	A	1449	C	C6-N1-C1'	-6.15	113.42	120.80
2	A	240	C	N3-C4-N4	6.15	122.30	118.00
2	A	921	G	O4'-C1'-N9	6.15	113.12	108.20
2	A	1228	U	O4'-C1'-N1	6.15	113.12	108.20
2	A	1328	A	C5-C6-N6	-6.15	118.78	123.70
2	A	1575	A	C4-C5-C6	6.15	120.07	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1602	A	O4'-C1'-N9	6.15	113.12	108.20
2	A	1852	G	C5-C6-O6	-6.15	124.91	128.60
2	A	460	G	P-O3'-C3'	6.15	127.08	119.70
2	A	18	C	N3-C4-N4	6.14	122.30	118.00
2	A	541	U	O4'-C1'-N1	6.14	113.11	108.20
2	A	177	G	C5-C6-O6	-6.14	124.92	128.60
2	A	854	A	C4-C5-C6	6.14	120.07	117.00
2	A	1526	A	C5-C6-N1	-6.14	114.63	117.70
2	A	2	A	C4-C5-C6	6.14	120.07	117.00
2	A	502	A	C4-C5-C6	6.14	120.07	117.00
2	A	554	A	C5-C6-N6	-6.14	118.79	123.70
2	A	1068	U	P-O3'-C3'	6.14	127.07	119.70
2	A	1271	G	C5-C6-O6	-6.14	124.92	128.60
2	A	1375	A	O4'-C1'-N9	6.14	113.11	108.20
2	A	877	G	O4'-C1'-N9	6.14	113.11	108.20
2	A	1632	A	C4-C5-C6	6.14	120.07	117.00
2	A	63	U	O4'-C1'-N1	6.13	113.11	108.20
2	A	221	A	C4-C5-C6	6.13	120.07	117.00
2	A	565	A	C4-C5-C6	6.13	120.07	117.00
2	A	1265	G	C5-C6-O6	-6.13	124.92	128.60
2	A	662	A	C4-C5-C6	6.13	120.07	117.00
2	A	1289	A	C5-C6-N6	-6.13	118.80	123.70
2	A	1405	A	C4-C5-C6	6.13	120.06	117.00
2	A	16	G	O4'-C1'-N9	6.13	113.10	108.20
2	A	61	A	C4-C5-C6	6.13	120.06	117.00
2	A	1236	A	C4-C5-C6	6.13	120.06	117.00
2	A	595	A	C4-C5-C6	6.13	120.06	117.00
2	A	644	A	C4-C5-C6	6.13	120.06	117.00
2	A	1540	A	C5'-C4'-O4'	6.13	116.45	109.10
2	A	1755	U	P-O5'-C5'	6.13	130.70	120.90
2	A	286	C	N3-C4-N4	6.12	122.29	118.00
2	A	498	A	C4-C5-C6	6.12	120.06	117.00
2	A	1289	A	C5-C6-N1	-6.12	114.64	117.70
2	A	1813	A	C4-C5-C6	6.12	120.06	117.00
20	X	173	PHE	CB-CG-CD2	-6.12	116.51	120.80
2	A	108	G	C5-C6-O6	-6.12	124.93	128.60
2	A	565	A	C5-C6-N6	-6.12	118.80	123.70
2	A	1306	U	O4'-C1'-N1	6.12	113.10	108.20
1	N	71	U	O4'-C1'-N1	6.12	113.10	108.20
2	A	1019	A	C4-C5-C6	6.12	120.06	117.00
2	A	467	G	C5-C6-O6	-6.12	124.93	128.60
2	A	1111	U	C5'-C4'-C3'	-6.12	106.21	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1435	A	C4-C5-C6	6.12	120.06	117.00
2	A	458	A	O4'-C1'-N9	6.12	113.09	108.20
2	A	990	C	N3-C4-N4	6.12	122.28	118.00
16	T	124	PHE	CB-CG-CD1	6.12	125.08	120.80
2	A	609	A	C4-C5-C6	6.12	120.06	117.00
2	A	987	G	O4'-C1'-N9	6.12	113.09	108.20
2	A	1366	A	C4-C5-C6	6.12	120.06	117.00
2	A	1137	G	P-O5'-C5'	6.12	130.68	120.90
2	A	1485	A	C4-C5-C6	6.12	120.06	117.00
3	F	4	A	C4-C5-C6	6.12	120.06	117.00
20	X	173	PHE	CB-CG-CD1	6.12	125.08	120.80
2	A	833	A	C4-C5-C6	6.11	120.06	117.00
2	A	850	A	C5-C6-N1	-6.11	114.64	117.70
2	A	269	C	N3-C4-N4	6.11	122.28	118.00
2	A	809	A	C5-C6-N6	-6.11	118.81	123.70
2	A	977	A	C5-C6-N6	-6.11	118.81	123.70
2	A	1016	A	C4-C5-C6	6.11	120.06	117.00
1	N	23	G	O4'-C1'-N9	6.11	113.09	108.20
2	A	419	C	N3-C4-N4	6.11	122.28	118.00
2	A	1135	C	N3-C4-N4	6.11	122.28	118.00
2	A	322	G	C5-C6-O6	-6.11	124.94	128.60
2	A	997	A	C4-C5-C6	6.11	120.05	117.00
2	A	1434	A	C4-C5-C6	6.11	120.05	117.00
2	A	171	A	O4'-C1'-N9	6.11	113.08	108.20
2	A	175	A	C4-C5-C6	6.11	120.05	117.00
2	A	1196	A	C5-C6-N1	-6.11	114.65	117.70
2	A	1272	A	C5-C6-N6	-6.11	118.81	123.70
2	A	1280	A	C4-C5-C6	6.11	120.05	117.00
2	A	1630	C	N3-C4-N4	6.11	122.27	118.00
2	A	1719	A	C5-C6-N1	-6.11	114.65	117.70
2	A	808	A	C4-C5-C6	6.10	120.05	117.00
1	N	41	A	C5-C6-N6	-6.10	118.82	123.70
2	A	1115	A	C4-C5-C6	6.10	120.05	117.00
2	A	1140	A	C4-C5-C6	6.10	120.05	117.00
2	A	1852	G	N3-C2-N2	6.10	124.17	119.90
2	A	1013	U	O4'-C1'-N1	6.10	113.08	108.20
2	A	1032	A	C4-C5-C6	6.10	120.05	117.00
2	A	27	A	C5-C6-N1	-6.10	114.65	117.70
2	A	812	A	C4-C5-C6	6.10	120.05	117.00
2	A	1625	A	C5-C6-N1	-6.10	114.65	117.70
1	N	75	A	C4-C5-C6	6.10	120.05	117.00
2	A	27	A	O4'-C1'-N9	6.10	113.08	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	55	C	N3-C4-N4	6.10	122.27	118.00
2	A	168	C	N3-C4-C5	-6.09	119.46	121.90
2	A	286	C	O4'-C1'-N1	6.09	113.08	108.20
2	A	1028	C	N3-C4-N4	6.09	122.27	118.00
2	A	388	A	C5-C6-N6	-6.09	118.83	123.70
2	A	812	A	O4'-C1'-N9	6.09	113.07	108.20
2	A	1205	A	C4-C5-C6	6.09	120.05	117.00
2	A	1444	A	C5-C6-N1	-6.09	114.65	117.70
2	A	1482	A	C5-C6-N1	-6.09	114.65	117.70
2	A	191	C	N3-C4-C5	-6.09	119.46	121.90
2	A	335	U	O4'-C1'-N1	6.09	113.07	108.20
2	A	580	A	C4-C5-C6	6.09	120.05	117.00
2	A	850	A	C4-C5-C6	6.09	120.05	117.00
1	N	16	C	N3-C4-N4	6.09	122.26	118.00
1	N	26	C	N3-C4-C5	-6.09	119.46	121.90
2	A	176	U	O4'-C1'-N1	6.09	113.07	108.20
2	A	1017	U	O4'-C1'-N1	6.09	113.07	108.20
2	A	1307	C	N3-C4-C5	-6.09	119.46	121.90
2	A	1410	A	C4-C5-C6	6.09	120.05	117.00
2	A	91	A	C5-C6-N6	-6.09	118.83	123.70
2	A	142	C	O4'-C1'-N1	6.09	113.07	108.20
2	A	934	A	C5-C6-N1	-6.09	114.66	117.70
2	A	1141	A	C4-C5-C6	6.09	120.04	117.00
2	A	1319	U	O4'-C1'-N1	6.09	113.07	108.20
3	F	18	A	C4-C5-C6	6.09	120.04	117.00
2	A	900	A	C4-C5-C6	6.08	120.04	117.00
2	A	432	C	N3-C4-N4	6.08	122.26	118.00
2	A	1184	A	C5-C6-N1	-6.08	114.66	117.70
2	A	22	A	C4-C5-C6	6.08	120.04	117.00
2	A	241	A	C5-C6-N6	-6.08	118.83	123.70
2	A	943	G	O4'-C1'-N9	6.08	113.06	108.20
2	A	1312	C	N3-C4-N4	6.08	122.26	118.00
2	A	1463	C	N3-C4-N4	6.08	122.26	118.00
2	A	1519	G	O4'-C1'-N9	6.08	113.06	108.20
2	A	1594	U	C5'-C4'-O4'	6.08	116.40	109.10
2	A	46	A	O4'-C1'-N9	6.08	113.06	108.20
2	A	624	A	C5-C6-N6	-6.08	118.84	123.70
2	A	283	A	C4-C5-C6	6.08	120.04	117.00
2	A	425	A	C5-C6-N1	-6.08	114.66	117.70
2	A	518	A	C4-C5-C6	6.08	120.04	117.00
2	A	861	A	O4'-C1'-N9	6.08	113.06	108.20
2	A	882	A	C5-C6-N1	-6.08	114.66	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	456	G	O4'-C1'-N9	6.08	113.06	108.20
2	A	218	A	C4-C5-C6	6.08	120.04	117.00
2	A	1674	A	C4-C5-C6	6.08	120.04	117.00
2	A	92	A	C4-C5-C6	6.07	120.04	117.00
2	A	437	A	C5-C6-N1	-6.07	114.66	117.70
2	A	1818	A	C4-C5-C6	6.07	120.04	117.00
2	A	1103	G	O4'-C1'-N9	6.07	113.06	108.20
2	A	213	C	N3-C4-N4	6.07	122.25	118.00
2	A	544	A	C4-C5-C6	6.07	120.03	117.00
2	A	573	A	C4-C5-C6	6.07	120.03	117.00
2	A	934	A	C4-C5-C6	6.07	120.04	117.00
2	A	1320	G	O4'-C1'-N9	6.07	113.06	108.20
2	A	1495	U	O4'-C1'-N1	6.07	113.06	108.20
2	A	379	A	C5-C6-N1	-6.07	114.67	117.70
2	A	1016	A	C5-C6-N1	-6.07	114.67	117.70
2	A	1736	U	O4'-C1'-N1	6.07	113.06	108.20
2	A	326	A	C4-C5-C6	6.07	120.03	117.00
2	A	426	G	O4'-C1'-N9	6.07	113.05	108.20
2	A	1079	A	C4-C5-C6	6.07	120.03	117.00
2	A	574	A	C4-C5-C6	6.07	120.03	117.00
2	A	490	A	C5-C6-N6	-6.06	118.85	123.70
2	A	600	G	O4'-C1'-N9	6.06	113.05	108.20
2	A	1031	A	O4'-C1'-N9	6.06	113.05	108.20
2	A	1119	C	N3-C4-N4	6.06	122.24	118.00
2	A	1372	A	O4'-C1'-N9	6.06	113.05	108.20
2	A	48	C	N3-C4-N4	6.06	122.24	118.00
2	A	328	G	O4'-C1'-N9	6.06	113.05	108.20
2	A	1556	A	C4-C5-C6	6.06	120.03	117.00
2	A	151	C	N3-C4-N4	6.06	122.24	118.00
2	A	640	A	C5-C6-N6	-6.06	118.85	123.70
2	A	1082	G	O4'-C1'-N9	6.06	113.05	108.20
2	A	1177	A	C4-C5-C6	6.06	120.03	117.00
2	A	1836	C	N3-C4-C5	-6.06	119.48	121.90
2	A	149	A	C4-C5-C6	6.06	120.03	117.00
2	A	233	A	C5-C6-N6	-6.06	118.85	123.70
2	A	423	A	C4-C5-C6	6.06	120.03	117.00
2	A	510	A	C5-C6-N6	-6.06	118.86	123.70
2	A	1207	G	O4'-C1'-N9	6.06	113.05	108.20
2	A	1628	A	C4-C5-C6	6.06	120.03	117.00
2	A	1784	A	C4-C5-C6	6.06	120.03	117.00
2	A	533	C	N3-C4-C5	-6.06	119.48	121.90
2	A	600	G	C5-C6-O6	-6.05	124.97	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1422	U	O4'-C1'-N1	6.05	113.04	108.20
2	A	493	C	N3-C4-N4	6.05	122.24	118.00
2	A	977	A	C4-C5-C6	6.05	120.03	117.00
2	A	33	G	O4'-C1'-N9	6.05	113.04	108.20
2	A	166	A	C4-C5-C6	6.05	120.03	117.00
2	A	1309	A	C4-C5-C6	6.05	120.03	117.00
2	A	922	A	C4-C5-C6	6.05	120.03	117.00
2	A	1580	U	O4'-C1'-N1	6.05	113.04	108.20
2	A	1003	C	N3-C4-N4	6.05	122.23	118.00
2	A	301	C	N3-C4-N4	6.04	122.23	118.00
2	A	1048	A	C4-C5-C6	6.04	120.02	117.00
2	A	1615	A	C1'-O4'-C4'	-6.04	105.06	109.90
2	A	230	C	N3-C4-N4	6.04	122.23	118.00
2	A	350	A	C4-C5-C6	6.04	120.02	117.00
2	A	916	A	C4-C5-C6	6.04	120.02	117.00
2	A	1763	C	N3-C4-C5	-6.04	119.48	121.90
2	A	194	C	N3-C4-N4	6.04	122.23	118.00
2	A	1418	G	O4'-C1'-N9	6.04	113.03	108.20
3	F	6	A	C4-C5-C6	6.04	120.02	117.00
2	A	462	C	N3-C4-C5	-6.04	119.48	121.90
2	A	964	U	O4'-C1'-N1	6.04	113.03	108.20
2	A	1524	C	N3-C4-N4	6.04	122.23	118.00
2	A	1618	A	O4'-C1'-N9	6.04	113.03	108.20
6	H	96	TYR	CB-CG-CD1	-6.04	117.38	121.00
2	A	45	A	C4-C5-C6	6.04	120.02	117.00
2	A	1726	A	C4-C5-C6	6.04	120.02	117.00
2	A	141	A	C4-C5-C6	6.04	120.02	117.00
2	A	1020	A	C5-C6-N6	-6.03	118.87	123.70
2	A	1527	C	N3-C4-N4	6.03	122.22	118.00
2	A	1537	C	N3-C4-N4	6.03	122.22	118.00
2	A	1714	A	C4-C5-C6	6.03	120.02	117.00
2	A	42	A	C4-C5-C6	6.03	120.02	117.00
2	A	158	A	C4-C5-C6	6.03	120.02	117.00
2	A	730	C	N3-C4-N4	6.03	122.22	118.00
2	A	167	G	O4'-C1'-N9	6.03	113.03	108.20
2	A	448	A	C5-C6-N6	-6.03	118.88	123.70
2	A	1332	C	N3-C4-N4	6.03	122.22	118.00
2	A	1800	A	C4-C5-C6	6.03	120.02	117.00
1	N	58	A	C5-C6-N6	-6.03	118.88	123.70
2	A	1139	A	O4'-C1'-N9	6.03	113.02	108.20
2	A	21	U	O4'-C1'-N1	6.03	113.02	108.20
2	A	778	C	N3-C4-C5	-6.03	119.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1219	A	C4-C5-C6	6.03	120.01	117.00
2	A	1219	A	O4'-C1'-N9	6.03	113.02	108.20
2	A	1263	C	N3-C4-N4	6.03	122.22	118.00
2	A	1349	A	C4-C5-C6	6.03	120.01	117.00
2	A	40	A	C4-C5-C6	6.02	120.01	117.00
2	A	222	G	O4'-C1'-N9	6.02	113.02	108.20
2	A	1043	C	N3-C4-N4	6.02	122.22	118.00
2	A	1060	C	N3-C4-C5	-6.02	119.49	121.90
2	A	1608	G	O4'-C1'-N9	6.02	113.02	108.20
2	A	1844	A	C4-C5-C6	6.02	120.01	117.00
2	A	22	A	C5-C6-N6	-6.02	118.88	123.70
2	A	736	C	O4'-C1'-N1	6.02	113.02	108.20
2	A	821	A	C4-C5-C6	6.02	120.01	117.00
2	A	976	A	O4'-C1'-N9	6.02	113.02	108.20
2	A	79	A	C4-C5-C6	6.02	120.01	117.00
1	N	58	A	C4-C5-C6	6.02	120.01	117.00
2	A	442	G	O4'-C1'-N9	6.02	113.01	108.20
2	A	46	A	C4-C5-C6	6.01	120.01	117.00
2	A	366	A	C5-C6-N1	-6.01	114.69	117.70
2	A	953	A	C4-C5-C6	6.01	120.01	117.00
2	A	1078	A	C5-C6-N6	-6.01	118.89	123.70
2	A	1242	A	C4-C5-C6	6.01	120.01	117.00
2	A	290	A	C4-C5-C6	6.01	120.01	117.00
2	A	1116	U	O4'-C1'-N1	6.01	113.01	108.20
2	A	1204	A	C4-C5-C6	6.01	120.01	117.00
2	A	1240	U	P-O3'-C3'	6.01	126.91	119.70
2	A	1341	G	O4'-C1'-N9	6.01	113.01	108.20
2	A	1596	A	C4-C5-C6	6.01	120.01	117.00
2	A	205	G	O4'-C1'-N9	6.01	113.01	108.20
2	A	992	A	C4-C5-C6	6.01	120.00	117.00
2	A	1378	A	C5-C6-N1	-6.01	114.69	117.70
2	A	1551	A	C4-C5-C6	6.01	120.00	117.00
2	A	476	A	C4-C5-C6	6.00	120.00	117.00
18	V	118	ASN	C-N-CA	6.00	136.71	121.70
2	A	500	G	O4'-C1'-N9	6.00	113.00	108.20
2	A	909	A	C4-C5-C6	6.00	120.00	117.00
2	A	1167	G	O4'-C1'-N9	6.00	113.00	108.20
2	A	1779	C	O4'-C1'-N1	6.00	113.00	108.20
2	A	95	G	O4'-C1'-N9	6.00	113.00	108.20
2	A	1816	A	C4-C5-C6	6.00	120.00	117.00
2	A	295	C	O4'-C1'-N1	6.00	113.00	108.20
2	A	952	G	O4'-C1'-N9	6.00	113.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1710	A	C5-C6-N1	-6.00	114.70	117.70
2	A	1337	C	N3-C4-N4	6.00	122.20	118.00
2	A	1695	C	O4'-C1'-N1	6.00	113.00	108.20
2	A	1701	G	O4'-C1'-N9	6.00	113.00	108.20
1	N	34	A	C4-C5-C6	6.00	120.00	117.00
2	A	488	C	O4'-C1'-N1	6.00	113.00	108.20
2	A	814	A	C4-C5-C6	6.00	120.00	117.00
1	N	33	C	N3-C4-N4	5.99	122.19	118.00
2	A	195	C	N3-C4-C5	-5.99	119.50	121.90
2	A	609	A	C5-C6-N6	-5.99	118.91	123.70
2	A	1340	A	C5-C6-N6	-5.99	118.90	123.70
2	A	408	A	O4'-C1'-N9	5.99	112.99	108.20
2	A	835	C	N3-C4-N4	5.99	122.19	118.00
2	A	850	A	O4'-C1'-N9	5.99	112.99	108.20
2	A	611	C	O4'-C1'-N1	5.99	112.99	108.20
2	A	919	G	O4'-C1'-N9	5.99	112.99	108.20
2	A	1859	C	C6-N1-C1'	-5.99	113.62	120.80
2	A	480	C	N3-C4-N4	5.99	122.19	118.00
2	A	510	A	C5-C6-N1	-5.99	114.71	117.70
2	A	85	A	C4-C5-C6	5.98	119.99	117.00
2	A	951	A	C5-C6-N6	-5.98	118.91	123.70
2	A	593	C	N3-C4-N4	5.98	122.19	118.00
2	A	1274	A	C5-C6-N6	-5.98	118.91	123.70
2	A	1274	A	O4'-C1'-N9	5.98	112.99	108.20
2	A	1293	U	O4'-C1'-N1	5.98	112.99	108.20
2	A	1400	U	O4'-C1'-N1	5.98	112.99	108.20
2	A	1749	C	N3-C4-N4	5.98	122.19	118.00
2	A	313	C	N3-C4-N4	5.98	122.19	118.00
2	A	510	A	C4-C5-C6	5.98	119.99	117.00
2	A	798	A	C5-C6-N6	-5.98	118.92	123.70
2	A	1374	A	C5-C6-N6	-5.98	118.92	123.70
2	A	1700	C	N3-C4-N4	5.98	122.19	118.00
1	N	55	C	O4'-C1'-N1	5.98	112.98	108.20
2	A	735	C	N3-C4-C5	-5.98	119.51	121.90
2	A	967	G	O4'-C1'-N9	5.98	112.98	108.20
1	N	37	A	C5-C6-N1	-5.98	114.71	117.70
2	A	1256	A	C5-C6-N1	-5.98	114.71	117.70
2	A	1278	A	C4-C5-C6	5.98	119.99	117.00
2	A	1762	A	C4-C5-C6	5.98	119.99	117.00
2	A	49	C	O4'-C1'-N1	5.97	112.98	108.20
2	A	1679	C	N3-C4-C5	-5.97	119.51	121.90
2	A	1847	C	N3-C4-N4	5.97	122.18	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	659	A	C4-C5-C6	5.97	119.99	117.00
2	A	845	A	C5-C6-N1	-5.97	114.71	117.70
2	A	1096	A	C4-C5-C6	5.97	119.99	117.00
2	A	463	A	C4-C5-C6	5.97	119.99	117.00
2	A	1247	A	C4-C5-C6	5.97	119.99	117.00
2	A	229	A	C4-C5-C6	5.97	119.98	117.00
2	A	238	G	O4'-C1'-N9	5.97	112.98	108.20
2	A	1222	G	C5-C6-O6	-5.97	125.02	128.60
2	A	1396	U	O4'-C1'-N1	5.97	112.97	108.20
2	A	1621	C	N3-C4-N4	5.97	122.18	118.00
2	A	1781	G	O4'-C1'-N9	5.97	112.97	108.20
2	A	69	C	N3-C4-N4	5.97	122.18	118.00
2	A	99	A	C5-C6-N6	-5.97	118.92	123.70
2	A	343	C	N3-C4-C5	-5.97	119.51	121.90
2	A	882	A	C5-C6-N6	-5.97	118.93	123.70
1	N	43	A	C4-C5-C6	5.97	119.98	117.00
2	A	806	A	C4-C5-C6	5.97	119.98	117.00
2	A	1031	A	C4-C5-C6	5.97	119.98	117.00
2	A	1669	G	N3-C2-N2	5.97	124.08	119.90
2	A	1417	A	C4-C5-C6	5.96	119.98	117.00
2	A	1646	A	C4-C5-C6	5.96	119.98	117.00
2	A	508	G	O4'-C1'-N9	5.96	112.97	108.20
2	A	1564	A	C5-C6-N1	-5.96	114.72	117.70
2	A	1264	C	O4'-C1'-N1	5.96	112.97	108.20
2	A	805	A	C5-C6-N6	-5.96	118.93	123.70
2	A	1252	G	C5-C6-O6	-5.96	125.02	128.60
2	A	1032	A	C5-C6-N6	-5.96	118.93	123.70
2	A	1472	A	C5-C6-N6	-5.96	118.93	123.70
2	A	1707	A	C4-C5-C6	5.96	119.98	117.00
2	A	353	A	C4-C5-C6	5.96	119.98	117.00
2	A	390	C	O4'-C1'-N1	5.96	112.97	108.20
2	A	904	A	C4-C5-C6	5.96	119.98	117.00
2	A	1096	A	C5-C6-N6	-5.96	118.94	123.70
2	A	1187	C	N3-C4-N4	5.96	122.17	118.00
2	A	232	A	C4-C5-C6	5.96	119.98	117.00
2	A	512	A	C4-C5-C6	5.95	119.98	117.00
2	A	535	A	C4-C5-C6	5.95	119.98	117.00
2	A	1008	A	C5-C6-N6	-5.95	118.94	123.70
2	A	1019	A	C5-C6-N6	-5.95	118.94	123.70
2	A	1670	A	C5-C6-N1	-5.95	114.72	117.70
2	A	127	C	N3-C4-C5	-5.95	119.52	121.90
2	A	231	C	N3-C4-N4	5.95	122.17	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	912	A	C5-C6-N6	-5.95	118.94	123.70
2	A	1691	C	N3-C4-C5	-5.95	119.52	121.90
1	N	14	A	C5-N7-C8	5.95	106.88	103.90
2	A	1226	C	N3-C4-C5	-5.95	119.52	121.90
2	A	1628	A	C5-C6-N6	-5.95	118.94	123.70
2	A	1656	A	O4'-C1'-N9	5.95	112.96	108.20
2	A	1810	G	O4'-C1'-N9	5.95	112.96	108.20
2	A	292	A	C4-C5-C6	5.95	119.97	117.00
2	A	338	A	C5-C6-N1	-5.95	114.73	117.70
2	A	127	C	N3-C4-N4	5.95	122.16	118.00
2	A	584	A	C5-C6-N6	-5.95	118.94	123.70
2	A	1281	G	O4'-C1'-N9	5.95	112.96	108.20
2	A	435	A	O4'-C1'-N9	5.95	112.96	108.20
2	A	1079	A	O4'-C1'-N9	5.94	112.96	108.20
2	A	1497	C	N3-C4-N4	5.94	122.16	118.00
2	A	841	G	O4'-C1'-N9	5.94	112.95	108.20
2	A	1397	A	C5-C6-N6	-5.94	118.95	123.70
2	A	1819	A	O4'-C1'-N9	5.94	112.95	108.20
2	A	1369	C	N3-C4-N4	5.94	122.16	118.00
2	A	1430	C	N3-C4-N4	5.94	122.16	118.00
2	A	1659	A	O4'-C1'-N9	5.94	112.95	108.20
2	A	1665	C	N3-C4-N4	5.94	122.16	118.00
1	N	37	A	C5-C6-N6	-5.94	118.95	123.70
2	A	666	C	N3-C4-C5	-5.94	119.53	121.90
2	A	807	A	O4'-C1'-N9	5.94	112.95	108.20
2	A	164	A	O4'-C1'-N9	5.94	112.95	108.20
2	A	911	G	C5-C6-O6	-5.94	125.04	128.60
25	c	67	TYR	CB-CG-CD2	-5.94	117.44	121.00
2	A	435	A	C4-C5-C6	5.93	119.97	117.00
2	A	445	A	C5-C6-N6	-5.93	118.96	123.70
2	A	391	A	C4-C5-C6	5.93	119.97	117.00
2	A	420	C	N3-C4-N4	5.93	122.15	118.00
2	A	550	A	C5-C6-N1	-5.93	114.73	117.70
2	A	631	A	C4-C5-C6	5.93	119.97	117.00
2	A	867	U	O4'-C1'-N1	5.93	112.94	108.20
2	A	1147	G	O4'-C1'-N9	5.93	112.94	108.20
2	A	1640	C	N3-C4-N4	5.93	122.15	118.00
1	N	65	C	N3-C4-C5	-5.93	119.53	121.90
2	A	1194	G	O4'-C1'-N9	5.93	112.94	108.20
2	A	1554	C	N3-C4-C5	-5.93	119.53	121.90
2	A	438	A	O4'-C1'-N9	5.93	112.94	108.20
2	A	497	G	O4'-C1'-N9	5.93	112.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	733	G	O4'-C1'-N9	5.93	112.94	108.20
2	A	1218	G	O4'-C1'-N9	5.93	112.94	108.20
2	A	1448	A	C5-C6-N6	-5.93	118.96	123.70
2	A	1693	C	N3-C4-N4	5.93	122.15	118.00
2	A	25	A	P-O5'-C5'	5.92	130.38	120.90
2	A	111	A	C5-C6-N1	-5.92	114.74	117.70
2	A	1058	A	C4-C5-C6	5.92	119.96	117.00
2	A	1832	U	O4'-C1'-N1	5.92	112.94	108.20
29	g	167	TYR	CB-CG-CD2	-5.92	117.45	121.00
2	A	17	C	O4'-C1'-N1	5.92	112.94	108.20
2	A	434	G	O4'-C1'-N9	5.92	112.94	108.20
2	A	127	C	O4'-C1'-N1	5.92	112.94	108.20
2	A	204	G	O4'-C1'-N9	5.92	112.94	108.20
2	A	329	A	C5-C6-N6	-5.92	118.96	123.70
2	A	416	A	C4-C5-C6	5.92	119.96	117.00
2	A	521	A	C5-C6-N1	-5.92	114.74	117.70
2	A	1007	A	C4-C5-C6	5.92	119.96	117.00
2	A	1038	A	C5-C6-N6	-5.92	118.96	123.70
2	A	1624	C	N3-C4-N4	5.92	122.15	118.00
2	A	1022	C	N3-C4-N4	5.92	122.14	118.00
2	A	1193	G	O4'-C1'-N9	5.92	112.94	108.20
2	A	1080	A	C5-C6-N6	-5.92	118.97	123.70
2	A	1398	A	C5-C6-N6	-5.92	118.97	123.70
2	A	1064	G	C5-C6-O6	-5.92	125.05	128.60
2	A	1262	C	O4'-C1'-N1	5.91	112.93	108.20
2	A	1333	C	N3-C4-N4	5.91	122.14	118.00
2	A	1449	C	N3-C4-C5	-5.91	119.53	121.90
2	A	1729	G	N3-C2-N2	5.91	124.04	119.90
2	A	44	U	O4'-C1'-N1	5.91	112.93	108.20
2	A	980	C	N3-C4-N4	5.91	122.14	118.00
2	A	1379	A	C5-C6-N1	-5.91	114.74	117.70
2	A	439	A	C4-C5-C6	5.91	119.96	117.00
2	A	551	A	C4-C5-C6	5.91	119.96	117.00
2	A	1130	G	O4'-C1'-N9	5.91	112.93	108.20
2	A	1398	A	C4-C5-C6	5.91	119.95	117.00
2	A	1670	A	C5-C6-N6	-5.91	118.97	123.70
2	A	1779	C	N3-C4-N4	5.91	122.14	118.00
1	N	4	A	C5-C6-N6	-5.91	118.97	123.70
2	A	379	A	C4-C5-C6	5.91	119.95	117.00
2	A	735	C	N3-C4-N4	5.91	122.14	118.00
2	A	1008	A	C4-C5-C6	5.91	119.95	117.00
2	A	1375	A	C5-C6-N1	-5.91	114.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	845	A	C4-C5-C6	5.91	119.95	117.00
2	A	1465	A	C4-C5-C6	5.91	119.95	117.00
2	A	1469	G	O4'-C1'-N9	5.91	112.93	108.20
2	A	1636	A	C4-C5-C6	5.91	119.95	117.00
2	A	1857	A	C4-C5-C6	5.91	119.95	117.00
2	A	446	C	N3-C4-N4	5.90	122.13	118.00
2	A	849	C	N3-C4-N4	5.90	122.13	118.00
2	A	1047	G	O4'-C1'-N9	5.90	112.92	108.20
2	A	1200	A	C4-C5-C6	5.90	119.95	117.00
2	A	181	A	C4-C5-C6	5.90	119.95	117.00
2	A	214	A	C4-C5-C6	5.90	119.95	117.00
2	A	509	A	C4-C5-C6	5.90	119.95	117.00
2	A	659	A	C5-C6-N6	-5.90	118.98	123.70
2	A	979	A	C4-C5-C6	5.90	119.95	117.00
2	A	1289	A	C4-C5-C6	5.90	119.95	117.00
2	A	1498	C	N3-C4-N4	5.90	122.13	118.00
2	A	1540	A	C4-C5-C6	5.90	119.95	117.00
2	A	1614	A	C4-C5-C6	5.90	119.95	117.00
2	A	1410	A	O4'-C1'-N9	5.90	112.92	108.20
2	A	1559	C	N3-C4-N4	5.90	122.13	118.00
2	A	653	C	N3-C4-N4	5.90	122.13	118.00
2	A	1106	G	O4'-C1'-N9	5.90	112.92	108.20
2	A	589	A	C4-C5-C6	5.90	119.95	117.00
2	A	1299	C	C6-N1-C1'	-5.90	113.72	120.80
2	A	1526	A	C4-C5-C6	5.90	119.95	117.00
2	A	471	C	N3-C4-N4	5.89	122.13	118.00
2	A	953	A	O4'-C1'-N9	5.89	112.92	108.20
2	A	1176	C	O4'-C1'-N1	5.89	112.92	108.20
2	A	99	A	C4-C5-C6	5.89	119.95	117.00
2	A	1656	A	C5-C6-N6	-5.89	118.99	123.70
2	A	1450	A	C5-C6-N6	-5.89	118.99	123.70
2	A	103	A	C5-C6-N6	-5.89	118.99	123.70
2	A	526	A	O4'-C1'-N9	5.89	112.91	108.20
2	A	1140	A	C5-C6-N6	-5.89	118.99	123.70
2	A	1195	A	C4-C5-C6	5.89	119.94	117.00
2	A	1268	C	N3-C4-N4	5.89	122.12	118.00
2	A	1282	G	O4'-C1'-N9	5.89	112.91	108.20
2	A	1735	C	N3-C4-C5	-5.89	119.54	121.90
2	A	755	C	N3-C4-N4	5.89	122.12	118.00
2	A	1102	C	N3-C4-N4	5.89	122.12	118.00
2	A	1583	A	C4-C5-C6	5.89	119.94	117.00
2	A	1629	A	C5-C6-N6	-5.89	118.99	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1813	A	C5-C6-N6	-5.89	118.99	123.70
1	N	67	C	N3-C4-C5	-5.88	119.55	121.90
2	A	125	C	N3-C4-N4	5.88	122.12	118.00
2	A	272	C	N3-C4-C5	-5.88	119.55	121.90
2	A	970	C	N3-C4-N4	5.88	122.12	118.00
2	A	1178	A	C5-C6-N1	-5.88	114.76	117.70
2	A	1262	C	N3-C4-C5	-5.88	119.55	121.90
2	A	1518	C	N3-C4-C5	-5.88	119.55	121.90
2	A	88	G	O4'-C1'-N9	5.88	112.91	108.20
2	A	1	U	O4'-C1'-N1	5.88	112.91	108.20
2	A	68	A	C4-C5-C6	5.88	119.94	117.00
2	A	507	C	N3-C4-C5	-5.88	119.55	121.90
2	A	968	A	C5-C6-N6	-5.88	118.99	123.70
2	A	979	A	O4'-C1'-N9	5.88	112.91	108.20
2	A	1027	A	C4-C5-C6	5.88	119.94	117.00
2	A	1515	G	C4-N9-C1'	5.88	134.15	126.50
2	A	1707	A	C5-C6-N1	-5.88	114.76	117.70
1	N	5	G	O4'-C1'-N9	5.88	112.90	108.20
2	A	517	C	N3-C4-N4	5.88	122.12	118.00
2	A	94	G	O4'-C1'-N9	5.88	112.90	108.20
2	A	450	A	O4'-C1'-N9	5.88	112.90	108.20
2	A	595	A	C5-C6-N6	-5.88	119.00	123.70
2	A	14	C	N3-C4-N4	5.88	122.11	118.00
2	A	474	A	C4-C5-C6	5.88	119.94	117.00
2	A	1049	C	N3-C4-N4	5.88	122.11	118.00
2	A	1113	C	C6-N1-C1'	-5.88	113.75	120.80
2	A	1178	A	C5-C6-N6	-5.88	119.00	123.70
2	A	1368	U	O4'-C1'-N1	5.88	112.90	108.20
2	A	1395	C	N3-C4-C5	-5.88	119.55	121.90
2	A	535	A	O4'-C1'-N9	5.88	112.90	108.20
2	A	684	A	C4-C5-C6	5.88	119.94	117.00
2	A	1803	A	C5-C6-N6	-5.88	119.00	123.70
2	A	145	G	O4'-C1'-N9	5.87	112.90	108.20
2	A	404	A	C4-C5-C6	5.87	119.94	117.00
2	A	404	A	C5-C6-N6	-5.87	119.00	123.70
2	A	1166	A	O4'-C1'-N9	5.87	112.90	108.20
2	A	1776	G	C5-C6-O6	-5.87	125.08	128.60
2	A	232	A	C5-C6-N6	-5.87	119.00	123.70
2	A	826	A	C5-C6-N6	-5.87	119.00	123.70
2	A	1750	C	N3-C4-C5	-5.87	119.55	121.90
2	A	652	G	C5-C6-O6	-5.87	125.08	128.60
2	A	988	A	C4-C5-C6	5.87	119.94	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1829	A	C4-C5-C6	5.87	119.94	117.00
2	A	1860	A	C4-C5-C6	5.87	119.94	117.00
2	A	937	C	N3-C4-N4	5.87	122.11	118.00
2	A	951	A	C4-C5-C6	5.87	119.94	117.00
2	A	1257	C	N3-C4-N4	5.87	122.11	118.00
2	A	511	A	C5-C6-N6	-5.87	119.01	123.70
2	A	976	A	C4-C5-C6	5.87	119.93	117.00
2	A	19	A	O4'-C1'-N9	5.87	112.89	108.20
2	A	182	C	N3-C4-N4	5.87	122.11	118.00
2	A	440	C	C2-N1-C1'	5.87	125.25	118.80
2	A	1690	A	C5-C6-N6	-5.87	119.01	123.70
2	A	398	A	C4-C5-C6	5.86	119.93	117.00
2	A	1169	A	C4-C5-C6	5.86	119.93	117.00
2	A	1216	A	C5-C6-N6	-5.86	119.01	123.70
2	A	440	C	N3-C4-N4	5.86	122.10	118.00
2	A	918	A	C4-C5-C6	5.86	119.93	117.00
3	F	13	G	O4'-C1'-N9	5.86	112.89	108.20
1	N	32	C	N3-C4-C5	-5.86	119.56	121.90
2	A	61	A	C5-C6-N6	-5.86	119.01	123.70
2	A	110	U	O4'-C1'-N1	5.86	112.89	108.20
2	A	1803	A	C4-C5-C6	5.86	119.93	117.00
2	A	1051	A	C4-C5-C6	5.86	119.93	117.00
2	A	1336	U	O4'-C1'-N1	5.86	112.89	108.20
2	A	1704	G	O4'-C1'-N9	5.86	112.89	108.20
2	A	1465	A	C5-C6-N6	-5.86	119.02	123.70
2	A	538	C	N3-C4-C5	-5.85	119.56	121.90
2	A	1470	A	C5-C6-N6	-5.85	119.02	123.70
2	A	606	A	C4-C5-C6	5.85	119.93	117.00
2	A	1049	C	N3-C4-C5	-5.85	119.56	121.90
2	A	1466	C	N3-C4-C5	-5.85	119.56	121.90
2	A	1263	C	N3-C4-C5	-5.85	119.56	121.90
2	A	85	A	C5-C6-N1	-5.85	114.78	117.70
2	A	498	A	O4'-C1'-N9	5.85	112.88	108.20
2	A	107	A	C5-C6-N1	-5.85	114.78	117.70
2	A	309	A	C5-C6-N6	-5.85	119.02	123.70
1	N	61	C	N3-C4-C5	-5.85	119.56	121.90
2	A	46	A	C5-C6-N1	-5.84	114.78	117.70
2	A	302	C	O4'-C1'-N1	5.84	112.88	108.20
2	A	1027	A	C5-C6-N6	-5.84	119.03	123.70
2	A	1181	C	N3-C4-N4	5.84	122.09	118.00
16	T	118	TYR	CB-CG-CD2	5.84	124.51	121.00
2	A	903	G	O4'-C1'-N9	5.84	112.87	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	61	A	O4'-C1'-N9	5.84	112.87	108.20
2	A	339	A	C4-C5-C6	5.84	119.92	117.00
2	A	387	G	O4'-C1'-N9	5.84	112.87	108.20
2	A	654	A	O4'-C1'-N9	5.84	112.87	108.20
1	N	14	A	C5-C6-N1	-5.84	114.78	117.70
2	A	195	C	N3-C4-N4	5.84	122.09	118.00
2	A	214	A	C5-C6-N6	-5.84	119.03	123.70
2	A	1185	A	C5-C6-N1	-5.84	114.78	117.70
2	A	1298	G	C5-C6-O6	-5.84	125.10	128.60
2	A	922	A	O4'-C1'-N9	5.84	112.87	108.20
2	A	1436	C	N3-C4-N4	5.84	122.09	118.00
2	A	666	C	N3-C4-N4	5.84	122.08	118.00
2	A	1026	A	C4-C5-C6	5.84	119.92	117.00
2	A	1140	A	C5-C6-N1	-5.84	114.78	117.70
2	A	1845	A	C4-C5-C6	5.84	119.92	117.00
2	A	41	G	C5-C6-O6	-5.83	125.10	128.60
2	A	1376	C	N3-C4-N4	5.83	122.08	118.00
2	A	635	C	N3-C4-N4	5.83	122.08	118.00
2	A	290	A	O4'-C1'-N9	5.83	112.86	108.20
2	A	476	A	C5-C6-N6	-5.83	119.04	123.70
2	A	487	C	N3-C4-N4	5.83	122.08	118.00
2	A	83	A	O4'-C1'-N9	5.83	112.86	108.20
2	A	236	C	N3-C4-N4	5.83	122.08	118.00
2	A	1237	A	C4-C5-C6	5.83	119.91	117.00
2	A	1291	A	C5-C6-N1	-5.83	114.79	117.70
2	A	1673	A	C5-C6-N1	-5.83	114.79	117.70
3	F	25	U	O4'-C1'-N1	5.83	112.86	108.20
2	A	91	A	O4'-C1'-N9	5.83	112.86	108.20
2	A	398	A	C5-C6-N1	-5.83	114.79	117.70
2	A	1307	C	N3-C4-N4	5.83	122.08	118.00
2	A	1349	A	C5-C6-N6	-5.83	119.04	123.70
2	A	1545	G	O4'-C1'-N9	5.83	112.86	108.20
2	A	425	A	C4-C5-C6	5.83	119.91	117.00
2	A	622	C	N3-C4-C5	-5.83	119.57	121.90
2	A	645	A	C5-C6-N1	-5.83	114.79	117.70
2	A	856	G	O4'-C1'-N9	5.83	112.86	108.20
2	A	1090	C	N3-C4-N4	5.83	122.08	118.00
2	A	1826	A	C4-C5-C6	5.83	119.91	117.00
2	A	1835	C	N3-C4-C5	-5.83	119.57	121.90
2	A	386	U	O4'-C1'-N1	5.82	112.86	108.20
2	A	1213	A	C5-C6-N1	-5.82	114.79	117.70
2	A	1417	A	C5-C6-N6	-5.82	119.04	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1587	C	N3-C4-N4	5.82	122.08	118.00
2	A	65	C	N3-C4-N4	5.82	122.08	118.00
2	A	60	A	C5-C6-N6	-5.82	119.04	123.70
2	A	388	A	C4-C5-C6	5.82	119.91	117.00
2	A	788	C	N3-C4-C5	-5.82	119.57	121.90
2	A	976	A	C5-C6-N6	-5.82	119.04	123.70
2	A	1708	C	N3-C4-N4	5.82	122.08	118.00
2	A	976	A	C5-C6-N1	-5.82	114.79	117.70
2	A	1374	A	C4-C5-C6	5.82	119.91	117.00
2	A	1163	G	O4'-C1'-N9	5.82	112.85	108.20
2	A	1297	A	C4-C5-C6	5.82	119.91	117.00
2	A	1476	A	C5-C6-N6	-5.82	119.05	123.70
2	A	1571	G	O4'-C1'-N9	5.82	112.85	108.20
2	A	159	A	C4-C5-C6	5.82	119.91	117.00
2	A	234	C	N3-C4-C5	-5.82	119.57	121.90
2	A	929	G	C5-C6-O6	-5.82	125.11	128.60
2	A	1711	C	N3-C4-N4	5.82	122.07	118.00
2	A	333	A	C5-C6-N6	-5.81	119.05	123.70
2	A	972	G	O4'-C1'-N9	5.81	112.85	108.20
2	A	1317	G	O4'-C1'-N9	5.81	112.85	108.20
2	A	1384	A	C5-C6-N1	-5.81	114.79	117.70
2	A	1602	A	C4-C5-C6	5.81	119.91	117.00
2	A	1461	A	C5-C6-N1	-5.81	114.79	117.70
2	A	38	A	C4-C5-C6	5.81	119.90	117.00
2	A	53	C	N3-C4-C5	-5.81	119.58	121.90
2	A	545	A	C5-C6-N6	-5.81	119.05	123.70
2	A	1378	A	C5-C6-N6	-5.81	119.05	123.70
2	A	193	C	N3-C4-N4	5.81	122.06	118.00
2	A	436	G	O4'-C1'-N9	5.81	112.85	108.20
2	A	1084	U	O4'-C1'-N1	5.81	112.85	108.20
2	A	1385	C	N3-C4-C5	-5.81	119.58	121.90
2	A	1502	A	C4-C5-C6	5.81	119.90	117.00
2	A	1528	A	C4-C5-C6	5.81	119.90	117.00
2	A	734	C	N3-C4-N4	5.81	122.06	118.00
1	N	37	A	C4-C5-C6	5.80	119.90	117.00
2	A	273	G	O4'-C1'-N9	5.80	112.84	108.20
2	A	1179	A	C5-C6-N1	-5.80	114.80	117.70
2	A	1466	C	N3-C4-N4	5.80	122.06	118.00
2	A	1661	C	N3-C4-C5	-5.80	119.58	121.90
2	A	1805	C	N3-C4-C5	-5.80	119.58	121.90
2	A	84	A	C4-C5-C6	5.80	119.90	117.00
2	A	1224	A	C4-C5-C6	5.80	119.90	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1661	C	N3-C4-N4	5.80	122.06	118.00
2	A	307	G	O4'-C1'-N9	5.80	112.84	108.20
2	A	1191	A	C5-C6-N6	-5.80	119.06	123.70
2	A	1787	A	C5-C6-N1	-5.80	114.80	117.70
2	A	272	C	N3-C4-N4	5.80	122.06	118.00
2	A	326	A	O4'-C1'-N9	5.80	112.84	108.20
2	A	643	A	C5-C6-N6	-5.80	119.06	123.70
2	A	815	G	O4'-C1'-N9	5.80	112.84	108.20
2	A	1129	A	C5-C6-N1	-5.80	114.80	117.70
2	A	1650	C	N3-C4-N4	5.80	122.06	118.00
2	A	1145	A	O4'-C1'-N9	5.80	112.84	108.20
2	A	1513	C	N3-C4-N4	5.80	122.06	118.00
2	A	78	C	N3-C4-N4	5.80	122.06	118.00
2	A	450	A	C4-C5-C6	5.80	119.90	117.00
2	A	598	C	N3-C4-N4	5.80	122.06	118.00
2	A	1202	G	O4'-C1'-N9	5.80	112.84	108.20
2	A	1303	U	P-O5'-C5'	5.80	130.18	120.90
2	A	1622	C	N3-C4-N4	5.80	122.06	118.00
2	A	1674	A	C5-C6-N1	-5.80	114.80	117.70
2	A	1688	G	O4'-C1'-N9	5.80	112.84	108.20
2	A	353	A	C5-C6-N6	-5.79	119.06	123.70
2	A	963	C	N3-C4-N4	5.79	122.06	118.00
2	A	268	G	C1'-O4'-C4'	-5.79	105.27	109.90
2	A	283	A	O4'-C1'-N9	5.79	112.83	108.20
2	A	577	A	C5-C6-N1	-5.79	114.80	117.70
2	A	643	A	C4-C5-C6	5.79	119.90	117.00
2	A	664	C	N3-C4-C5	-5.79	119.58	121.90
2	A	1076	A	C4-C5-C6	5.79	119.90	117.00
2	A	654	A	C4-C5-C6	5.79	119.90	117.00
2	A	382	A	C5-C6-N6	-5.79	119.07	123.70
2	A	455	A	C5-C6-N1	-5.79	114.81	117.70
2	A	1479	A	C4-C5-C6	5.79	119.89	117.00
2	A	1484	C	N3-C4-N4	5.79	122.05	118.00
2	A	1859	C	N3-C4-N4	5.79	122.05	118.00
2	A	13	C	N3-C4-N4	5.79	122.05	118.00
2	A	359	C	C6-N1-C1'	-5.79	113.85	120.80
2	A	1086	C	N3-C4-N4	5.79	122.05	118.00
2	A	376	C	N3-C4-C5	-5.79	119.58	121.90
2	A	424	G	O4'-C1'-N9	5.79	112.83	108.20
2	A	923	C	N3-C4-C5	-5.79	119.58	121.90
2	A	1002	C	N3-C4-N4	5.79	122.05	118.00
2	A	1761	C	N3-C4-C5	-5.79	119.58	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	157	U	O4'-C1'-N1	5.79	112.83	108.20
2	A	855	G	O4'-C1'-N9	5.79	112.83	108.20
2	A	1249	A	C5-C6-N6	-5.79	119.07	123.70
1	N	21	G	O4'-C1'-N9	5.78	112.83	108.20
2	A	661	A	C4-C5-C6	5.78	119.89	117.00
2	A	838	C	N3-C4-N4	5.78	122.05	118.00
2	A	1023	A	C5-C6-N6	-5.78	119.07	123.70
2	A	1302	U	O4'-C1'-N1	5.78	112.83	108.20
2	A	1392	A	C5-C6-N6	-5.78	119.07	123.70
2	A	1602	A	C5-C6-N6	-5.78	119.07	123.70
2	A	83	A	C5-C6-N1	-5.78	114.81	117.70
2	A	605	C	N3-C4-C5	-5.78	119.59	121.90
2	A	896	C	N3-C4-N4	5.78	122.05	118.00
2	A	1677	C	N3-C4-N4	5.78	122.05	118.00
2	A	1124	C	N3-C4-C5	-5.78	119.59	121.90
2	A	623	C	N3-C4-C5	-5.78	119.59	121.90
2	A	1201	C	N3-C4-N4	5.78	122.05	118.00
2	A	471	C	N3-C4-C5	-5.78	119.59	121.90
2	A	660	A	C5-C6-N1	-5.78	114.81	117.70
2	A	1464	C	N3-C4-N4	5.78	122.04	118.00
2	A	1863	A	C5-C6-N1	-5.77	114.81	117.70
3	F	11	A	C5-C6-N6	-5.77	119.08	123.70
2	A	507	C	N3-C4-N4	5.77	122.04	118.00
2	A	513	A	C4-C5-C6	5.77	119.89	117.00
2	A	1375	A	C4-C5-C6	5.77	119.89	117.00
2	A	1604	C	N3-C4-N4	5.77	122.04	118.00
1	N	14	A	O4'-C1'-N9	5.77	112.82	108.20
2	A	750	G	O4'-C1'-N9	5.77	112.82	108.20
2	A	1366	A	C5-C6-N6	-5.77	119.08	123.70
2	A	159	A	O4'-C1'-N9	5.77	112.82	108.20
2	A	190	A	P-O3'-C3'	5.77	126.62	119.70
2	A	432	C	N3-C4-C5	-5.77	119.59	121.90
2	A	582	C	N3-C4-N4	5.77	122.04	118.00
2	A	630	A	C4-C5-C6	5.77	119.89	117.00
2	A	872	C	N3-C4-N4	5.77	122.04	118.00
2	A	1504	A	C5-C6-N1	-5.77	114.82	117.70
2	A	1754	G	O4'-C1'-N9	5.77	112.81	108.20
2	A	1777	C	N3-C4-N4	5.77	122.04	118.00
2	A	628	C	N3-C4-N4	5.77	122.04	118.00
2	A	852	C	N3-C4-N4	5.77	122.04	118.00
2	A	1004	A	C5-C6-N1	-5.77	114.82	117.70
2	A	1353	A	C4-C5-C6	5.77	119.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1410	A	C5-C6-N6	-5.77	119.09	123.70
2	A	1796	C	N3-C4-N4	5.77	122.04	118.00
2	A	166	A	C5-C6-N6	-5.77	119.09	123.70
2	A	338	A	C4-C5-C6	5.77	119.88	117.00
2	A	1131	C	N3-C4-N4	5.77	122.04	118.00
2	A	425	A	O4'-C1'-N9	5.76	112.81	108.20
2	A	1518	C	N3-C4-N4	5.76	122.03	118.00
2	A	1699	C	P-O3'-C3'	5.76	126.61	119.70
2	A	1807	A	C4-C5-C6	5.76	119.88	117.00
2	A	1696	C	N3-C4-N4	5.76	122.03	118.00
16	T	125	PHE	CB-CG-CD2	-5.76	116.77	120.80
28	f	139	TYR	CB-CG-CD2	-5.76	117.54	121.00
2	A	293	A	C5-C6-N1	-5.76	114.82	117.70
2	A	1327	C	N3-C4-N4	5.76	122.03	118.00
2	A	175	A	C5-C6-N1	-5.76	114.82	117.70
3	F	10	C	N3-C4-N4	5.76	122.03	118.00
1	N	59	A	C4-C5-C6	5.75	119.88	117.00
2	A	791	A	C5-C6-N6	-5.75	119.10	123.70
2	A	994	A	C5-C6-N1	-5.75	114.82	117.70
1	N	39	C	N3-C4-N4	5.75	122.03	118.00
2	A	675	A	C4-C5-C6	5.75	119.88	117.00
2	A	1046	A	C4-C5-C6	5.75	119.88	117.00
2	A	1230	C	N3-C4-N4	5.75	122.03	118.00
2	A	340	C	N3-C4-C5	-5.75	119.60	121.90
2	A	1211	C	N3-C4-N4	5.75	122.03	118.00
2	A	1224	A	C5-C6-N1	-5.75	114.82	117.70
2	A	1399	C	C2-N1-C1'	5.75	125.13	118.80
2	A	1479	A	O4'-C1'-N9	5.75	112.80	108.20
2	A	1269	C	N3-C4-N4	5.75	122.03	118.00
2	A	1482	A	C4-C5-C6	5.75	119.88	117.00
2	A	1698	C	N3-C4-C5	-5.75	119.60	121.90
2	A	1179	A	C5-C6-N6	-5.75	119.10	123.70
2	A	527	C	N3-C4-C5	-5.75	119.60	121.90
2	A	1210	A	O4'-C1'-N9	5.75	112.80	108.20
2	A	1275	C	N3-C4-N4	5.75	122.02	118.00
2	A	171	A	C5-C6-N1	-5.75	114.83	117.70
2	A	223	A	O4'-C1'-N9	5.75	112.80	108.20
2	A	352	C	N3-C4-N4	5.75	122.02	118.00
2	A	1037	G	O4'-C1'-N9	5.75	112.80	108.20
2	A	1524	C	N3-C4-C5	-5.75	119.60	121.90
2	A	539	C	N3-C4-N4	5.74	122.02	118.00
2	A	1171	G	O4'-C1'-N9	5.74	112.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1677	C	N3-C4-C5	-5.74	119.60	121.90
2	A	1372	A	C4-C5-C6	5.74	119.87	117.00
2	A	1560	C	N3-C4-N4	5.74	122.02	118.00
2	A	904	A	C5-C6-N1	-5.74	114.83	117.70
2	A	933	C	N3-C4-N4	5.74	122.02	118.00
2	A	944	C	N3-C4-C5	-5.74	119.60	121.90
2	A	1843	G	O4'-C1'-N9	5.74	112.79	108.20
2	A	321	C	N3-C4-C5	-5.74	119.61	121.90
2	A	1081	C	N3-C4-N4	5.74	122.02	118.00
2	A	1692	A	C4-C5-C6	5.74	119.87	117.00
1	N	31	C	N3-C4-N4	5.74	122.02	118.00
2	A	312	C	N3-C4-N4	5.74	122.02	118.00
2	A	861	A	C5-C6-N1	-5.74	114.83	117.70
2	A	960	A	C5-C6-N1	-5.74	114.83	117.70
2	A	535	A	C5-C6-N6	-5.74	119.11	123.70
2	A	1117	G	O4'-C1'-N9	5.74	112.79	108.20
2	A	1190	A	C5-C6-N1	-5.74	114.83	117.70
2	A	1472	A	C5-C6-N1	-5.74	114.83	117.70
2	A	1585	C	N3-C4-N4	5.74	122.01	118.00
2	A	129	C	O4'-C1'-C2'	-5.73	100.07	105.80
2	A	272	C	O4'-C1'-N1	5.73	112.79	108.20
2	A	554	A	C5-C6-N1	-5.73	114.83	117.70
2	A	825	C	N3-C4-N4	5.73	122.01	118.00
2	A	880	C	N3-C4-C5	-5.73	119.61	121.90
2	A	1262	C	N3-C4-N4	5.73	122.01	118.00
2	A	833	A	C5-C6-N6	-5.73	119.12	123.70
2	A	835	C	N3-C4-C5	-5.73	119.61	121.90
2	A	1327	C	C2-N1-C1'	5.73	125.10	118.80
2	A	1442	A	C5-C6-N6	-5.73	119.11	123.70
2	A	1584	A	C4-C5-C6	5.73	119.86	117.00
2	A	89	C	N3-C4-C5	-5.73	119.61	121.90
2	A	1854	A	C5-C6-N6	-5.73	119.12	123.70
3	F	11	A	C4-C5-C6	5.73	119.86	117.00
2	A	569	C	N3-C4-N4	5.73	122.01	118.00
2	A	1237	A	C5-C6-N6	-5.73	119.12	123.70
2	A	495	G	O4'-C1'-N9	5.73	112.78	108.20
2	A	574	A	C5-C6-N6	-5.73	119.12	123.70
2	A	1764	G	C5-C6-O6	-5.73	125.16	128.60
2	A	459	A	O4'-C1'-N9	5.72	112.78	108.20
2	A	1854	A	C4-C5-C6	5.72	119.86	117.00
2	A	1267	C	N3-C4-N4	5.72	122.00	118.00
2	A	1475	G	O4'-C1'-N9	5.72	112.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	120	U	O4'-C1'-N1	5.72	112.78	108.20
2	A	1109	A	O4'-C1'-N9	5.72	112.78	108.20
2	A	1246	A	C5-C6-N1	-5.72	114.84	117.70
2	A	1395	C	N3-C4-N4	5.72	122.00	118.00
2	A	1609	A	C4-C5-C6	5.72	119.86	117.00
2	A	506	A	C5-C6-N1	-5.72	114.84	117.70
2	A	1020	A	O4'-C1'-N9	5.72	112.77	108.20
2	A	1379	A	C5-C6-N6	-5.72	119.13	123.70
1	N	13	C	N3-C4-N4	5.71	122.00	118.00
2	A	458	A	C4-C5-C6	5.71	119.86	117.00
2	A	996	C	N3-C4-N4	5.71	122.00	118.00
2	A	1846	C	N3-C4-N4	5.71	122.00	118.00
2	A	17	C	N3-C4-N4	5.71	122.00	118.00
2	A	77	A	C4-C5-C6	5.71	119.86	117.00
2	A	1401	A	C4-C5-C6	5.71	119.86	117.00
2	A	1456	C	N3-C4-C5	-5.71	119.61	121.90
2	A	27	A	C4-C5-C6	5.71	119.86	117.00
2	A	102	A	C5-C6-N1	-5.71	114.84	117.70
2	A	684	A	C5-C6-N6	-5.71	119.13	123.70
2	A	980	C	N3-C4-C5	-5.71	119.62	121.90
2	A	993	A	C4-C5-C6	5.71	119.86	117.00
1	N	1	A	C4-C5-C6	5.71	119.86	117.00
2	A	1179	A	C4-C5-C6	5.71	119.86	117.00
2	A	1549	C	N3-C4-N4	5.71	122.00	118.00
2	A	405	A	C5-C6-N6	-5.71	119.13	123.70
2	A	624	A	C4-C5-C6	5.71	119.85	117.00
2	A	499	G	O4'-C1'-N9	5.71	112.77	108.20
2	A	533	C	N3-C4-N4	5.71	121.99	118.00
2	A	1405	A	C5-C6-N1	-5.71	114.85	117.70
3	F	17	C	N3-C4-N4	5.71	121.99	118.00
2	A	23	G	O4'-C1'-N9	5.71	112.76	108.20
1	N	74	C	N3-C4-C5	-5.70	119.62	121.90
2	A	60	A	O4'-C1'-N9	5.70	112.76	108.20
2	A	730	C	O4'-C1'-N1	5.70	112.76	108.20
2	A	1081	C	N3-C4-C5	-5.70	119.62	121.90
2	A	1144	A	C5-C6-N1	-5.70	114.85	117.70
2	A	1351	C	O4'-C1'-N1	5.70	112.76	108.20
2	A	1433	C	N3-C4-N4	5.70	121.99	118.00
3	F	19	C	N3-C4-N4	5.70	121.99	118.00
2	A	512	A	C5-C6-N1	-5.70	114.85	117.70
2	A	525	G	O4'-C1'-N9	5.70	112.76	108.20
2	A	731	C	N3-C4-N4	5.70	121.99	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	899	A	C5-C6-N6	-5.70	119.14	123.70
2	A	1166	A	C5-C6-N6	-5.70	119.14	123.70
2	A	147	A	P-O3'-C3'	5.70	126.54	119.70
2	A	284	C	N3-C4-C5	-5.70	119.62	121.90
2	A	377	C	N3-C4-N4	5.70	121.99	118.00
2	A	576	G	C5-C6-O6	-5.70	125.18	128.60
2	A	813	G	O4'-C1'-N9	5.70	112.76	108.20
2	A	1081	C	C5'-C4'-C3'	-5.70	106.88	116.00
2	A	1795	A	C5-C6-N1	-5.70	114.85	117.70
2	A	1508	C	N3-C4-C5	-5.70	119.62	121.90
2	A	158	A	O4'-C1'-N9	5.70	112.76	108.20
2	A	333	A	O4'-C1'-N9	5.70	112.76	108.20
2	A	1408	C	N3-C4-N4	5.70	121.99	118.00
2	A	159	A	C5-C6-N6	-5.69	119.14	123.70
2	A	475	A	C5-C6-N6	-5.69	119.14	123.70
2	A	1584	A	C5-C6-N1	-5.69	114.85	117.70
2	A	117	C	N3-C4-C5	-5.69	119.62	121.90
2	A	519	A	C4-C5-C6	5.69	119.85	117.00
2	A	596	G	P-O3'-C3'	5.69	126.53	119.70
2	A	603	C	N3-C4-N4	5.69	121.98	118.00
2	A	957	G	O4'-C1'-N9	5.69	112.75	108.20
2	A	1854	A	O4'-C1'-N9	5.69	112.75	108.20
2	A	158	A	C5-C6-N6	-5.69	119.15	123.70
2	A	170	A	C4-C5-C6	5.69	119.85	117.00
2	A	354	A	C4-C5-C6	5.69	119.85	117.00
2	A	454	A	C5-C6-N6	-5.69	119.15	123.70
2	A	736	C	N3-C4-N4	5.69	121.98	118.00
2	A	822	A	O4'-C1'-N9	5.69	112.75	108.20
2	A	969	C	N3-C4-N4	5.69	121.98	118.00
2	A	1431	C	P-O5'-C5'	5.69	130.00	120.90
2	A	1584	A	C5-C6-N6	-5.69	119.15	123.70
2	A	1761	C	N3-C4-N4	5.69	121.98	118.00
2	A	25	A	C4-C5-C6	5.69	119.84	117.00
2	A	438	A	C4-C5-C6	5.69	119.84	117.00
2	A	473	C	N3-C4-C5	-5.69	119.62	121.90
2	A	1238	U	C2-N1-C1'	5.69	124.52	117.70
2	A	1618	A	C5-C6-N6	-5.69	119.15	123.70
2	A	2	A	C5-C6-N6	-5.69	119.15	123.70
1	N	32	C	N3-C4-N4	5.68	121.98	118.00
2	A	779	C	N3-C4-N4	5.68	121.98	118.00
2	A	988	A	C5-C6-N6	-5.68	119.15	123.70
2	A	1267	C	N3-C4-C5	-5.68	119.63	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1699	C	N3-C4-C5	-5.68	119.63	121.90
1	N	6	A	C5-C6-N6	-5.68	119.15	123.70
2	A	428	G	C5-C6-O6	-5.68	125.19	128.60
2	A	459	A	C5-C6-N1	-5.68	114.86	117.70
2	A	835	C	C6-N1-C1'	-5.68	113.98	120.80
2	A	1613	C	N3-C4-N4	5.68	121.98	118.00
2	A	431	C	N3-C4-C5	-5.68	119.63	121.90
2	A	580	A	C5-C6-N6	-5.68	119.16	123.70
2	A	1264	C	N3-C4-C5	-5.68	119.63	121.90
2	A	1287	A	C5-C6-N1	-5.68	114.86	117.70
2	A	513	A	C5-C6-N6	-5.68	119.16	123.70
2	A	1061	G	O4'-C1'-N9	5.68	112.74	108.20
2	A	1138	G	O4'-C1'-N9	5.68	112.74	108.20
2	A	1442	A	C4-C5-C6	5.68	119.84	117.00
2	A	1497	C	N3-C4-C5	-5.68	119.63	121.90
2	A	177	G	O4'-C1'-N9	5.68	112.74	108.20
2	A	429	A	C4-C5-C6	5.68	119.84	117.00
2	A	496	G	O4'-C1'-N9	5.68	112.74	108.20
2	A	882	A	C4-C5-C6	5.68	119.84	117.00
2	A	1212	C	C6-N1-C1'	-5.68	113.99	120.80
2	A	1705	C	N3-C4-N4	5.68	121.97	118.00
2	A	465	C	N3-C4-N4	5.67	121.97	118.00
2	A	1119	C	N3-C4-C5	-5.67	119.63	121.90
2	A	1301	C	N3-C4-C5	-5.67	119.63	121.90
2	A	829	C	N3-C4-N4	5.67	121.97	118.00
2	A	854	A	C5-C6-N1	-5.67	114.86	117.70
2	A	973	C	N3-C4-C5	-5.67	119.63	121.90
2	A	1070	C	N3-C4-C5	-5.67	119.63	121.90
2	A	1188	U	O4'-C1'-N1	5.67	112.74	108.20
2	A	50	A	C5-C6-N6	-5.67	119.16	123.70
2	A	361	A	C5-C6-N6	-5.67	119.16	123.70
2	A	757	C	N3-C4-C5	-5.67	119.63	121.90
2	A	1004	A	C4-C5-C6	5.67	119.84	117.00
40	r	114	TYR	CB-CG-CD2	5.67	124.40	121.00
2	A	98	C	N3-C4-N4	5.67	121.97	118.00
2	A	1260	C	N3-C4-N4	5.67	121.97	118.00
2	A	1646	A	C5-C6-N1	-5.67	114.87	117.70
2	A	1699	C	N3-C4-N4	5.67	121.97	118.00
1	N	43	A	C5-C6-N6	-5.67	119.17	123.70
2	A	575	C	N3-C4-N4	5.67	121.97	118.00
2	A	994	A	C5-C6-N6	-5.67	119.17	123.70
2	A	1694	A	C5-C6-N1	-5.67	114.87	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	445	A	C4-C5-C6	5.67	119.83	117.00
1	N	19	A	C5-C6-N6	-5.66	119.17	123.70
1	N	63	U	O4'-C1'-N1	5.66	112.73	108.20
2	A	39	A	C5-C6-N6	-5.66	119.17	123.70
2	A	58	C	O4'-C1'-N1	5.66	112.73	108.20
2	A	206	A	C5-C6-N6	-5.66	119.17	123.70
2	A	658	A	C4-C5-C6	5.66	119.83	117.00
2	A	1105	C	N3-C4-N4	5.66	121.97	118.00
2	A	1549	C	C6-N1-C1'	-5.66	114.00	120.80
2	A	1782	A	O4'-C1'-N9	5.66	112.73	108.20
2	A	448	A	C4-C5-C6	5.66	119.83	117.00
2	A	866	A	C4-C5-C6	5.66	119.83	117.00
4	P	115	VAL	C-N-CA	5.66	135.85	121.70
2	A	89	C	N3-C4-N4	5.66	121.96	118.00
2	A	382	A	C5-C6-N1	-5.66	114.87	117.70
2	A	731	C	N3-C4-C5	-5.66	119.64	121.90
2	A	1274	A	C4-C5-C6	5.66	119.83	117.00
2	A	1569	C	N3-C4-C5	-5.66	119.64	121.90
2	A	1574	A	C4-C5-C6	5.66	119.83	117.00
2	A	46	A	C5-C6-N6	-5.66	119.17	123.70
2	A	190	A	C5-C6-N6	-5.66	119.17	123.70
2	A	519	A	C5-C6-N6	-5.66	119.17	123.70
2	A	584	A	C5-C6-N1	-5.66	114.87	117.70
2	A	956	U	O4'-C1'-N1	5.66	112.73	108.20
2	A	1071	C	N3-C4-N4	5.66	121.96	118.00
2	A	1166	A	C4-C5-C6	5.66	119.83	117.00
2	A	1436	C	N3-C4-C5	-5.66	119.64	121.90
2	A	1542	C	N3-C4-N4	5.66	121.96	118.00
2	A	491	C	N3-C4-N4	5.66	121.96	118.00
2	A	1224	A	C5-C6-N6	-5.66	119.17	123.70
2	A	1716	U	C2-N1-C1'	5.66	124.49	117.70
1	N	70	C	N3-C4-C5	-5.66	119.64	121.90
2	A	779	C	N3-C4-C5	-5.66	119.64	121.90
2	A	1212	C	N3-C4-N4	5.66	121.96	118.00
2	A	1817	A	C5-C6-N6	-5.65	119.18	123.70
2	A	220	C	N3-C4-N4	5.65	121.96	118.00
2	A	932	G	O4'-C1'-N9	5.65	112.72	108.20
2	A	72	C	N3-C4-N4	5.65	121.96	118.00
2	A	179	C	N3-C4-N4	5.65	121.95	118.00
2	A	654	A	C5-C6-N6	-5.65	119.18	123.70
2	A	656	U	O4'-C1'-N1	5.65	112.72	108.20
2	A	797	U	O4'-C1'-N1	5.65	112.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1003	C	N3-C4-C5	-5.65	119.64	121.90
2	A	1008	A	C5-C6-N1	-5.65	114.88	117.70
2	A	1201	C	N3-C4-C5	-5.65	119.64	121.90
2	A	1844	A	C5-C6-N6	-5.65	119.18	123.70
2	A	860	A	C5-C6-N6	-5.65	119.18	123.70
2	A	1625	A	C4-C5-C6	5.65	119.82	117.00
1	N	34	A	C5-C6-N6	-5.65	119.18	123.70
2	A	181	A	C5-C6-N6	-5.65	119.18	123.70
2	A	283	A	C5-C6-N6	-5.65	119.18	123.70
2	A	416	A	C5-C6-N6	-5.65	119.18	123.70
2	A	559	A	C5-C6-N1	-5.65	114.88	117.70
2	A	644	A	C5-C6-N6	-5.65	119.18	123.70
2	A	915	A	C5-C6-N1	-5.65	114.88	117.70
2	A	1121	C	N3-C4-C5	-5.65	119.64	121.90
2	A	1457	G	N3-C2-N2	5.65	123.85	119.90
1	N	6	A	C4-C5-C6	5.65	119.82	117.00
2	A	1219	A	C5-C6-N6	-5.65	119.18	123.70
2	A	1455	G	O4'-C1'-N9	5.65	112.72	108.20
2	A	1630	C	N3-C4-C5	-5.65	119.64	121.90
2	A	1825	A	C4-C5-C6	5.65	119.82	117.00
2	A	133	C	N3-C4-N4	5.64	121.95	118.00
2	A	509	A	C5-C6-N6	-5.64	119.18	123.70
2	A	1775	A	C5-C6-N1	-5.64	114.88	117.70
2	A	98	C	N3-C4-C5	-5.64	119.64	121.90
2	A	155	G	O4'-C1'-N9	5.64	112.71	108.20
2	A	1054	A	C5-C6-N6	-5.64	119.19	123.70
1	N	73	C	N3-C4-C5	-5.64	119.64	121.90
2	A	1024	A	O4'-C1'-N9	5.64	112.71	108.20
2	A	1691	C	N3-C4-N4	5.64	121.95	118.00
2	A	594	A	C5-C6-N1	-5.64	114.88	117.70
2	A	940	A	C4-C5-C6	5.64	119.82	117.00
2	A	1087	C	N3-C4-N4	5.64	121.95	118.00
2	A	92	A	C5-C6-N6	-5.64	119.19	123.70
2	A	686	G	O4'-C1'-N9	5.64	112.71	108.20
2	A	1305	C	N3-C4-N4	5.64	121.95	118.00
2	A	1536	G	O4'-C1'-N9	5.64	112.71	108.20
3	F	14	G	O4'-C1'-N9	5.64	112.71	108.20
2	A	22	A	C5-C6-N1	-5.63	114.88	117.70
2	A	111	A	C5-C6-N6	-5.63	119.19	123.70
2	A	915	A	C5-C6-N6	-5.63	119.19	123.70
2	A	1045	A	C5-C6-N1	-5.63	114.88	117.70
2	A	1080	A	C5-C6-N1	-5.63	114.88	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1434	A	C5-C6-N1	-5.63	114.88	117.70
2	A	1734	C	N3-C4-N4	5.63	121.94	118.00
2	A	19	A	C4-C5-C6	5.63	119.82	117.00
2	A	1839	A	C4-C5-C6	5.63	119.82	117.00
2	A	1839	A	C5-C6-N1	-5.63	114.88	117.70
2	A	82	G	N3-C2-N2	5.63	123.84	119.90
2	A	196	U	O4'-C1'-N1	5.63	112.70	108.20
2	A	470	G	O4'-C1'-N9	5.63	112.71	108.20
2	A	1655	C	N3-C4-C5	-5.63	119.65	121.90
2	A	118	C	N3-C4-N4	5.63	121.94	118.00
2	A	633	A	C5-C6-N6	-5.63	119.20	123.70
2	A	837	G	C4'-C3'-C2'	-5.63	96.97	102.60
2	A	907	C	N3-C4-C5	-5.63	119.65	121.90
2	A	73	C	O4'-C1'-N1	5.63	112.70	108.20
2	A	169	U	O4'-C1'-N1	5.63	112.70	108.20
2	A	1295	A	C5-C6-N6	-5.63	119.20	123.70
2	A	1146	A	C4-C5-C6	5.63	119.81	117.00
2	A	1158	C	N3-C4-N4	5.63	121.94	118.00
2	A	1596	A	C5-C6-N1	-5.63	114.89	117.70
2	A	1857	A	O4'-C1'-N9	5.63	112.70	108.20
1	N	62	A	C4-C5-C6	5.62	119.81	117.00
2	A	777	C	N3-C4-N4	5.62	121.94	118.00
2	A	1185	A	C5-C6-N6	-5.62	119.20	123.70
2	A	54	A	C5-C6-N6	-5.62	119.20	123.70
2	A	142	C	C2-N1-C1'	5.62	124.98	118.80
2	A	490	A	C5-C6-N1	-5.62	114.89	117.70
2	A	521	A	C4-C5-C6	5.62	119.81	117.00
2	A	944	C	N3-C4-N4	5.62	121.94	118.00
2	A	994	A	O4'-C1'-N9	5.62	112.70	108.20
7	I	242	LYS	N-CA-CB	5.62	120.72	110.60
2	A	951	A	C5-C6-N1	-5.62	114.89	117.70
2	A	1563	C	N3-C4-C5	-5.62	119.65	121.90
2	A	1628	A	C5-C6-N1	-5.62	114.89	117.70
1	N	66	U	O4'-C1'-N1	5.62	112.70	108.20
2	A	223	A	C5-C6-N6	-5.62	119.20	123.70
3	F	9	C	N3-C4-N4	5.62	121.93	118.00
2	A	60	A	C5-C6-N1	-5.62	114.89	117.70
2	A	111	A	C4-C5-C6	5.62	119.81	117.00
2	A	340	C	N3-C4-N4	5.62	121.93	118.00
2	A	491	C	O4'-C1'-N1	5.62	112.69	108.20
2	A	1333	C	N3-C4-C5	-5.62	119.65	121.90
2	A	1483	A	C4-C5-C6	5.62	119.81	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	405	A	O4'-C1'-N9	5.62	112.69	108.20
2	A	481	C	N3-C4-C5	-5.62	119.65	121.90
2	A	1433	C	N3-C4-C5	-5.62	119.65	121.90
2	A	1483	A	C5-C6-N1	-5.62	114.89	117.70
2	A	123	G	O4'-C1'-N9	5.61	112.69	108.20
2	A	229	A	C5-C6-N6	-5.61	119.21	123.70
2	A	983	A	C5-C6-N6	-5.61	119.21	123.70
2	A	1190	A	C5-C6-N6	-5.61	119.21	123.70
2	A	1719	A	C4-C5-C6	5.61	119.81	117.00
2	A	1742	C	N3-C4-C5	-5.61	119.65	121.90
3	F	23	A	C5-C6-N6	-5.61	119.21	123.70
2	A	1127	G	O4'-C1'-N9	5.61	112.69	108.20
2	A	447	C	N3-C4-N4	5.61	121.93	118.00
2	A	1551	A	C5-C6-N6	-5.61	119.21	123.70
2	A	1740	A	C5-C6-N6	-5.61	119.21	123.70
2	A	452	C	N3-C4-C5	-5.61	119.66	121.90
2	A	634	G	O4'-C1'-N9	5.61	112.69	108.20
2	A	1114	C	N3-C4-N4	5.61	121.92	118.00
2	A	1453	U	O4'-C1'-N1	5.61	112.69	108.20
2	A	133	C	N3-C4-C5	-5.61	119.66	121.90
2	A	147	A	O4'-C1'-N9	5.61	112.68	108.20
2	A	393	G	O4'-C1'-N9	5.61	112.69	108.20
2	A	1301	C	N3-C4-N4	5.61	121.92	118.00
2	A	366	A	C4-C5-C6	5.60	119.80	117.00
2	A	1063	C	N3-C4-N4	5.60	121.92	118.00
2	A	1397	A	C4-C5-C6	5.60	119.80	117.00
2	A	1464	C	N3-C4-C5	-5.60	119.66	121.90
2	A	1713	G	O4'-C1'-N9	5.60	112.68	108.20
2	A	1827	C	N3-C4-N4	5.60	121.92	118.00
3	F	20	C	N3-C4-N4	5.60	121.92	118.00
2	A	376	C	N3-C4-N4	5.60	121.92	118.00
2	A	1212	C	N3-C4-C5	-5.60	119.66	121.90
2	A	50	A	O4'-C1'-N9	5.60	112.68	108.20
2	A	1139	A	C4-C5-C6	5.60	119.80	117.00
2	A	1399	C	N3-C4-N4	5.60	121.92	118.00
2	A	359	C	N3-C4-C5	-5.60	119.66	121.90
2	A	751	C	O4'-C1'-N1	5.60	112.68	108.20
2	A	873	C	N3-C4-N4	5.60	121.92	118.00
2	A	1784	A	O4'-C1'-N9	5.60	112.68	108.20
2	A	142	C	N3-C4-N4	5.59	121.92	118.00
2	A	389	C	N3-C4-N4	5.59	121.92	118.00
2	A	623	C	N3-C4-N4	5.59	121.92	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	635	C	N3-C4-C5	-5.59	119.66	121.90
2	A	790	A	C5-C6-N1	-5.59	114.90	117.70
2	A	798	A	C5-C6-N1	-5.59	114.90	117.70
2	A	959	A	O4'-C1'-N9	5.59	112.68	108.20
2	A	1250	C	N3-C4-N4	5.59	121.92	118.00
2	A	1669	G	O4'-C1'-N9	5.59	112.67	108.20
3	F	3	C	N3-C4-N4	5.59	121.92	118.00
39	q	48	TYR	CB-CG-CD2	5.59	124.36	121.00
2	A	617	U	O4'-C1'-N1	5.59	112.67	108.20
2	A	1080	A	P-O3'-C3'	5.59	126.41	119.70
2	A	1161	G	O4'-C1'-N9	5.59	112.67	108.20
2	A	1236	A	C5-C6-N6	-5.59	119.23	123.70
2	A	1522	C	N3-C4-N4	5.59	121.91	118.00
2	A	1714	A	O4'-C1'-N9	5.59	112.67	108.20
2	A	221	A	C5-C6-N1	-5.59	114.91	117.70
2	A	324	C	N3-C4-N4	5.59	121.91	118.00
2	A	358	U	O4'-C1'-N1	5.59	112.67	108.20
2	A	839	C	N3-C4-N4	5.59	121.91	118.00
2	A	993	A	C5-C6-N6	-5.59	119.23	123.70
2	A	1502	A	C5-C6-N6	-5.59	119.23	123.70
2	A	1835	C	N3-C4-N4	5.59	121.91	118.00
2	A	440	C	C6-N1-C1'	-5.59	114.09	120.80
2	A	1576	C	N3-C4-N4	5.59	121.91	118.00
2	A	131	C	N3-C4-N4	5.59	121.91	118.00
2	A	397	G	O4'-C1'-N9	5.59	112.67	108.20
2	A	865	A	C5-C6-N6	-5.59	119.23	123.70
2	A	1640	C	N3-C4-C5	-5.59	119.67	121.90
2	A	1768	C	N3-C4-N4	5.59	121.91	118.00
2	A	1588	C	N3-C4-N4	5.58	121.91	118.00
7	I	69	PHE	CB-CG-CD1	5.58	124.71	120.80
2	A	315	C	N3-C4-C5	-5.58	119.67	121.90
2	A	347	C	N3-C4-N4	5.58	121.91	118.00
2	A	427	G	O4'-C1'-N9	5.58	112.67	108.20
2	A	958	A	C5-C6-N1	-5.58	114.91	117.70
2	A	1549	C	N3-C4-C5	-5.58	119.67	121.90
2	A	1817	A	C5-C6-N1	-5.58	114.91	117.70
1	N	72	A	C5-C6-N1	-5.58	114.91	117.70
2	A	286	C	N3-C4-C5	-5.58	119.67	121.90
2	A	449	C	N3-C4-N4	5.58	121.91	118.00
2	A	614	C	N3-C4-C5	-5.58	119.67	121.90
2	A	1249	A	C4-C5-C6	5.58	119.79	117.00
2	A	1632	A	C5-C6-N1	-5.58	114.91	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	398	A	C5-C6-N6	-5.58	119.24	123.70
2	A	473	C	N3-C4-N4	5.58	121.90	118.00
2	A	594	A	C5-C6-N6	-5.58	119.24	123.70
2	A	831	C	N3-C4-C5	-5.58	119.67	121.90
2	A	1135	C	N3-C4-C5	-5.58	119.67	121.90
2	A	354	A	C5-C6-N1	-5.58	114.91	117.70
2	A	1175	G	O4'-C1'-N9	5.58	112.66	108.20
2	A	1801	C	N3-C4-C5	-5.58	119.67	121.90
2	A	321	C	N3-C4-N4	5.58	121.90	118.00
2	A	1071	C	N3-C4-C5	-5.58	119.67	121.90
2	A	1186	A	C5-C6-N1	-5.58	114.91	117.70
2	A	1650	C	N3-C4-C5	-5.58	119.67	121.90
2	A	486	C	N3-C4-N4	5.57	121.90	118.00
2	A	1269	C	O4'-C1'-N1	5.57	112.66	108.20
9	K	165	TYR	CB-CG-CD2	-5.57	117.66	121.00
2	A	309	A	C4-C5-C6	5.57	119.79	117.00
2	A	997	A	C5-C6-N1	-5.57	114.91	117.70
2	A	1251	G	O4'-C1'-N9	5.57	112.66	108.20
2	A	1552	C	O4'-C1'-N1	5.57	112.66	108.20
2	A	493	C	N3-C4-C5	-5.57	119.67	121.90
2	A	1658	A	C5-C6-N6	-5.57	119.24	123.70
3	F	8	A	C5-C6-N6	-5.57	119.24	123.70
2	A	218	A	O4'-C1'-N9	5.57	112.66	108.20
2	A	408	A	C5-C6-N6	-5.57	119.25	123.70
2	A	1227	C	N3-C4-C5	-5.57	119.67	121.90
2	A	1129	A	C4-C5-C6	5.57	119.78	117.00
2	A	1531	G	O4'-C1'-N9	5.57	112.65	108.20
2	A	1726	A	C5-C6-N6	-5.57	119.25	123.70
1	N	10	G	O4'-C1'-N9	5.57	112.65	108.20
2	A	488	C	N3-C4-C5	-5.57	119.67	121.90
2	A	629	C	N3-C4-C5	-5.57	119.67	121.90
2	A	664	C	N3-C4-N4	5.57	121.90	118.00
2	A	988	A	C5-C6-N1	-5.57	114.92	117.70
2	A	1046	A	O4'-C1'-N9	5.57	112.65	108.20
2	A	1159	C	N3-C4-N4	5.57	121.89	118.00
2	A	1215	C	N3-C4-N4	5.57	121.90	118.00
2	A	1615	A	C5-C6-N1	-5.57	114.92	117.70
2	A	466	A	O4'-C1'-N9	5.56	112.65	108.20
2	A	979	A	C5-C6-N6	-5.56	119.25	123.70
1	N	72	A	C4-C5-C6	5.56	119.78	117.00
2	A	129	C	N3-C4-N4	5.56	121.89	118.00
2	A	407	C	N3-C4-N4	5.56	121.89	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	960	A	C5-C6-N6	-5.56	119.25	123.70
2	A	1385	C	N3-C4-N4	5.56	121.89	118.00
2	A	1738	G	N3-C2-N2	5.56	123.79	119.90
2	A	1854	A	C5-C6-N1	-5.56	114.92	117.70
2	A	231	C	N3-C4-C5	-5.56	119.68	121.90
2	A	454	A	C5-C6-N1	-5.56	114.92	117.70
2	A	973	C	N3-C4-N4	5.56	121.89	118.00
2	A	1557	C	N3-C4-C5	-5.56	119.68	121.90
2	A	87	U	O4'-C1'-N1	5.56	112.65	108.20
2	A	304	A	C4-C5-C6	5.56	119.78	117.00
2	A	619	A	C4-C5-C6	5.56	119.78	117.00
2	A	675	A	C5-C6-N1	-5.56	114.92	117.70
2	A	736	C	N3-C4-C5	-5.56	119.68	121.90
2	A	806	A	C5-C6-N6	-5.56	119.25	123.70
2	A	1614	A	C5-C6-N6	-5.56	119.25	123.70
2	A	1783	G	N3-C2-N2	5.56	123.79	119.90
2	A	1844	A	C5-C6-N1	-5.56	114.92	117.70
1	N	55	C	N3-C4-C5	-5.56	119.68	121.90
2	A	42	A	C5-C6-N6	-5.56	119.25	123.70
2	A	138	C	N3-C4-N4	5.56	121.89	118.00
2	A	518	A	C5-C6-N6	-5.56	119.25	123.70
2	A	677	C	C2-N1-C1'	5.56	124.91	118.80
2	A	907	C	N3-C4-N4	5.56	121.89	118.00
2	A	984	C	O4'-C1'-N1	5.56	112.64	108.20
2	A	1102	C	N3-C4-C5	-5.56	119.68	121.90
2	A	1226	C	N3-C4-N4	5.56	121.89	118.00
2	A	1311	U	P-O3'-C3'	5.56	126.37	119.70
2	A	1539	C	N3-C4-C5	-5.56	119.68	121.90
2	A	91	A	C5-C6-N1	-5.55	114.92	117.70
2	A	661	A	C5-C6-N1	-5.55	114.92	117.70
2	A	926	C	N3-C4-C5	-5.55	119.68	121.90
1	N	75	A	C5-C6-N6	-5.55	119.26	123.70
2	A	492	C	N3-C4-N4	5.55	121.89	118.00
2	A	1502	A	C5-C6-N1	-5.55	114.92	117.70
2	A	1583	A	C5-C6-N1	-5.55	114.92	117.70
2	A	112	U	P-O3'-C3'	5.55	126.36	119.70
2	A	847	C	N3-C4-N4	5.55	121.89	118.00
3	F	9	C	N3-C4-C5	-5.55	119.68	121.90
2	A	580	A	O4'-C1'-N9	5.55	112.64	108.20
2	A	812	A	C5-C6-N6	-5.55	119.26	123.70
2	A	1002	C	N3-C4-C5	-5.55	119.68	121.90
2	A	1146	A	C5-C6-N1	-5.55	114.92	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	58	C	N3-C4-N4	5.55	121.88	118.00
2	A	618	A	C5-C6-N6	-5.55	119.26	123.70
2	A	643	A	O4'-C1'-N9	5.55	112.64	108.20
2	A	1247	A	C5-C6-N6	-5.55	119.26	123.70
1	N	26	C	N3-C4-N4	5.55	121.88	118.00
2	A	84	A	C5-C6-N6	-5.55	119.26	123.70
2	A	429	A	O4'-C1'-N9	5.55	112.64	108.20
2	A	564	A	C5-C6-N6	-5.55	119.26	123.70
2	A	1211	C	N3-C4-C5	-5.55	119.68	121.90
2	A	1399	C	N3-C4-C5	-5.55	119.68	121.90
2	A	1567	C	N3-C4-C5	-5.55	119.68	121.90
2	A	1850	C	N3-C4-N4	5.55	121.88	118.00
2	A	969	C	N3-C4-C5	-5.54	119.68	121.90
2	A	1664	G	O4'-C1'-N9	5.54	112.64	108.20
2	A	1819	A	C5-C6-N6	-5.54	119.26	123.70
2	A	453	C	N3-C4-N4	5.54	121.88	118.00
2	A	577	A	C5-C6-N6	-5.54	119.27	123.70
2	A	1099	C	N3-C4-N4	5.54	121.88	118.00
2	A	1309	A	C5-C6-N1	-5.54	114.93	117.70
2	A	1382	A	C5-C6-N6	-5.54	119.27	123.70
2	A	134	C	N3-C4-N4	5.54	121.88	118.00
2	A	228	A	C4-C5-C6	5.54	119.77	117.00
2	A	348	C	N3-C4-N4	5.54	121.88	118.00
2	A	479	A	C5-C6-N1	-5.54	114.93	117.70
2	A	1109	A	C5-C6-N1	-5.54	114.93	117.70
2	A	1144	A	C4-C5-C6	5.54	119.77	117.00
3	F	17	C	N3-C4-C5	-5.54	119.68	121.90
2	A	19	A	C5-C6-N6	-5.54	119.27	123.70
2	A	104	A	C5-C6-N1	-5.54	114.93	117.70
2	A	381	C	N3-C4-C5	-5.54	119.68	121.90
2	A	630	A	C5-C6-N1	-5.54	114.93	117.70
2	A	1288	C	N3-C4-C5	-5.54	119.68	121.90
2	A	1581	U	O4'-C1'-N1	5.54	112.63	108.20
1	N	31	C	N3-C4-C5	-5.54	119.69	121.90
2	A	609	A	O4'-C1'-N9	5.54	112.63	108.20
2	A	515	A	C4-C5-C6	5.54	119.77	117.00
2	A	1139	A	C5-C6-N6	-5.54	119.27	123.70
2	A	1703	C	N3-C4-N4	5.54	121.88	118.00
2	A	233	A	C5-C6-N1	-5.54	114.93	117.70
2	A	326	A	C5-C6-N1	-5.54	114.93	117.70
2	A	611	C	N3-C4-C5	-5.54	119.69	121.90
2	A	868	A	C5-C6-N6	-5.54	119.27	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1216	A	O4'-C1'-N9	5.54	112.63	108.20
2	A	1245	C	N3-C4-N4	5.54	121.88	118.00
2	A	1485	A	C5-C6-N1	-5.54	114.93	117.70
1	N	2	G	O4'-C1'-N9	5.53	112.63	108.20
2	A	390	C	N3-C4-N4	5.53	121.87	118.00
2	A	660	A	C4-C5-C6	5.53	119.77	117.00
2	A	1765	G	O4'-C1'-N9	5.53	112.63	108.20
2	A	491	C	N3-C4-C5	-5.53	119.69	121.90
2	A	918	A	C5-C6-N6	-5.53	119.27	123.70
2	A	1063	C	N3-C4-C5	-5.53	119.69	121.90
2	A	1195	A	C5-C6-N1	-5.53	114.93	117.70
2	A	435	A	C5-C6-N6	-5.53	119.28	123.70
2	A	1742	C	N3-C4-N4	5.53	121.87	118.00
2	A	1800	A	C5-C6-N1	-5.53	114.93	117.70
2	A	1845	A	C5-C6-N6	-5.53	119.28	123.70
2	A	1246	A	C5-C6-N6	-5.53	119.28	123.70
2	A	1365	A	C5-C6-N6	-5.53	119.28	123.70
1	N	4	A	C5-C6-N1	-5.53	114.94	117.70
2	A	77	A	C5-C6-N6	-5.53	119.28	123.70
2	A	329	A	C5-C6-N1	-5.53	114.94	117.70
2	A	404	A	C5-C6-N1	-5.53	114.94	117.70
2	A	1076	A	C5-C6-N6	-5.53	119.28	123.70
2	A	1219	A	C5-C6-N1	-5.53	114.94	117.70
2	A	1410	A	C5-C6-N1	-5.53	114.94	117.70
2	A	293	A	C4-C5-C6	5.52	119.76	117.00
2	A	1118	A	C5-C6-N6	-5.52	119.28	123.70
2	A	1552	C	N3-C4-N4	5.52	121.87	118.00
2	A	1692	A	C5-C6-N1	-5.52	114.94	117.70
2	A	526	A	C5-C6-N1	-5.52	114.94	117.70
2	A	904	A	C5-C6-N6	-5.52	119.28	123.70
2	A	1158	C	N3-C4-C5	-5.52	119.69	121.90
2	A	1639	C	N3-C4-C5	-5.52	119.69	121.90
15	S	84	ASN	C-N-CA	5.52	135.50	121.70
2	A	1249	A	O4'-C1'-N9	5.52	112.62	108.20
3	F	24	C	O4'-C1'-N1	5.52	112.62	108.20
2	A	45	A	C5-C6-N6	-5.52	119.28	123.70
2	A	1450	A	C4-C5-C6	5.52	119.76	117.00
2	A	1530	U	O4'-C1'-N1	5.52	112.62	108.20
2	A	1611	U	O4'-C1'-N1	5.52	112.61	108.20
2	A	1642	A	C4-C5-C6	5.52	119.76	117.00
2	A	1642	A	C5-C6-N1	-5.52	114.94	117.70
1	N	41	A	C5-C6-N1	-5.52	114.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	11	A	C4-C5-C6	5.52	119.76	117.00
2	A	13	C	N3-C4-C5	-5.52	119.69	121.90
2	A	18	C	N3-C4-C5	-5.52	119.69	121.90
2	A	206	A	C5-C6-N1	-5.52	114.94	117.70
2	A	391	A	C5-C6-N6	-5.52	119.29	123.70
2	A	897	G	O4'-C1'-N9	5.52	112.61	108.20
2	A	1051	A	O4'-C1'-N9	5.52	112.61	108.20
2	A	369	C	N3-C4-C5	-5.52	119.69	121.90
2	A	1131	C	N3-C4-C5	-5.52	119.69	121.90
2	A	1298	G	P-O5'-C5'	-5.52	112.07	120.90
2	A	102	A	C5-C6-N6	-5.51	119.29	123.70
2	A	187	C	N3-C4-N4	5.51	121.86	118.00
2	A	673	G	O4'-C1'-N9	5.51	112.61	108.20
2	A	805	A	C5-C6-N1	-5.51	114.94	117.70
2	A	1330	G	O4'-C1'-N9	5.51	112.61	108.20
2	A	1554	C	N3-C4-N4	5.51	121.86	118.00
2	A	1596	A	C5-C6-N6	-5.51	119.29	123.70
1	N	41	A	C4-C5-C6	5.51	119.76	117.00
2	A	429	A	C5-C6-N1	-5.51	114.94	117.70
2	A	1328	A	C5-C6-N1	-5.51	114.94	117.70
1	N	3	C	N3-C4-C5	-5.51	119.69	121.90
1	N	59	A	C5-C6-N1	-5.51	114.94	117.70
2	A	40	A	C5-C6-N1	-5.51	114.94	117.70
2	A	211	U	O4'-C1'-N1	5.51	112.61	108.20
2	A	330	C	N3-C4-N4	5.51	121.86	118.00
2	A	866	A	C5-C6-N6	-5.51	119.29	123.70
2	A	1334	G	O4'-C1'-N9	5.51	112.61	108.20
2	A	1353	A	C5-C6-N1	-5.51	114.94	117.70
1	N	36	A	C5-C6-N6	-5.51	119.29	123.70
2	A	306	C	N3-C4-C5	-5.51	119.70	121.90
2	A	475	A	C4-C5-C6	5.51	119.75	117.00
2	A	922	A	C5-C6-N6	-5.51	119.29	123.70
2	A	1327	C	O4'-C1'-N1	5.51	112.61	108.20
2	A	1845	A	O4'-C1'-N9	5.51	112.61	108.20
2	A	937	C	N3-C4-C5	-5.51	119.70	121.90
2	A	993	A	C5-C6-N1	-5.51	114.95	117.70
2	A	1005	A	C4-C5-C6	5.51	119.75	117.00
2	A	170	A	O4'-C1'-N9	5.51	112.61	108.20
2	A	799	C	N3-C4-C5	-5.51	119.70	121.90
2	A	918	A	C5-C6-N1	-5.51	114.95	117.70
2	A	1254	A	C5-C6-N6	-5.50	119.30	123.70
2	A	1734	C	N3-C4-C5	-5.50	119.70	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	732	C	N3-C4-C5	-5.50	119.70	121.90
2	A	1576	C	N3-C4-C5	-5.50	119.70	121.90
2	A	313	C	N3-C4-C5	-5.50	119.70	121.90
2	A	320	G	O4'-C1'-N9	5.50	112.60	108.20
2	A	509	A	C5-C6-N1	-5.50	114.95	117.70
2	A	660	A	C5-C6-N6	-5.50	119.30	123.70
2	A	1247	A	C5-C6-N1	-5.50	114.95	117.70
2	A	1030	A	C5-C6-N6	-5.50	119.30	123.70
3	F	24	C	N3-C4-C5	-5.50	119.70	121.90
1	N	17	G	C5-C6-O6	-5.50	125.30	128.60
2	A	304	A	C5-C6-N1	-5.50	114.95	117.70
2	A	1023	A	O4'-C1'-N9	5.50	112.60	108.20
2	A	1083	A	C5-C6-N1	-5.50	114.95	117.70
2	A	1145	A	C5-C6-N1	-5.50	114.95	117.70
2	A	1759	C	N3-C4-N4	5.50	121.85	118.00
2	A	1767	C	N3-C4-N4	5.50	121.85	118.00
2	A	450	A	C5-C6-N1	-5.50	114.95	117.70
2	A	458	A	C5-C6-N1	-5.50	114.95	117.70
2	A	1331	G	N3-C2-N2	5.50	123.75	119.90
2	A	1735	C	N3-C4-N4	5.50	121.85	118.00
2	A	42	A	C5-C6-N1	-5.49	114.95	117.70
2	A	193	C	N3-C4-C5	-5.49	119.70	121.90
2	A	643	A	C5-C6-N1	-5.49	114.95	117.70
2	A	777	C	N3-C4-C5	-5.49	119.70	121.90
2	A	1092	G	O4'-C1'-N9	5.49	112.59	108.20
2	A	1112	C	N3-C4-N4	5.49	121.85	118.00
2	A	1345	G	O4'-C1'-N9	5.49	112.59	108.20
2	A	1622	C	P-O3'-C3'	5.49	126.29	119.70
2	A	1623	C	N3-C4-C5	-5.49	119.70	121.90
2	A	419	C	N3-C4-C5	-5.49	119.70	121.90
2	A	1045	A	C5-C6-N6	-5.49	119.31	123.70
2	A	1747	C	N3-C4-N4	5.49	121.84	118.00
2	A	292	A	C5-C6-N1	-5.49	114.95	117.70
2	A	1015	C	N3-C4-C5	-5.49	119.70	121.90
2	A	40	A	C5-C6-N6	-5.49	119.31	123.70
2	A	150	A	C4-C5-C6	5.49	119.74	117.00
2	A	420	C	N3-C4-C5	-5.49	119.70	121.90
2	A	1035	C	N3-C4-C5	-5.49	119.70	121.90
2	A	1486	G	O4'-C1'-N9	5.49	112.59	108.20
2	A	1839	A	C5-C6-N6	-5.49	119.31	123.70
2	A	282	G	O4'-C1'-N9	5.49	112.59	108.20
2	A	407	C	N3-C4-C5	-5.49	119.70	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	443	C	N3-C4-N4	5.49	121.84	118.00
2	A	480	C	N3-C4-C5	-5.49	119.71	121.90
2	A	1123	C	N3-C4-N4	5.49	121.84	118.00
2	A	1586	C	N3-C4-N4	5.49	121.84	118.00
2	A	1120	C	N3-C4-N4	5.48	121.84	118.00
2	A	1143	C	N3-C4-N4	5.48	121.84	118.00
2	A	1435	A	C5-C6-N6	-5.48	119.31	123.70
1	N	43	A	C5-C6-N1	-5.48	114.96	117.70
2	A	559	A	C5-C6-N6	-5.48	119.31	123.70
2	A	983	A	C5-C6-N1	-5.48	114.96	117.70
2	A	1129	A	C5-C6-N6	-5.48	119.31	123.70
2	A	1382	A	C5-C6-N1	-5.48	114.96	117.70
2	A	1412	C	N3-C4-C5	-5.48	119.71	121.90
2	A	1478	C	N3-C4-N4	5.48	121.84	118.00
2	A	1825	A	C5-C6-N1	-5.48	114.96	117.70
3	F	26	C	N3-C4-N4	5.48	121.84	118.00
2	A	27	A	C5-C6-N6	-5.48	119.31	123.70
2	A	53	C	N3-C4-N4	5.48	121.84	118.00
2	A	147	A	C5-C6-N6	-5.48	119.32	123.70
2	A	166	A	O4'-C1'-N9	5.48	112.58	108.20
2	A	481	C	N3-C4-N4	5.48	121.84	118.00
2	A	781	C	N3-C4-C5	-5.48	119.71	121.90
2	A	1295	A	C5-C6-N1	-5.48	114.96	117.70
2	A	455	A	C5-C6-N6	-5.48	119.32	123.70
2	A	1471	G	O4'-C1'-N9	5.48	112.58	108.20
2	A	1485	A	C5-C6-N6	-5.48	119.32	123.70
1	N	72	A	C5-C6-N6	-5.48	119.32	123.70
2	A	125	C	O4'-C1'-N1	5.48	112.58	108.20
2	A	279	G	O4'-C1'-N9	5.48	112.58	108.20
2	A	1340	A	C5-C6-N1	-5.48	114.96	117.70
2	A	337	G	O4'-C1'-N9	5.47	112.58	108.20
2	A	2	A	C5-C6-N1	-5.47	114.96	117.70
2	A	309	A	C5-C6-N1	-5.47	114.96	117.70
2	A	346	C	C6-N1-C1'	-5.47	114.23	120.80
2	A	482	C	O4'-C1'-N1	5.47	112.58	108.20
2	A	630	A	O4'-C1'-N9	5.47	112.58	108.20
2	A	1005	A	C5-C6-N1	-5.47	114.96	117.70
2	A	1337	C	N3-C4-C5	-5.47	119.71	121.90
2	A	1533	C	N3-C4-N4	5.47	121.83	118.00
2	A	1572	G	O4'-C1'-N9	5.47	112.58	108.20
2	A	416	A	O4'-C1'-N9	5.47	112.58	108.20
2	A	860	A	O4'-C1'-N9	5.47	112.58	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	1	A	O4'-C1'-N9	5.47	112.58	108.20
2	A	339	A	C5-C6-N1	-5.47	114.97	117.70
2	A	754	C	N3-C4-N4	5.47	121.83	118.00
2	A	860	A	C5-C6-N1	-5.47	114.97	117.70
2	A	1026	A	O4'-C1'-N9	5.47	112.58	108.20
2	A	1266	G	O4'-C1'-N9	5.47	112.58	108.20
2	A	1387	C	N3-C4-N4	5.47	121.83	118.00
2	A	128	U	P-O3'-C3'	5.47	126.26	119.70
2	A	400	G	O4'-C1'-N9	5.47	112.57	108.20
2	A	1105	C	N3-C4-C5	-5.47	119.71	121.90
2	A	589	A	C5-C6-N1	-5.47	114.97	117.70
2	A	593	C	N3-C4-C5	-5.47	119.71	121.90
2	A	834	G	O4'-C1'-N9	5.47	112.57	108.20
2	A	1123	C	N3-C4-C5	-5.47	119.71	121.90
2	A	1649	G	O4'-C1'-N9	5.47	112.57	108.20
2	A	191	C	N3-C4-N4	5.46	121.83	118.00
2	A	429	A	C5-C6-N6	-5.46	119.33	123.70
2	A	638	A	C4-C5-C6	5.46	119.73	117.00
2	A	975	C	N3-C4-C5	-5.46	119.72	121.90
3	F	30	A	C5-C6-N6	-5.46	119.33	123.70
2	A	17	C	N3-C4-C5	-5.46	119.72	121.90
2	A	67	C	N3-C4-N4	5.46	121.82	118.00
2	A	662	A	C5-C6-N6	-5.46	119.33	123.70
2	A	846	C	N3-C4-N4	5.46	121.82	118.00
2	A	963	C	N3-C4-C5	-5.46	119.72	121.90
2	A	1073	A	C5-C6-N6	-5.46	119.33	123.70
2	A	1412	C	N3-C4-N4	5.46	121.82	118.00
2	A	1479	A	C5-C6-N6	-5.46	119.33	123.70
2	A	425	A	C5-C6-N6	-5.46	119.33	123.70
2	A	1257	C	N3-C4-C5	-5.46	119.72	121.90
2	A	1527	C	N3-C4-C5	-5.46	119.72	121.90
2	A	1639	C	N3-C4-N4	5.46	121.82	118.00
2	A	1144	A	C5-C6-N6	-5.46	119.33	123.70
2	A	1184	A	O4'-C1'-N9	5.46	112.57	108.20
2	A	1489	C	O4'-C1'-N1	5.46	112.57	108.20
2	A	1499	C	N3-C4-C5	-5.46	119.72	121.90
2	A	1693	C	N3-C4-C5	-5.46	119.72	121.90
2	A	609	A	C5-C6-N1	-5.46	114.97	117.70
2	A	916	A	C5-C6-N1	-5.46	114.97	117.70
2	A	1176	C	N3-C4-N4	5.46	121.82	118.00
2	A	1379	A	C4-C5-C6	5.46	119.73	117.00
2	A	1480	A	O4'-C1'-N9	5.46	112.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1552	C	N3-C4-C5	-5.46	119.72	121.90
2	A	1556	A	C5-C6-N6	-5.46	119.33	123.70
2	A	518	A	C5-C6-N1	-5.46	114.97	117.70
2	A	923	C	N3-C4-N4	5.46	121.82	118.00
2	A	1018	U	C6-N1-C1'	-5.46	113.56	121.20
2	A	1766	C	N3-C4-N4	5.46	121.82	118.00
2	A	1863	A	O4'-C1'-N9	5.46	112.57	108.20
2	A	493	C	O4'-C1'-N1	5.46	112.56	108.20
2	A	821	A	C5-C6-N6	-5.46	119.34	123.70
2	A	14	C	N3-C4-C5	-5.45	119.72	121.90
2	A	139	C	N3-C4-N4	5.45	121.82	118.00
2	A	1575	A	C5-C6-N6	-5.45	119.34	123.70
2	A	171	A	C5-C6-N6	-5.45	119.34	123.70
2	A	557	C	N3-C4-N4	5.45	121.82	118.00
2	A	613	G	O4'-C1'-N9	5.45	112.56	108.20
2	A	759	A	C5-C6-N1	-5.45	114.97	117.70
2	A	836	C	N3-C4-N4	5.45	121.81	118.00
2	A	512	A	O4'-C1'-N9	5.45	112.56	108.20
2	A	583	C	N3-C4-N4	5.45	121.81	118.00
2	A	868	A	C5-C6-N1	-5.45	114.98	117.70
2	A	1258	C	N3-C4-N4	5.45	121.81	118.00
2	A	1658	A	O4'-C1'-N9	5.45	112.56	108.20
2	A	49	C	N3-C4-C5	-5.45	119.72	121.90
1	N	6	A	O4'-C1'-N9	5.45	112.56	108.20
2	A	3	C	N3-C4-C5	-5.45	119.72	121.90
2	A	350	A	C5-C6-N1	-5.45	114.98	117.70
2	A	757	C	N3-C4-N4	5.45	121.81	118.00
2	A	1124	C	O4'-C1'-N1	5.45	112.56	108.20
2	A	1190	A	C4-C5-C6	5.45	119.72	117.00
2	A	453	C	N3-C4-C5	-5.44	119.72	121.90
2	A	1760	C	N3-C4-N4	5.44	121.81	118.00
2	A	151	C	N3-C4-C5	-5.44	119.72	121.90
2	A	596	G	N3-C2-N2	5.44	123.71	119.90
2	A	1079	A	C5-C6-N1	-5.44	114.98	117.70
2	A	1113	C	N3-C4-C5	-5.44	119.72	121.90
2	A	1803	A	C5-C6-N1	-5.44	114.98	117.70
2	A	1822	C	N3-C4-N4	5.44	121.81	118.00
2	A	292	A	C5-C6-N6	-5.44	119.35	123.70
2	A	308	C	N3-C4-C5	-5.44	119.72	121.90
2	A	455	A	O4'-C1'-N9	5.44	112.55	108.20
2	A	876	G	C5-C6-O6	-5.44	125.33	128.60
3	F	27	C	N3-C4-N4	5.44	121.81	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	483	A	O4'-C1'-N9	5.44	112.55	108.20
2	A	1016	A	C5-C6-N6	-5.44	119.35	123.70
2	A	1820	G	O4'-C1'-N9	5.44	112.55	108.20
2	A	290	A	C5-C6-N6	-5.44	119.35	123.70
2	A	860	A	C4-C5-C6	5.44	119.72	117.00
2	A	1024	A	C5-C6-N1	-5.44	114.98	117.70
2	A	1756	C	N3-C4-N4	5.44	121.81	118.00
2	A	331	C	N3-C4-N4	5.43	121.81	118.00
2	A	751	C	N3-C4-C5	-5.43	119.73	121.90
2	A	814	A	C5-C6-N1	-5.43	114.98	117.70
2	A	1807	A	C5-C6-N6	-5.43	119.35	123.70
2	A	1812	A	C4-C5-C6	5.43	119.72	117.00
7	I	69	PHE	CB-CG-CD2	-5.43	117.00	120.80
2	A	946	C	N3-C4-N4	5.43	121.80	118.00
2	A	1056	A	C5-C6-N1	-5.43	114.98	117.70
2	A	1149	C	C2-N1-C1'	5.43	124.78	118.80
2	A	3	C	N3-C4-N4	5.43	121.80	118.00
2	A	1215	C	N3-C4-C5	-5.43	119.73	121.90
1	N	74	C	N3-C4-N4	5.43	121.80	118.00
2	A	117	C	N3-C4-N4	5.43	121.80	118.00
2	A	306	C	N3-C4-N4	5.43	121.80	118.00
2	A	624	A	C5-C6-N1	-5.43	114.98	117.70
2	A	825	C	O4'-C1'-N1	5.43	112.54	108.20
2	A	1242	A	C5-C6-N1	-5.43	114.98	117.70
2	A	684	A	P-O5'-C5'	5.43	129.59	120.90
2	A	839	C	N3-C4-C5	-5.43	119.73	121.90
2	A	295	C	N3-C4-N4	5.43	121.80	118.00
2	A	316	C	N3-C4-N4	5.43	121.80	118.00
2	A	759	A	C5-C6-N6	-5.43	119.36	123.70
2	A	1079	A	C5-C6-N6	-5.43	119.36	123.70
2	A	1362	G	O4'-C1'-N9	5.43	112.54	108.20
2	A	1618	A	C5-C6-N1	-5.43	114.99	117.70
2	A	1656	A	C5-C6-N1	-5.43	114.99	117.70
2	A	221	A	C5-C6-N6	-5.42	119.36	123.70
2	A	595	A	C5-C6-N1	-5.42	114.99	117.70
2	A	1328	A	C4-C5-C6	5.42	119.71	117.00
2	A	1526	A	C5-C6-N6	-5.42	119.36	123.70
2	A	1690	A	C5-C6-N1	-5.42	114.99	117.70
2	A	70	G	O4'-C1'-N9	5.42	112.54	108.20
2	A	469	C	N3-C4-C5	-5.42	119.73	121.90
2	A	953	A	C5-C6-N6	-5.42	119.36	123.70
2	A	1374	A	C5-C6-N1	-5.42	114.99	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1415	C	C6-N1-C2	-5.42	118.13	120.30
2	A	11	A	C5-C6-N6	-5.42	119.36	123.70
2	A	174	C	N3-C4-N4	5.42	121.80	118.00
2	A	381	C	N3-C4-N4	5.42	121.80	118.00
2	A	355	C	N3-C4-N4	5.42	121.79	118.00
2	A	823	A	C5-C6-N6	-5.42	119.36	123.70
2	A	1588	C	N3-C4-C5	-5.42	119.73	121.90
2	A	38	A	C5-C6-N6	-5.42	119.36	123.70
2	A	149	A	C5-C6-N1	-5.42	114.99	117.70
2	A	1065	U	O4'-C1'-N1	5.42	112.53	108.20
3	F	24	C	N3-C4-N4	5.42	121.79	118.00
2	A	1456	C	N3-C4-N4	5.42	121.79	118.00
2	A	1609	A	C5-C6-N1	-5.42	114.99	117.70
1	N	58	A	O4'-C1'-N9	5.41	112.53	108.20
2	A	1043	C	N3-C4-C5	-5.41	119.73	121.90
2	A	1114	C	N3-C4-C5	-5.41	119.73	121.90
2	A	1390	G	C2'-C3'-O3'	5.41	122.36	113.70
2	A	487	C	N3-C4-C5	-5.41	119.73	121.90
2	A	1416	G	O4'-C1'-N9	5.41	112.53	108.20
2	A	355	C	N3-C4-C5	-5.41	119.74	121.90
2	A	476	A	C5-C6-N1	-5.41	115.00	117.70
2	A	516	A	C4-C5-C6	5.41	119.70	117.00
2	A	900	A	C5-C6-N1	-5.41	115.00	117.70
2	A	1015	C	N3-C4-N4	5.41	121.79	118.00
2	A	1055	G	O4'-C1'-N9	5.41	112.53	108.20
2	A	1204	A	C5-C6-N1	-5.41	115.00	117.70
2	A	1560	C	N3-C4-C5	-5.41	119.74	121.90
2	A	1567	C	N3-C4-N4	5.41	121.79	118.00
2	A	1623	C	N3-C4-N4	5.41	121.79	118.00
3	F	7	C	N3-C4-N4	5.41	121.79	118.00
2	A	440	C	N3-C4-C5	-5.41	119.74	121.90
2	A	1449	C	N3-C4-N4	5.41	121.79	118.00
2	A	1470	A	C5'-C4'-C3'	-5.41	107.34	116.00
2	A	1749	C	N3-C4-C5	-5.41	119.74	121.90
16	T	321	PHE	CB-CG-CD2	5.41	124.59	120.80
2	A	104	A	C5-C6-N6	-5.41	119.38	123.70
3	F	18	A	C5-C6-N6	-5.41	119.37	123.70
2	A	78	C	O4'-C1'-N1	5.41	112.52	108.20
2	A	354	A	C5-C6-N6	-5.41	119.38	123.70
2	A	479	A	C5-C6-N6	-5.41	119.38	123.70
2	A	550	A	C5-C6-N6	-5.41	119.38	123.70
2	A	996	C	N3-C4-C5	-5.41	119.74	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1109	A	C5-C6-N6	-5.41	119.38	123.70
2	A	1819	A	C5-C6-N1	-5.41	115.00	117.70
2	A	993	A	O4'-C1'-N9	5.40	112.52	108.20
2	A	214	A	C5-C6-N1	-5.40	115.00	117.70
2	A	321	C	P-O3'-C3'	5.40	126.18	119.70
2	A	814	A	C5-C6-N6	-5.40	119.38	123.70
2	A	1031	A	C5-C6-N1	-5.40	115.00	117.70
2	A	1205	A	C5-C6-N6	-5.40	119.38	123.70
2	A	1726	A	C5-C6-N1	-5.40	115.00	117.70
2	A	391	A	C5-C6-N1	-5.40	115.00	117.70
2	A	1104	G	O4'-C1'-N9	5.40	112.52	108.20
2	A	1243	C	N3-C4-C5	-5.40	119.74	121.90
2	A	1682	C	N3-C4-C5	-5.40	119.74	121.90
2	A	1738	G	O4'-C1'-N9	5.40	112.52	108.20
2	A	1859	C	N3-C4-C5	-5.40	119.74	121.90
1	N	13	C	N3-C4-C5	-5.40	119.74	121.90
2	A	218	A	C5-C6-N6	-5.40	119.38	123.70
2	A	284	C	O4'-C1'-N1	5.40	112.52	108.20
2	A	315	C	N3-C4-N4	5.40	121.78	118.00
2	A	449	C	N3-C4-C5	-5.40	119.74	121.90
2	A	544	A	C5-C6-N6	-5.40	119.38	123.70
2	A	1772	C	N3-C4-C5	-5.40	119.74	121.90
2	A	1780	U	O4'-C1'-N1	5.40	112.52	108.20
2	A	1261	A	C5-C6-N1	-5.40	115.00	117.70
2	A	1351	C	N3-C4-N4	5.40	121.78	118.00
3	F	19	C	N3-C4-C5	-5.40	119.74	121.90
2	A	755	C	N3-C4-C5	-5.39	119.74	121.90
2	A	1255	A	O4'-C1'-N9	5.39	112.52	108.20
2	A	1775	A	C5-C6-N6	-5.39	119.39	123.70
3	F	4	A	C5-C6-N6	-5.39	119.38	123.70
2	A	294	C	N3-C4-C5	-5.39	119.74	121.90
2	A	465	C	O4'-C1'-N1	5.39	112.51	108.20
2	A	1278	A	O4'-C1'-N9	5.39	112.51	108.20
2	A	1463	C	N3-C4-C5	-5.39	119.74	121.90
2	A	1805	C	N3-C4-N4	5.39	121.78	118.00
2	A	293	A	C5-C6-N6	-5.39	119.39	123.70
2	A	636	G	O4'-C1'-N9	5.39	112.51	108.20
2	A	842	G	O4'-C1'-N9	5.39	112.51	108.20
2	A	924	G	O4'-C1'-N9	5.39	112.51	108.20
2	A	953	A	C5-C6-N1	-5.39	115.00	117.70
2	A	1031	A	C5-C6-N6	-5.39	119.39	123.70
3	F	11	A	C5-C6-N1	-5.39	115.00	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	85	A	C5-C6-N6	-5.39	119.39	123.70
2	A	369	C	N3-C4-N4	5.39	121.77	118.00
2	A	443	C	N3-C4-C5	-5.39	119.74	121.90
2	A	482	C	N3-C4-C5	-5.39	119.74	121.90
2	A	1318	G	O4'-C1'-N9	5.39	112.51	108.20
2	A	1548	C	N3-C4-N4	5.39	121.77	118.00
2	A	569	C	N3-C4-C5	-5.39	119.75	121.90
2	A	804	A	C5-C6-N1	-5.39	115.01	117.70
2	A	1083	A	C5-C6-N6	-5.39	119.39	123.70
3	F	6	A	C5-C6-N6	-5.39	119.39	123.70
2	A	125	C	N3-C4-C5	-5.39	119.75	121.90
2	A	129	C	N3-C4-C5	-5.39	119.75	121.90
2	A	227	A	O4'-C1'-N9	5.39	112.51	108.20
2	A	529	C	N3-C4-C5	-5.39	119.75	121.90
2	A	1051	A	C5-C6-N6	-5.39	119.39	123.70
2	A	1177	A	C5-C6-N6	-5.39	119.39	123.70
2	A	178	C	N3-C4-N4	5.38	121.77	118.00
2	A	308	C	N3-C4-N4	5.38	121.77	118.00
2	A	612	C	N3-C4-N4	5.38	121.77	118.00
2	A	1005	A	C5-C6-N6	-5.38	119.39	123.70
2	A	1075	C	N3-C4-N4	5.38	121.77	118.00
2	A	1532	A	C5-C6-N1	-5.38	115.01	117.70
2	A	143	U	O4'-C1'-N1	5.38	112.51	108.20
2	A	1745	C	N3-C4-N4	5.38	121.77	118.00
2	A	803	G	O4'-C1'-N9	5.38	112.50	108.20
2	A	1744	G	O4'-C1'-N9	5.38	112.50	108.20
2	A	1818	A	C5-C6-N6	-5.38	119.39	123.70
2	A	662	A	C5-C6-N1	-5.38	115.01	117.70
2	A	677	C	N3-C4-C5	-5.38	119.75	121.90
2	A	1785	A	C5-C6-N1	-5.38	115.01	117.70
2	A	422	G	O4'-C1'-N9	5.38	112.50	108.20
2	A	435	A	C5-C6-N1	-5.38	115.01	117.70
2	A	477	U	O4'-C1'-N1	5.38	112.50	108.20
2	A	900	A	C5-C6-N6	-5.38	119.40	123.70
2	A	1088	G	O4'-C1'-N9	5.38	112.50	108.20
2	A	1258	C	N3-C4-C5	-5.38	119.75	121.90
2	A	1801	C	N3-C4-N4	5.38	121.76	118.00
2	A	1120	C	N3-C4-C5	-5.38	119.75	121.90
2	A	1813	A	C5-C6-N1	-5.38	115.01	117.70
1	N	3	C	N3-C4-N4	5.37	121.76	118.00
1	N	36	A	C5-C6-N1	-5.37	115.01	117.70
2	A	142	C	N3-C4-C5	-5.37	119.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	515	A	C5-C6-N6	-5.37	119.40	123.70
2	A	1090	C	N3-C4-C5	-5.37	119.75	121.90
2	A	54	A	C5-C6-N1	-5.37	115.01	117.70
2	A	535	A	C5-C6-N1	-5.37	115.02	117.70
2	A	1419	C	N3-C4-N4	5.37	121.76	118.00
2	A	1665	C	N3-C4-C5	-5.37	119.75	121.90
2	A	1719	A	C5-C6-N6	-5.37	119.40	123.70
2	A	1772	C	N3-C4-N4	5.37	121.76	118.00
2	A	452	C	N3-C4-N4	5.37	121.76	118.00
2	A	628	C	N3-C4-C5	-5.37	119.75	121.90
2	A	857	A	C5-C6-N6	-5.37	119.41	123.70
2	A	1086	C	N3-C4-C5	-5.37	119.75	121.90
2	A	901	C	N3-C4-C5	-5.37	119.75	121.90
1	N	57	A	C5-C6-N1	-5.37	115.02	117.70
2	A	69	C	N3-C4-C5	-5.37	119.75	121.90
2	A	986	A	O4'-C1'-N9	5.37	112.49	108.20
2	A	1187	C	N3-C4-C5	-5.37	119.75	121.90
2	A	6	G	O4'-C1'-N9	5.36	112.49	108.20
2	A	667	G	O4'-C1'-N9	5.36	112.49	108.20
2	A	922	A	C5-C6-N1	-5.36	115.02	117.70
2	A	1115	A	C5-C6-N1	-5.36	115.02	117.70
2	A	1243	C	N3-C4-N4	5.36	121.75	118.00
2	A	1480	A	C4-C5-C6	5.36	119.68	117.00
2	A	1658	A	C4-C5-C6	5.36	119.68	117.00
2	A	587	G	O4'-C1'-N9	5.36	112.49	108.20
2	A	658	A	C5-C6-N6	-5.36	119.41	123.70
2	A	82	G	O4'-C1'-N9	5.36	112.49	108.20
2	A	523	A	C5-C6-N1	-5.36	115.02	117.70
2	A	1255	A	C5-C6-N6	-5.36	119.41	123.70
2	A	1673	A	C5-C6-N6	-5.36	119.41	123.70
2	A	107	A	C5-C6-N6	-5.36	119.41	123.70
2	A	399	C	N3-C4-C5	-5.36	119.76	121.90
2	A	1578	C	N3-C4-N4	5.36	121.75	118.00
1	N	36	A	O4'-C1'-N9	5.36	112.49	108.20
2	A	490	A	O4'-C1'-N9	5.36	112.49	108.20
2	A	1252	G	O4'-C1'-N9	5.36	112.48	108.20
2	A	1392	A	C5-C6-N1	-5.36	115.02	117.70
2	A	1426	C	N3-C4-N4	5.36	121.75	118.00
2	A	107	A	O4'-C1'-N9	5.36	112.48	108.20
2	A	228	A	O4'-C1'-N9	5.36	112.48	108.20
2	A	873	C	N3-C4-C5	-5.36	119.76	121.90
2	A	1415	C	N3-C4-C5	-5.36	119.76	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1583	A	C5-C6-N6	-5.36	119.42	123.70
2	A	1850	C	N3-C4-C5	-5.36	119.76	121.90
2	A	564	A	C5-C6-N1	-5.35	115.02	117.70
2	A	61	A	C5-C6-N1	-5.35	115.02	117.70
2	A	1026	A	C5-C6-N1	-5.35	115.02	117.70
2	A	1113	C	N3-C4-N4	5.35	121.75	118.00
2	A	1213	A	C5-C6-N6	-5.35	119.42	123.70
2	A	1149	C	N3-C4-N4	5.35	121.75	118.00
2	A	1249	A	C5-C6-N1	-5.35	115.02	117.70
2	A	1632	A	C5-C6-N6	-5.35	119.42	123.70
2	A	1776	G	C5'-C4'-C3'	5.35	124.56	116.00
2	A	1788	C	N3-C4-C5	-5.35	119.76	121.90
2	A	74	G	O4'-C1'-N9	5.35	112.48	108.20
2	A	173	A	C5-C6-N1	-5.35	115.03	117.70
2	A	1149	C	N3-C4-C5	-5.35	119.76	121.90
2	A	1431	C	N3-C4-N4	5.35	121.75	118.00
2	A	1812	A	O4'-C1'-N9	5.35	112.48	108.20
2	A	466	A	C5-C6-N6	-5.35	119.42	123.70
2	A	1038	A	C5-C6-N1	-5.35	115.03	117.70
2	A	1236	A	C5-C6-N1	-5.35	115.03	117.70
2	A	1255	A	C5'-C4'-O4'	5.35	115.52	109.10
2	A	1419	C	N3-C4-C5	-5.35	119.76	121.90
2	A	1845	A	C5-C6-N1	-5.35	115.03	117.70
3	F	26	C	N3-C4-C5	-5.35	119.76	121.90
2	A	526	A	C5-C6-N6	-5.35	119.42	123.70
2	A	1134	C	N3-C4-N4	5.35	121.74	118.00
2	A	1155	G	O4'-C1'-N9	5.35	112.48	108.20
1	N	47	C	N3-C4-N4	5.34	121.74	118.00
2	A	290	A	C5-C6-N1	-5.34	115.03	117.70
2	A	1070	C	N3-C4-N4	5.34	121.74	118.00
2	A	1209	C	N3-C4-N4	5.34	121.74	118.00
2	A	1782	A	C5-C6-N6	-5.34	119.42	123.70
2	A	73	C	N3-C4-N4	5.34	121.74	118.00
2	A	234	C	N3-C4-N4	5.34	121.74	118.00
2	A	1863	A	C5-C6-N6	-5.34	119.42	123.70
2	A	659	A	C5-C6-N1	-5.34	115.03	117.70
2	A	1498	C	N3-C4-C5	-5.34	119.76	121.90
1	N	39	C	N3-C4-C5	-5.34	119.77	121.90
2	A	182	C	N3-C4-C5	-5.34	119.77	121.90
2	A	147	A	C5-C6-N1	-5.34	115.03	117.70
2	A	227	A	C5-C6-N1	-5.34	115.03	117.70
2	A	559	A	O4'-C1'-N9	5.34	112.47	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	630	A	C5-C6-N6	-5.34	119.43	123.70
2	A	1280	A	C5-C6-N1	-5.34	115.03	117.70
2	A	1380	C	N3-C4-C5	-5.34	119.77	121.90
2	A	1674	A	C5-C6-N6	-5.34	119.43	123.70
2	A	1737	C	N3-C4-N4	5.34	121.74	118.00
2	A	1795	A	C4-C5-C6	5.34	119.67	117.00
2	A	1822	C	N3-C4-C5	-5.34	119.77	121.90
3	F	23	A	C5-C6-N1	-5.34	115.03	117.70
2	A	19	A	C5-C6-N1	-5.33	115.03	117.70
2	A	474	A	C5-C6-N6	-5.33	119.43	123.70
2	A	658	A	C5-C6-N1	-5.33	115.03	117.70
2	A	871	A	C5-C6-N1	-5.33	115.03	117.70
2	A	970	C	N3-C4-C5	-5.33	119.77	121.90
2	A	1008	A	O4'-C1'-N9	5.33	112.47	108.20
2	A	1763	C	N3-C4-N4	5.33	121.73	118.00
2	A	38	A	C5-C6-N1	-5.33	115.03	117.70
2	A	173	A	O4'-C1'-N9	5.33	112.47	108.20
2	A	414	C	N3-C4-C5	-5.33	119.77	121.90
2	A	449	C	C5'-C4'-O4'	5.33	115.50	109.10
2	A	933	C	N3-C4-C5	-5.33	119.77	121.90
2	A	1635	A	C5-C6-N1	-5.33	115.03	117.70
14	R	21	PHE	CB-CG-CD2	5.33	124.53	120.80
2	A	106	C	N3-C4-C5	-5.33	119.77	121.90
2	A	529	C	N3-C4-N4	5.33	121.73	118.00
1	N	49	A	C5-C6-N6	-5.33	119.44	123.70
2	A	1019	A	C5-C6-N1	-5.33	115.03	117.70
2	A	1375	A	C5-C6-N6	-5.33	119.44	123.70
1	N	75	A	C5-C6-N1	-5.33	115.04	117.70
2	A	975	C	N3-C4-N4	5.33	121.73	118.00
2	A	1251	G	C5'-C4'-O4'	5.33	115.49	109.10
2	A	1327	C	C6-N1-C1'	-5.33	114.41	120.80
2	A	912	A	C5-C6-N1	-5.33	115.04	117.70
2	A	1051	A	C5-C6-N1	-5.33	115.04	117.70
2	A	1426	C	N3-C4-C5	-5.33	119.77	121.90
2	A	1613	C	N3-C4-C5	-5.33	119.77	121.90
2	A	1655	C	N3-C4-N4	5.33	121.73	118.00
2	A	134	C	N3-C4-C5	-5.32	119.77	121.90
2	A	150	A	C5-C6-N6	-5.32	119.44	123.70
2	A	40	A	O4'-C1'-N9	5.32	112.46	108.20
2	A	373	G	O4'-C1'-N9	5.32	112.46	108.20
2	A	1099	C	N3-C4-C5	-5.32	119.77	121.90
2	A	1840	G	O4'-C1'-N9	5.32	112.46	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	179	C	N3-C4-C5	-5.32	119.77	121.90
2	A	229	A	O4'-C1'-N9	5.32	112.46	108.20
2	A	633	A	C4-C5-C6	5.32	119.66	117.00
2	A	865	A	C4-C5-C6	5.32	119.66	117.00
2	A	1791	U	O4'-C1'-N1	5.32	112.46	108.20
2	A	294	C	N3-C4-N4	5.32	121.72	118.00
2	A	631	A	C5-C6-N6	-5.32	119.44	123.70
2	A	820	C	N3-C4-N4	5.32	121.72	118.00
2	A	1305	C	N3-C4-C5	-5.32	119.77	121.90
2	A	1479	A	C5-C6-N1	-5.32	115.04	117.70
2	A	1522	C	N3-C4-C5	-5.32	119.77	121.90
2	A	1564	A	C5-C6-N6	-5.32	119.45	123.70
2	A	1631	G	O4'-C1'-N9	5.32	112.45	108.20
2	A	1792	C	N3-C4-C5	-5.32	119.77	121.90
20	X	115	LYS	N-CA-CB	5.32	120.17	110.60
1	N	34	A	C5-C6-N1	-5.32	115.04	117.70
2	A	1361	G	O4'-C1'-N9	5.32	112.45	108.20
2	A	1405	A	C5-C6-N6	-5.32	119.45	123.70
2	A	139	C	N3-C4-C5	-5.31	119.78	121.90
2	A	83	A	C5-C6-N6	-5.31	119.45	123.70
2	A	324	C	N3-C4-C5	-5.31	119.78	121.90
2	A	512	A	C5-C6-N6	-5.31	119.45	123.70
2	A	732	C	N3-C4-N4	5.31	121.72	118.00
2	A	985	C	N3-C4-C5	-5.31	119.78	121.90
2	A	1075	C	N3-C4-C5	-5.31	119.78	121.90
2	A	1540	A	C5-C6-N1	-5.31	115.04	117.70
2	A	1730	A	O4'-C1'-N9	5.31	112.45	108.20
3	F	6	A	O4'-C1'-N9	5.31	112.45	108.20
2	A	184	G	C5-C6-O6	-5.31	125.41	128.60
2	A	1540	A	C5-C6-N6	-5.31	119.45	123.70
7	I	196	THR	N-CA-CB	5.31	120.39	110.30
2	A	24	C	N3-C4-N4	5.31	121.72	118.00
2	A	1372	A	C5-C6-N1	-5.31	115.05	117.70
2	A	1372	A	C5-C6-N6	-5.31	119.45	123.70
1	N	16	C	N3-C4-C5	-5.31	119.78	121.90
2	A	947	C	N3-C4-C5	-5.31	119.78	121.90
2	A	947	C	P-O5'-C5'	5.31	129.39	120.90
33	k	97	PRO	N-CA-CB	-5.31	96.76	102.60
2	A	831	C	N3-C4-N4	5.31	121.71	118.00
2	A	909	A	C5-C6-N1	-5.31	115.05	117.70
2	A	1535	G	O4'-C1'-N9	5.31	112.44	108.20
2	A	1548	C	N3-C4-C5	-5.30	119.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1578	C	N3-C4-C5	-5.30	119.78	121.90
2	A	1365	A	C5-C6-N1	-5.30	115.05	117.70
2	A	1425	G	O4'-C1'-N9	5.30	112.44	108.20
2	A	1594	U	C2-N1-C1'	5.30	124.06	117.70
2	A	1705	C	N3-C4-C5	-5.30	119.78	121.90
2	A	1245	C	N3-C4-C5	-5.30	119.78	121.90
2	A	77	A	C5-C6-N1	-5.30	115.05	117.70
2	A	522	C	N3-C4-C5	-5.30	119.78	121.90
2	A	1181	C	N3-C4-C5	-5.30	119.78	121.90
2	A	1445	G	O4'-C1'-N9	5.30	112.44	108.20
3	F	8	A	C5-C6-N1	-5.30	115.05	117.70
7	I	2	ALA	N-CA-CB	5.30	117.52	110.10
2	A	232	A	C5-C6-N1	-5.30	115.05	117.70
2	A	554	A	P-O3'-C3'	5.30	126.06	119.70
2	A	645	A	C5-C6-N6	-5.30	119.46	123.70
2	A	1759	C	N3-C4-C5	-5.30	119.78	121.90
3	F	4	A	C5-C6-N1	-5.30	115.05	117.70
2	A	792	G	O4'-C1'-N9	5.29	112.44	108.20
2	A	1624	C	N3-C4-C5	-5.29	119.78	121.90
2	A	1829	A	C5-C6-N1	-5.29	115.05	117.70
2	A	103	A	C5-C6-N1	-5.29	115.05	117.70
2	A	327	C	N3-C4-N4	5.29	121.70	118.00
2	A	675	A	C5-C6-N6	-5.29	119.47	123.70
2	A	1777	C	N3-C4-C5	-5.29	119.78	121.90
2	A	1792	C	N3-C4-N4	5.29	121.71	118.00
2	A	25	A	C5-C6-N6	-5.29	119.47	123.70
9	K	165	TYR	CB-CG-CD1	5.29	124.17	121.00
2	A	302	C	N3-C4-N4	5.29	121.70	118.00
2	A	363	G	C5-C6-O6	-5.29	125.43	128.60
2	A	1112	C	C2-N1-C1'	5.29	124.62	118.80
2	A	1384	A	O4'-C1'-N9	5.29	112.43	108.20
2	A	1621	C	N3-C4-C5	-5.29	119.78	121.90
2	A	392	C	N3-C4-C5	-5.29	119.78	121.90
2	A	744	C	O4'-C1'-N1	5.29	112.43	108.20
2	A	1056	A	C5-C6-N6	-5.29	119.47	123.70
2	A	1365	A	O4'-C1'-N9	5.29	112.43	108.20
2	A	1695	C	N3-C4-N4	5.29	121.70	118.00
2	A	1818	A	C5-C6-N1	-5.29	115.06	117.70
2	A	78	C	N3-C4-C5	-5.29	119.78	121.90
3	F	30	A	C5-C6-N1	-5.29	115.06	117.70
2	A	850	A	C5-C6-N6	-5.29	119.47	123.70
2	A	857	A	C5-C6-N1	-5.29	115.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1196	A	C5-C6-N6	-5.29	119.47	123.70
2	A	159	A	C5-C6-N1	-5.28	115.06	117.70
2	A	446	C	N3-C4-C5	-5.28	119.79	121.90
2	A	560	C	N3-C4-N4	5.28	121.70	118.00
2	A	1033	G	O4'-C1'-N9	5.28	112.43	108.20
2	A	1053	C	N3-C4-C5	-5.28	119.79	121.90
2	A	1857	A	C5-C6-N6	-5.28	119.47	123.70
2	A	1499	C	N3-C4-N4	5.28	121.70	118.00
2	A	330	C	N3-C4-C5	-5.28	119.79	121.90
2	A	343	C	N3-C4-N4	5.28	121.70	118.00
2	A	1592	C	N3-C4-N4	5.28	121.70	118.00
2	A	806	A	C5-C6-N1	-5.28	115.06	117.70
2	A	1291	A	C5-C6-N6	-5.28	119.48	123.70
2	A	1829	A	C5-C6-N6	-5.28	119.48	123.70
3	F	7	C	N3-C4-C5	-5.28	119.79	121.90
2	A	190	A	C5-C6-N1	-5.28	115.06	117.70
2	A	243	C	N3-C4-C5	-5.28	119.79	121.90
2	A	542	G	P-O5'-C5'	5.28	129.34	120.90
2	A	875	C	N3-C4-N4	5.28	121.69	118.00
2	A	909	A	C5-C6-N6	-5.28	119.48	123.70
2	A	1528	A	C5-C6-N6	-5.28	119.48	123.70
2	A	901	C	N3-C4-N4	5.28	121.69	118.00
2	A	974	G	O4'-C1'-N9	5.28	112.42	108.20
2	A	1731	G	O4'-C1'-N9	5.28	112.42	108.20
2	A	1857	A	C5-C6-N1	-5.28	115.06	117.70
6	H	96	TYR	CB-CG-CD2	5.28	124.17	121.00
2	A	1177	A	C5-C6-N1	-5.27	115.06	117.70
2	A	1683	C	N3-C4-N4	5.27	121.69	118.00
2	A	208	G	C6-C5-N7	-5.27	127.24	130.40
2	A	558	C	N3-C4-C5	-5.27	119.79	121.90
2	A	1260	C	O4'-C1'-N1	5.27	112.42	108.20
2	A	1309	A	C5-C6-N6	-5.27	119.48	123.70
2	A	1794	A	C5-C6-N6	-5.27	119.48	123.70
2	A	1795	A	C5-C6-N6	-5.27	119.48	123.70
2	A	626	C	N3-C4-C5	-5.27	119.79	121.90
2	A	1800	A	C5-C6-N6	-5.27	119.48	123.70
2	A	1860	A	C5-C6-N1	-5.27	115.06	117.70
2	A	4	C	N3-C4-C5	-5.27	119.79	121.90
2	A	85	A	O4'-C1'-N9	5.27	112.42	108.20
2	A	214	A	O4'-C1'-N9	5.27	112.42	108.20
2	A	1460	C	N3-C4-C5	-5.27	119.79	121.90
2	A	1482	A	C5-C6-N6	-5.27	119.48	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	486	C	N3-C4-C5	-5.27	119.79	121.90
2	A	949	C	N3-C4-N4	5.27	121.69	118.00
2	A	1073	A	C5-C6-N1	-5.27	115.07	117.70
2	A	1261	A	C5-C6-N6	-5.27	119.49	123.70
2	A	598	C	N3-C4-C5	-5.27	119.79	121.90
3	F	18	A	C5-C6-N1	-5.27	115.07	117.70
2	A	37	C	N3-C4-C5	-5.26	119.79	121.90
2	A	411	G	O4'-C1'-N9	5.26	112.41	108.20
2	A	661	A	C5-C6-N6	-5.26	119.49	123.70
2	A	833	A	C5-C6-N1	-5.26	115.07	117.70
2	A	1694	A	C5-C6-N6	-5.26	119.49	123.70
2	A	854	A	C5-C6-N6	-5.26	119.49	123.70
2	A	1209	C	N3-C4-C5	-5.26	119.80	121.90
2	A	1429	C	N3-C4-C5	-5.26	119.80	121.90
1	N	47	C	P-O3'-C3'	5.26	126.01	119.70
2	A	289	G	O4'-C1'-N9	5.26	112.41	108.20
2	A	845	A	C5-C6-N6	-5.26	119.49	123.70
2	A	946	C	N3-C4-C5	-5.26	119.80	121.90
2	A	1537	C	N3-C4-C5	-5.26	119.80	121.90
2	A	1746	C	N3-C4-N4	5.26	121.68	118.00
2	A	1787	A	C5-C6-N6	-5.26	119.49	123.70
2	A	1828	A	C5-C6-N6	-5.26	119.49	123.70
2	A	580	A	C5-C6-N1	-5.26	115.07	117.70
2	A	583	C	N3-C4-C5	-5.26	119.80	121.90
2	A	1046	A	C5-C6-N6	-5.26	119.49	123.70
2	A	677	C	N3-C4-N4	5.26	121.68	118.00
2	A	1366	A	C5-C6-N1	-5.26	115.07	117.70
2	A	1694	A	P-O3'-C3'	-5.26	113.39	119.70
14	R	93	SER	N-CA-CB	5.26	118.39	110.50
2	A	50	A	C5-C6-N1	-5.25	115.07	117.70
2	A	72	C	N3-C4-C5	-5.25	119.80	121.90
2	A	76	U	O4'-C1'-N1	5.25	112.40	108.20
2	A	669	A	C4-C5-C6	5.25	119.63	117.00
2	A	1154	G	O4'-C1'-N9	5.25	112.40	108.20
2	A	822	A	C5-C6-N1	-5.25	115.07	117.70
2	A	852	C	N3-C4-C5	-5.25	119.80	121.90
2	A	1023	A	C5-C6-N1	-5.25	115.07	117.70
2	A	1237	A	C5-C6-N1	-5.25	115.07	117.70
2	A	1695	C	N3-C4-C5	-5.25	119.80	121.90
2	A	1254	A	C5-C6-N1	-5.25	115.08	117.70
2	A	1779	C	N3-C4-C5	-5.25	119.80	121.90
2	A	492	C	N3-C4-C5	-5.25	119.80	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	574	A	C5-C6-N1	-5.25	115.08	117.70
2	A	1096	A	O4'-C1'-N9	5.25	112.40	108.20
2	A	1291	A	O4'-C1'-N9	5.25	112.40	108.20
2	A	1423	C	N3-C4-N4	5.25	121.67	118.00
2	A	1827	C	N3-C4-C5	-5.25	119.80	121.90
2	A	809	A	O4'-C1'-N9	5.25	112.40	108.20
2	A	1287	A	C5-C6-N6	-5.25	119.50	123.70
2	A	408	A	C5-C6-N1	-5.25	115.08	117.70
2	A	1248	C	N3-C4-N4	5.25	121.67	118.00
2	A	338	A	C5-C6-N6	-5.24	119.50	123.70
2	A	830	C	N3-C4-N4	5.24	121.67	118.00
2	A	1124	C	N3-C4-N4	5.24	121.67	118.00
2	A	1184	A	C5-C6-N6	-5.24	119.51	123.70
2	A	1186	A	C5-C6-N6	-5.24	119.50	123.70
2	A	1224	A	O4'-C1'-N9	5.24	112.39	108.20
2	A	1533	C	N3-C4-C5	-5.24	119.80	121.90
2	A	1796	C	N3-C4-C5	-5.24	119.80	121.90
2	A	801	U	O4'-C1'-N1	5.24	112.39	108.20
2	A	1327	C	N3-C4-C5	-5.24	119.80	121.90
2	A	684	A	C5-C6-N1	-5.24	115.08	117.70
2	A	788	C	N3-C4-N4	5.24	121.67	118.00
2	A	1645	A	C5-C6-N6	-5.24	119.51	123.70
42	t	43	LEU	N-CA-CB	5.24	120.87	110.40
2	A	367	G	O4'-C1'-N9	5.24	112.39	108.20
3	F	20	C	N3-C4-C5	-5.24	119.81	121.90
2	A	137	U	C1'-O4'-C4'	-5.23	105.71	109.90
2	A	366	A	C5-C6-N6	-5.23	119.51	123.70
2	A	540	C	N3-C4-N4	5.23	121.66	118.00
2	A	796	U	P-O5'-C5'	5.23	129.27	120.90
2	A	1112	C	N3-C4-C5	-5.23	119.81	121.90
2	A	1214	C	N3-C4-C5	-5.23	119.81	121.90
2	A	1312	C	N3-C4-C5	-5.23	119.81	121.90
1	N	64	C	N3-C4-C5	-5.23	119.81	121.90
2	A	39	A	C4-C5-C6	5.23	119.61	117.00
2	A	54	A	O4'-C1'-N9	5.23	112.39	108.20
2	A	931	G	O4'-C1'-N9	5.23	112.39	108.20
2	A	958	A	O4'-C1'-N9	5.23	112.39	108.20
2	A	1004	A	C5-C6-N6	-5.23	119.52	123.70
2	A	1032	A	C5-C6-N1	-5.23	115.08	117.70
2	A	1696	C	N3-C4-C5	-5.23	119.81	121.90
2	A	820	C	N3-C4-C5	-5.23	119.81	121.90
2	A	846	C	N3-C4-C5	-5.23	119.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	73	C	N3-C4-C5	-5.23	119.81	121.90
2	A	650	C	N3-C4-C5	-5.23	119.81	121.90
2	A	951	A	P-O3'-C3'	5.23	125.97	119.70
2	A	1413	C	C5'-C4'-C3'	5.23	124.36	116.00
1	N	22	C	N3-C4-N4	5.22	121.66	118.00
2	A	241	A	C5-C6-N1	-5.22	115.09	117.70
2	A	517	C	N3-C4-C5	-5.22	119.81	121.90
2	A	649	G	O4'-C1'-N9	5.22	112.38	108.20
2	A	1465	A	C5-C6-N1	-5.22	115.09	117.70
2	A	158	A	C5-C6-N1	-5.22	115.09	117.70
2	A	823	A	C5-C6-N1	-5.22	115.09	117.70
2	A	1279	C	N3-C4-C5	-5.22	119.81	121.90
2	A	450	A	C5-C6-N6	-5.22	119.52	123.70
2	A	1508	C	N3-C4-N4	5.22	121.66	118.00
2	A	73	C	C2-N1-C1'	5.22	124.54	118.80
2	A	138	C	N3-C4-C5	-5.22	119.81	121.90
2	A	283	A	C5-C6-N1	-5.22	115.09	117.70
2	A	354	A	O4'-C1'-N9	5.22	112.38	108.20
2	A	361	A	C5-C6-N1	-5.22	115.09	117.70
2	A	670	G	O4'-C1'-N9	5.22	112.38	108.20
2	A	1812	A	C5-C6-N6	-5.22	119.52	123.70
2	A	316	C	N3-C4-C5	-5.22	119.81	121.90
2	A	388	A	C5-C6-N1	-5.22	115.09	117.70
2	A	474	A	C5-C6-N1	-5.22	115.09	117.70
2	A	612	C	N3-C4-C5	-5.22	119.81	121.90
2	A	645	A	O4'-C1'-N9	5.22	112.37	108.20
2	A	1816	A	C5-C6-N1	-5.22	115.09	117.70
39	q	48	TYR	CB-CG-CD1	-5.22	117.87	121.00
2	A	988	A	O4'-C1'-N9	5.21	112.37	108.20
2	A	1387	C	N3-C4-C5	-5.21	119.81	121.90
2	A	1629	A	C5-C6-N1	-5.21	115.09	117.70
2	A	1799	G	O4'-C1'-N9	5.21	112.37	108.20
3	F	27	C	N3-C4-C5	-5.21	119.81	121.90
38	p	106	TYR	N-CA-CB	5.21	119.99	110.60
2	A	753	C	N3-C4-N4	5.21	121.65	118.00
2	A	1121	C	N3-C4-N4	5.21	121.65	118.00
2	A	608	C	N3-C4-N4	5.21	121.65	118.00
2	A	880	C	N3-C4-N4	5.21	121.65	118.00
2	A	1227	C	N3-C4-N4	5.21	121.65	118.00
2	A	1248	C	N3-C4-C5	-5.21	119.82	121.90
2	A	1030	A	C4-C5-C6	5.21	119.60	117.00
2	A	1713	G	N3-C2-N2	5.21	123.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	37	C	N3-C4-N4	5.21	121.64	118.00
2	A	1094	C	N3-C4-N4	5.20	121.64	118.00
2	A	1737	C	N3-C4-C5	-5.20	119.82	121.90
2	A	861	A	C5-C6-N6	-5.20	119.54	123.70
2	A	1084	U	P-O3'-C3'	5.20	125.94	119.70
2	A	1250	C	N3-C4-C5	-5.20	119.82	121.90
2	A	1264	C	N3-C4-N4	5.20	121.64	118.00
2	A	1762	A	C5-C6-N6	-5.20	119.54	123.70
2	A	275	C	N3-C4-N4	5.20	121.64	118.00
2	A	1259	U	P-O3'-C3'	5.20	125.94	119.70
2	A	1528	A	C5-C6-N1	-5.20	115.10	117.70
2	A	1614	A	C5-C6-N1	-5.20	115.10	117.70
2	A	226	A	C5-C6-N1	-5.20	115.10	117.70
2	A	521	A	C5-C6-N6	-5.20	119.54	123.70
2	A	1269	C	N3-C4-C5	-5.20	119.82	121.90
2	A	164	A	C5-C6-N1	-5.20	115.10	117.70
2	A	1809	A	O4'-C1'-N9	5.20	112.36	108.20
2	A	64	A	C5-C6-N1	-5.20	115.10	117.70
2	A	67	C	N3-C4-C5	-5.20	119.82	121.90
2	A	1191	A	C4-C5-C6	5.20	119.60	117.00
2	A	1490	U	O4'-C1'-N1	5.19	112.36	108.20
2	A	48	C	N3-C4-C5	-5.19	119.82	121.90
2	A	149	A	C5-C6-N6	-5.19	119.55	123.70
2	A	1140	A	O4'-C1'-N9	5.19	112.36	108.20
2	A	1376	C	N3-C4-C5	-5.19	119.82	121.90
2	A	1622	C	N3-C4-C5	-5.19	119.82	121.90
2	A	141	A	C5-C6-N1	-5.19	115.11	117.70
2	A	557	C	N3-C4-C5	-5.19	119.82	121.90
2	A	977	A	O4'-C1'-N9	5.19	112.35	108.20
2	A	1569	C	N3-C4-N4	5.19	121.63	118.00
4	P	47	LEU	C-N-CA	5.19	134.68	121.70
2	A	64	A	C4-C5-C6	5.19	119.59	117.00
2	A	1044	G	N3-C2-N2	5.19	123.53	119.90
2	A	1204	A	C5-C6-N6	-5.19	119.55	123.70
2	A	1349	A	C5-C6-N1	-5.19	115.11	117.70
2	A	1442	A	C5-C6-N1	-5.19	115.11	117.70
2	A	1712	C	N3-C4-N4	5.19	121.63	118.00
2	A	3	C	O4'-C1'-N1	5.19	112.35	108.20
2	A	1159	C	N3-C4-C5	-5.19	119.83	121.90
2	A	1094	C	N3-C4-C5	-5.19	119.83	121.90
2	A	1323	G	O4'-C1'-N9	5.19	112.35	108.20
2	A	131	C	N3-C4-C5	-5.18	119.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	228	A	C5-C6-N6	-5.18	119.55	123.70
2	A	934	A	O4'-C1'-N9	5.18	112.35	108.20
2	A	1707	A	C5-C6-N6	-5.18	119.55	123.70
6	H	19	ALA	N-CA-CB	5.18	117.36	110.10
2	A	174	C	N3-C4-C5	-5.18	119.83	121.90
2	A	181	A	C5-C6-N1	-5.18	115.11	117.70
2	A	793	C	N3-C4-C5	-5.18	119.83	121.90
2	A	1642	A	C5-C6-N6	-5.18	119.56	123.70
20	X	108	SER	N-CA-CB	5.18	118.27	110.50
2	A	136	C	N3-C4-C5	-5.18	119.83	121.90
2	A	509	A	O4'-C1'-N9	5.18	112.34	108.20
2	A	1391	C	N3-C4-N4	5.18	121.62	118.00
3	F	3	C	N3-C4-C5	-5.18	119.83	121.90
2	A	644	A	C5-C6-N1	-5.18	115.11	117.70
2	A	1794	A	O4'-C1'-N9	5.18	112.34	108.20
2	A	414	C	N3-C4-N4	5.18	121.62	118.00
2	A	926	C	N3-C4-N4	5.18	121.62	118.00
2	A	1058	A	C5-C6-N6	-5.18	119.56	123.70
2	A	1391	C	N3-C4-C5	-5.18	119.83	121.90
2	A	1807	A	C5-C6-N1	-5.18	115.11	117.70
2	A	1826	A	C5-C6-N1	-5.18	115.11	117.70
2	A	804	A	O4'-C1'-N9	5.17	112.34	108.20
2	A	847	C	N3-C4-C5	-5.17	119.83	121.90
2	A	1275	C	N3-C4-C5	-5.17	119.83	121.90
2	A	275	C	N3-C4-C5	-5.17	119.83	121.90
2	A	4	C	N3-C4-N4	5.17	121.62	118.00
2	A	1496	G	O4'-C1'-N9	5.17	112.34	108.20
2	A	1526	A	O4'-C1'-N9	5.17	112.34	108.20
2	A	1558	G	O4'-C1'-N9	5.17	112.34	108.20
3	F	10	C	N3-C4-C5	-5.17	119.83	121.90
2	A	1413	C	C5'-C4'-O4'	-5.17	102.90	109.10
2	A	297	C	O4'-C1'-N1	5.17	112.33	108.20
2	A	812	A	C5-C6-N1	-5.17	115.12	117.70
2	A	1038	A	O4'-C1'-N9	5.17	112.33	108.20
2	A	1539	C	N3-C4-N4	5.17	121.62	118.00
2	A	1718	G	O4'-C1'-N9	5.17	112.33	108.20
2	A	24	C	C4'-C3'-C2'	-5.17	97.43	102.60
2	A	237	G	O4'-C1'-N9	5.17	112.33	108.20
2	A	1516	C	N3-C4-N4	5.17	121.62	118.00
2	A	908	C	N3-C4-C5	-5.16	119.83	121.90
2	A	1221	U	O4'-C1'-N1	5.16	112.33	108.20
2	A	749	C	N3-C4-N4	5.16	121.61	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1480	A	C5-C6-N6	-5.16	119.57	123.70
2	A	1762	A	C5-C6-N1	-5.16	115.12	117.70
1	N	34	A	O4'-C1'-N9	5.16	112.33	108.20
2	A	551	A	C5-C6-N1	-5.16	115.12	117.70
2	A	918	A	O4'-C1'-N9	5.16	112.33	108.20
2	A	965	U	O4'-C1'-N1	5.16	112.33	108.20
2	A	359	C	N3-C4-N4	5.16	121.61	118.00
2	A	608	C	N3-C4-C5	-5.16	119.84	121.90
2	A	1332	C	N3-C4-C5	-5.16	119.84	121.90
2	A	1398	A	O4'-C1'-N9	5.16	112.33	108.20
2	A	445	A	O4'-C1'-N9	5.16	112.33	108.20
2	A	1520	C	N3-C4-C5	-5.16	119.84	121.90
16	T	48	TYR	CB-CG-CD1	-5.16	117.91	121.00
2	A	45	A	C5-C6-N1	-5.16	115.12	117.70
2	A	640	A	C5-C6-N1	-5.16	115.12	117.70
2	A	1057	U	O4'-C1'-N1	5.16	112.32	108.20
2	A	655	G	O4'-C1'-N9	5.15	112.32	108.20
2	A	1692	A	C5-C6-N6	-5.15	119.58	123.70
2	A	1697	G	O4'-C1'-N9	5.15	112.32	108.20
3	F	6	A	C5-C6-N1	-5.15	115.12	117.70
2	A	332	C	N3-C4-C5	-5.15	119.84	121.90
2	A	836	C	N3-C4-C5	-5.15	119.84	121.90
2	A	1141	A	O4'-C1'-N9	5.15	112.32	108.20
2	A	43	U	O4'-C1'-N1	5.15	112.32	108.20
2	A	348	C	N3-C4-C5	-5.15	119.84	121.90
2	A	1432	C	P-O3'-C3'	5.15	125.88	119.70
2	A	1760	C	N3-C4-C5	-5.15	119.84	121.90
3	F	18	A	O4'-C1'-N9	5.15	112.32	108.20
2	A	326	A	C5-C6-N6	-5.15	119.58	123.70
2	A	1847	C	N3-C4-C5	-5.15	119.84	121.90
2	A	458	A	C5-C6-N6	-5.15	119.58	123.70
2	A	821	A	C5-C6-N1	-5.15	115.13	117.70
2	A	984	C	N3-C4-C5	-5.15	119.84	121.90
2	A	1411	C	N3-C4-C5	-5.15	119.84	121.90
2	A	1614	A	O4'-C1'-N9	5.15	112.32	108.20
42	t	12	TYR	CB-CG-CD2	-5.15	117.91	121.00
2	A	754	C	N3-C4-C5	-5.15	119.84	121.90
2	A	1162	G	O4'-C1'-N9	5.15	112.32	108.20
2	A	269	C	N3-C4-C5	-5.14	119.84	121.90
2	A	1076	A	C5-C6-N1	-5.14	115.13	117.70
2	A	1087	C	N3-C4-C5	-5.14	119.84	121.90
2	A	1382	A	O4'-C1'-N9	5.14	112.31	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	511	A	C5-C6-N1	-5.14	115.13	117.70
2	A	537	G	P-O3'-C3'	5.14	125.87	119.70
2	A	863	G	O4'-C1'-N9	5.14	112.31	108.20
2	A	1351	C	N3-C4-C5	-5.14	119.84	121.90
2	A	1546	U	C2-N1-C1'	5.14	123.87	117.70
2	A	79	A	C5-C6-N6	-5.14	119.59	123.70
2	A	1636	A	C5-C6-N6	-5.14	119.59	123.70
2	A	189	G	O4'-C1'-N9	5.14	112.31	108.20
2	A	243	C	N3-C4-N4	5.14	121.60	118.00
2	A	990	C	N3-C4-C5	-5.14	119.84	121.90
2	A	1272	A	C5-C6-N1	-5.14	115.13	117.70
2	A	1360	U	C6-N1-C1'	-5.14	114.00	121.20
2	A	1708	C	N3-C4-C5	-5.14	119.84	121.90
2	A	459	A	C5-C6-N6	-5.14	119.59	123.70
2	A	1553	C	N3-C4-N4	5.14	121.60	118.00
2	A	118	C	N3-C4-C5	-5.14	119.84	121.90
2	A	416	A	C5-C6-N1	-5.14	115.13	117.70
2	A	1808	G	O4'-C1'-N9	5.14	112.31	108.20
2	A	809	A	C5-C6-N1	-5.13	115.13	117.70
2	A	1232	G	N3-C2-N2	5.13	123.50	119.90
2	A	1743	G	O4'-C1'-N9	5.13	112.31	108.20
2	A	301	C	N3-C4-C5	-5.13	119.85	121.90
2	A	423	A	C5-C6-N6	-5.13	119.59	123.70
2	A	1774	G	C4'-C3'-C2'	-5.13	97.47	102.60
2	A	781	C	N3-C4-N4	5.13	121.59	118.00
2	A	1277	G	O4'-C1'-N9	5.13	112.31	108.20
2	A	1299	C	N3-C4-C5	-5.13	119.85	121.90
2	A	1575	A	C5-C6-N1	-5.13	115.13	117.70
2	A	491	C	C6-N1-C2	-5.13	118.25	120.30
2	A	1210	A	C5-C6-N1	-5.13	115.14	117.70
2	A	181	A	O4'-C1'-N9	5.13	112.30	108.20
2	A	295	C	N3-C4-C5	-5.13	119.85	121.90
2	A	1740	A	C5-C6-N1	-5.13	115.14	117.70
2	A	1745	C	N3-C4-C5	-5.13	119.85	121.90
28	f	67	ALA	N-CA-CB	5.13	117.28	110.10
2	A	1629	A	O4'-C1'-N9	5.12	112.30	108.20
2	A	206	A	O4'-C1'-N9	5.12	112.30	108.20
2	A	300	G	P-O5'-C5'	5.12	129.10	120.90
2	A	565	A	C5-C6-N1	-5.12	115.14	117.70
2	A	1467	C	N3-C4-C5	-5.12	119.85	121.90
2	A	1711	C	N3-C4-C5	-5.12	119.85	121.90
2	A	838	C	P-O5'-C5'	5.12	129.09	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	40	C	N3-C4-C5	-5.12	119.85	121.90
2	A	866	A	C5-C6-N1	-5.12	115.14	117.70
2	A	940	A	O4'-C1'-N9	5.12	112.29	108.20
2	A	1559	C	N3-C4-C5	-5.12	119.85	121.90
2	A	150	A	O4'-C1'-N9	5.12	112.29	108.20
2	A	226	A	P-O3'-C3'	5.12	125.84	119.70
2	A	227	A	C5-N7-C8	5.12	106.46	103.90
2	A	667	G	N3-C2-N2	5.11	123.48	119.90
2	A	1128	C	N3-C4-C5	-5.11	119.86	121.90
2	A	1448	A	C5-C6-N1	-5.11	115.14	117.70
2	A	270	G	O4'-C1'-N9	5.11	112.29	108.20
2	A	1054	A	C5-C6-N1	-5.11	115.14	117.70
2	A	1118	A	C5-C6-N1	-5.11	115.14	117.70
2	A	1233	C	N3-C4-C5	-5.11	119.86	121.90
2	A	1241	G	O4'-C1'-N9	5.11	112.29	108.20
2	A	1359	C	N3-C4-C5	-5.11	119.86	121.90
2	A	1378	A	O4'-C1'-N9	5.11	112.29	108.20
2	A	1529	C	N3-C4-N4	5.11	121.58	118.00
1	N	45	G	C5-C6-O6	-5.11	125.53	128.60
2	A	1551	A	C5-C6-N1	-5.11	115.15	117.70
1	N	53	A	C5-C6-N1	-5.11	115.15	117.70
2	A	371	C	N3-C4-C5	-5.11	119.86	121.90
2	A	1180	G	O4'-C1'-N9	5.11	112.29	108.20
2	A	1407	G	O4'-C1'-N9	5.11	112.29	108.20
2	A	1435	A	C5-C6-N1	-5.11	115.15	117.70
2	A	1552	C	C2-N1-C1'	5.11	124.42	118.80
2	A	1700	C	N3-C4-C5	-5.11	119.86	121.90
2	A	395	G	O4'-C1'-N9	5.10	112.28	108.20
2	A	1331	G	O4'-C1'-N9	5.10	112.28	108.20
2	A	804	A	C5-C6-N6	-5.10	119.62	123.70
2	A	822	A	C4-C5-C6	5.10	119.55	117.00
2	A	1058	A	O4'-C1'-N9	5.10	112.28	108.20
2	A	1289	A	O4'-C1'-N9	5.10	112.28	108.20
2	A	1615	A	C3'-C2'-C1'	-5.10	97.42	101.50
2	A	1653	G	O4'-C1'-N9	5.10	112.28	108.20
2	A	1411	C	N3-C4-N4	5.10	121.57	118.00
2	A	1517	A	C5-C6-N1	-5.10	115.15	117.70
2	A	209	C	N3-C4-C5	-5.10	119.86	121.90
2	A	1678	C	N3-C4-C5	-5.10	119.86	121.90
2	A	223	A	C5-C6-N1	-5.10	115.15	117.70
2	A	447	C	N3-C4-C5	-5.10	119.86	121.90
2	A	1577	C	N3-C4-C5	-5.10	119.86	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1816	A	C5-C6-N6	-5.10	119.62	123.70
14	R	21	PHE	CB-CG-CD1	-5.09	117.23	120.80
2	A	421	G	O4'-C1'-N9	5.09	112.28	108.20
2	A	560	C	N3-C4-C5	-5.09	119.86	121.90
2	A	437	A	C5-C6-N6	-5.09	119.63	123.70
2	A	808	A	O4'-C1'-N9	5.09	112.27	108.20
2	A	317	G	C2'-C3'-O3'	5.09	121.84	113.70
2	A	606	A	C5-C6-N1	-5.09	115.16	117.70
2	A	1271	G	O4'-C1'-N9	5.09	112.27	108.20
2	A	1483	A	O4'-C1'-N9	5.09	112.27	108.20
2	A	1643	G	C5'-C4'-C3'	-5.09	107.86	116.00
15	S	194	LYS	N-CA-CB	5.09	119.76	110.60
2	A	985	C	N3-C4-N4	5.09	121.56	118.00
2	A	1447	G	O4'-C1'-N9	5.09	112.27	108.20
2	A	220	C	N3-C4-C5	-5.09	119.86	121.90
2	A	338	A	O4'-C1'-N9	5.09	112.27	108.20
2	A	1278	A	C5-C6-N6	-5.09	119.63	123.70
2	A	1429	C	N3-C4-N4	5.09	121.56	118.00
2	A	1529	C	N3-C4-C5	-5.09	119.86	121.90
2	A	1600	G	N3-C2-N2	5.09	123.46	119.90
2	A	1784	A	C5-C6-N1	-5.09	115.16	117.70
2	A	603	C	N3-C4-C5	-5.08	119.87	121.90
2	A	744	C	N3-C4-N4	5.08	121.56	118.00
2	A	940	A	C5-C6-N6	-5.08	119.63	123.70
2	A	1134	C	N3-C4-C5	-5.08	119.87	121.90
2	A	1746	C	N3-C4-C5	-5.08	119.87	121.90
2	A	233	A	O4'-C1'-N9	5.08	112.27	108.20
2	A	1096	A	C5-C6-N1	-5.08	115.16	117.70
2	A	99	A	C5-C6-N1	-5.08	115.16	117.70
2	A	1592	C	N3-C4-C5	-5.08	119.87	121.90
42	t	1	MET	CG-SD-CE	-5.08	92.07	100.20
2	A	1816	A	O4'-C1'-N9	5.08	112.26	108.20
2	A	175	A	C5-C6-N6	-5.07	119.64	123.70
2	A	979	A	C5-C6-N1	-5.07	115.16	117.70
2	A	1192	A	C5-C6-N1	-5.07	115.16	117.70
2	A	39	A	O4'-C1'-N9	5.07	112.26	108.20
2	A	213	C	N3-C4-C5	-5.07	119.87	121.90
2	A	1260	C	N3-C4-C5	-5.07	119.87	121.90
2	A	1311	U	C6-N1-C1'	-5.07	114.10	121.20
2	A	657	U	O4'-C1'-N1	5.07	112.25	108.20
2	A	1417	A	C5-C6-N1	-5.07	115.17	117.70
2	A	1483	A	C5-C6-N6	-5.07	119.64	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	345	G	O4'-C1'-N9	5.07	112.25	108.20
2	A	572	U	C5'-C4'-C3'	-5.07	107.89	116.00
2	A	1139	A	C5-C6-N1	-5.07	115.17	117.70
2	A	1641	C	O4'-C1'-N1	5.07	112.25	108.20
35	m	113	PHE	CB-CG-CD1	5.07	124.35	120.80
2	A	433	U	O4'-C1'-N1	5.06	112.25	108.20
1	N	46	U	O4'-C1'-N1	5.06	112.25	108.20
2	A	271	G	O4'-C1'-N9	5.06	112.25	108.20
2	A	653	C	N3-C4-C5	-5.06	119.88	121.90
2	A	827	G	N3-C2-N2	5.06	123.44	119.90
2	A	1089	A	O4'-C1'-N9	5.06	112.25	108.20
2	A	99	A	O4'-C1'-N9	5.06	112.25	108.20
2	A	235	C	N3-C4-C5	-5.06	119.88	121.90
2	A	949	C	N3-C4-C5	-5.06	119.88	121.90
2	A	1782	A	C5-C6-N1	-5.06	115.17	117.70
2	A	540	C	O3'-P-O5'	-5.06	94.39	104.00
2	A	579	G	O4'-C1'-N9	5.06	112.25	108.20
2	A	209	C	P-O3'-C3'	5.05	125.77	119.70
2	A	1195	A	C5-C6-N6	-5.05	119.66	123.70
2	A	288	A	C5-C6-N1	-5.05	115.17	117.70
2	A	448	A	C5-C6-N1	-5.05	115.17	117.70
2	A	1511	G	O4'-C1'-N9	5.05	112.24	108.20
2	A	1523	G	O4'-C1'-N9	5.05	112.24	108.20
25	c	67	TYR	CB-CG-CD1	5.05	124.03	121.00
2	A	1295	A	O4'-C1'-N9	5.05	112.24	108.20
2	A	1451	A	O4'-C1'-N9	5.05	112.24	108.20
2	A	1747	C	N3-C4-C5	-5.05	119.88	121.90
2	A	172	U	O4'-C1'-N1	5.05	112.24	108.20
2	A	875	C	N3-C4-C5	-5.05	119.88	121.90
2	A	1756	C	N3-C4-C5	-5.05	119.88	121.90
2	A	353	A	C5-C6-N1	-5.05	115.18	117.70
2	A	1413	C	N3-C4-C5	-5.05	119.88	121.90
2	A	1853	A	O4'-C1'-N9	5.05	112.24	108.20
42	t	1	MET	C-N-CA	5.05	134.31	121.70
2	A	633	A	C5-C6-N1	-5.04	115.18	117.70
2	A	1470	A	C5-C6-N1	-5.04	115.18	117.70
2	A	79	A	C5-C6-N1	-5.04	115.18	117.70
2	A	136	C	N3-C4-N4	5.04	121.53	118.00
2	A	789	G	O4'-C1'-N9	5.04	112.23	108.20
1	N	13	C	P-O3'-C3'	5.04	125.75	119.70
1	N	20	A	C5-C6-N6	-5.04	119.67	123.70
2	A	1129	A	O4'-C1'-N9	5.04	112.23	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1283	A	C5-C6-N6	-5.04	119.67	123.70
2	A	1283	A	O4'-C1'-N9	5.04	112.23	108.20
2	A	131	C	O4'-C1'-N1	5.04	112.23	108.20
2	A	614	C	N3-C4-N4	5.04	121.53	118.00
2	A	1178	A	O4'-C1'-N9	5.04	112.23	108.20
2	A	1274	A	C5-C6-N1	-5.04	115.18	117.70
2	A	483	A	C4-C5-C6	5.04	119.52	117.00
2	A	806	A	O4'-C1'-N9	5.04	112.23	108.20
2	A	927	C	N3-C4-C5	-5.04	119.89	121.90
2	A	1821	U	P-O3'-C3'	5.04	125.74	119.70
2	A	156	G	O4'-C1'-N9	5.03	112.23	108.20
2	A	575	C	N3-C4-C5	-5.03	119.89	121.90
2	A	906	G	O4'-C1'-N9	5.03	112.23	108.20
2	A	1399	C	C6-N1-C1'	-5.03	114.76	120.80
2	A	1444	A	O4'-C1'-N9	5.03	112.23	108.20
2	A	1625	A	C5-C6-N6	-5.03	119.67	123.70
2	A	25	A	P-O3'-C3'	5.03	125.74	119.70
2	A	1205	A	C5-C6-N1	-5.03	115.18	117.70
2	A	1634	G	O4'-C1'-N9	5.03	112.23	108.20
2	A	297	C	N3-C4-N4	5.03	121.52	118.00
2	A	86	C	N3-C4-C5	-5.03	119.89	121.90
2	A	347	C	N3-C4-C5	-5.03	119.89	121.90
2	A	370	G	O4'-C1'-N9	5.03	112.22	108.20
2	A	1112	C	C6-N1-C1'	-5.03	114.77	120.80
2	A	1200	A	O4'-C1'-N9	5.03	112.22	108.20
2	A	218	A	C5-C6-N1	-5.03	115.19	117.70
2	A	310	G	C4'-C3'-C2'	-5.03	97.57	102.60
2	A	1491	G	C5-C6-O6	-5.03	125.58	128.60
2	A	1012	U	C2-N1-C1'	5.02	123.73	117.70
2	A	1216	A	C5-C6-N1	-5.02	115.19	117.70
2	A	1510	G	O4'-C1'-N9	5.02	112.22	108.20
2	A	1532	A	O4'-C1'-N9	5.02	112.22	108.20
2	A	584	A	O4'-C1'-N9	5.02	112.22	108.20
2	A	1287	A	O4'-C1'-N9	5.02	112.22	108.20
2	A	1024	A	C5-C6-N6	-5.02	119.69	123.70
2	A	1297	A	C5-C6-N1	-5.02	115.19	117.70
2	A	1683	C	N3-C4-C5	-5.02	119.89	121.90
2	A	178	C	N3-C4-C5	-5.02	119.89	121.90
2	A	405	A	C5-C6-N1	-5.02	115.19	117.70
2	A	194	C	N3-C4-C5	-5.01	119.89	121.90
2	A	521	A	O4'-C4'-C3'	-5.01	98.98	104.00
2	A	807	A	C4-C5-C6	5.01	119.51	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	955	G	O4'-C1'-N9	5.01	112.21	108.20
2	A	1628	A	O4'-C1'-N9	5.01	112.21	108.20
2	A	1230	C	N3-C4-C5	-5.01	119.90	121.90
1	N	33	C	N3-C4-C5	-5.01	119.90	121.90
2	A	389	C	N3-C4-C5	-5.01	119.90	121.90
2	A	390	C	P-O3'-C3'	5.01	125.71	119.70
2	A	900	A	O4'-C1'-N9	5.01	112.21	108.20
2	A	992	A	C5-C6-N1	-5.01	115.19	117.70
2	A	1085	G	O4'-C1'-N9	5.01	112.21	108.20
2	A	327	C	N3-C4-C5	-5.01	119.90	121.90
2	A	916	A	C5-C6-N6	-5.01	119.69	123.70
2	A	312	C	N3-C4-C5	-5.01	119.90	121.90
2	A	506	A	C5-C6-N6	-5.00	119.70	123.70
2	A	463	A	C5-C6-N1	-5.00	115.20	117.70
2	A	843	A	C5-C6-N1	-5.00	115.20	117.70
2	A	1297	A	C5-C6-N6	-5.00	119.70	123.70
2	A	339	A	O4'-C1'-N9	5.00	112.20	108.20
2	A	1461	A	C5-C6-N6	-5.00	119.70	123.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	794	G	C4'
7	I	171	ASP	CA
41	s	86	GLU	CA

All (185) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1075	C	Sidechain
2	A	1122	G	Sidechain
2	A	1136	G	Sidechain
2	A	1140	A	Sidechain
2	A	1144	A	Sidechain
2	A	1171	G	Sidechain
2	A	1199	G	Sidechain
2	A	1207	G	Sidechain
2	A	1232	G	Sidechain
2	A	1236	A	Sidechain
2	A	1286	G	Sidechain
2	A	1304	U	Sidechain
2	A	1325	U	Sidechain

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Mol	Chain	Res	Type	Group
2	A	1359	C	Sidechain
2	A	1393	U	Sidechain
2	A	1418	G	Sidechain
2	A	146	G	Sidechain
2	A	1508	C	Sidechain
2	A	1517	A	Sidechain
2	A	1523	G	Sidechain
2	A	1574	A	Sidechain
2	A	1600	G	Sidechain
2	A	1619	U	Sidechain
2	A	1684	C	Sidechain
2	A	1736	U	Sidechain
2	A	1744	G	Sidechain
2	A	1769	U	Sidechain
2	A	1771	G	Sidechain
2	A	1776	G	Sidechain
2	A	1828	A	Sidechain
2	A	1831	G	Sidechain
2	A	184	G	Sidechain
2	A	185	C	Sidechain
2	A	1854	A	Sidechain
2	A	1858	U	Sidechain
2	A	187	C	Sidechain
2	A	204	G	Sidechain
2	A	210	G	Sidechain
2	A	239	U	Sidechain
2	A	240	C	Sidechain
2	A	26	U	Sidechain
2	A	267	G	Sidechain
2	A	270	G	Sidechain
2	A	271	G	Sidechain
2	A	280	G	Sidechain
2	A	287	U	Sidechain
2	A	300	G	Sidechain
2	A	325	G	Sidechain
2	A	341	G	Sidechain
2	A	351	U	Sidechain
2	A	374	U	Sidechain
2	A	425	A	Sidechain
2	A	442	G	Sidechain
2	A	472	G	Sidechain
2	A	541	U	Sidechain

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Mol	Chain	Res	Type	Group
2	A	543	U	Sidechain
2	A	570	U	Sidechain
2	A	605	C	Sidechain
2	A	649	G	Sidechain
2	A	652	G	Sidechain
2	A	74	G	Sidechain
2	A	750	G	Sidechain
2	A	8	U	Sidechain
2	A	857	A	Sidechain
2	A	869	G	Sidechain
2	A	872	C	Sidechain
2	A	884	U	Sidechain
2	A	915	A	Sidechain
5	G	147	LYS	Peptide
5	G	152	LYS	Peptide
5	G	18	GLN	Peptide
5	G	27	GLU	Peptide
6	H	31	LEU	Peptide
6	H	43	GLU	Peptide
7	I	1	MET	Peptide
7	I	129	ILE	Peptide
9	K	118	GLY	Peptide
9	K	146	SER	Peptide
9	K	162	ARG	Peptide
10	L	10	GLN	Peptide
10	L	141	ARG	Peptide
10	L	15	VAL	Peptide
10	L	8	LYS	Peptide
10	L	9	PHE	Peptide
10	L	94	LYS	Peptide
1	N	1	A	Sidechain
1	N	12	G	Sidechain
1	N	2	G	Sidechain
1	N	22	C	Sidechain
1	N	72	A	Sidechain
1	N	73	C	Sidechain
4	P	117	GLU	Peptide
4	P	122	THR	Peptide
4	P	126	GLN	Peptide
4	P	141	LYS	Peptide
4	P	157	VAL	Peptide
4	P	159	ASP	Peptide

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Mol	Chain	Res	Type	Group
4	P	160	PRO	Peptide
4	P	165	SER	Peptide
4	P	171	ASP	Peptide
4	P	183	ARG	Sidechain
4	P	184	LEU	Peptide
4	P	187	GLN	Peptide
4	P	188	ALA	Peptide
4	P	225	ILE	Peptide
4	P	236	VAL	Peptide
4	P	46	ILE	Peptide
4	P	67	ARG	Peptide
14	R	142	LYS	Peptide
15	S	110	PRO	Peptide
15	S	133	THR	Peptide
15	S	322	LEU	Peptide
15	S	373	ALA	Peptide
15	S	86	LEU	Peptide
16	T	248	GLY	Peptide
17	U	43	GLU	Peptide
17	U	44	LYS	Peptide
17	U	79	HIS	Peptide
18	V	97	GLU	Peptide
19	W	41	ARG	Peptide
19	W	93	SER	Peptide
20	X	105	THR	Peptide
20	X	108	SER	Peptide
20	X	16	PRO	Peptide
20	X	17	ASP	Peptide
20	X	190	PRO	Peptide
20	X	193	GLN	Peptide
21	Y	2	PRO	Peptide
21	Y	36	LYS	Peptide
21	Y	37	CYS	Peptide
23	a	2	VAL	Peptide
24	b	25	GLY	Peptide
24	b	48	GLY	Peptide
24	b	49	GLN	Peptide
24	b	81	GLN	Peptide
24	b	9	VAL	Peptide
25	c	160	GLY	Peptide
27	e	122	PRO	Peptide
27	e	88	VAL	Peptide

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Mol	Chain	Res	Type	Group
27	e	89	SER	Peptide
28	f	4	ALA	Peptide
28	f	97	THR	Peptide
29	g	144	GLY	Peptide
30	h	108	PRO	Peptide
30	h	46	LYS	Peptide
30	h	50	VAL	Peptide
30	h	68	THR	Peptide
30	h	70	CYS	Peptide
31	i	146	CYS	Peptide
31	i	75	GLN	Peptide
31	i	76	ASN	Peptide
32	j	42	VAL	Peptide
35	m	12	LYS	Peptide
35	m	160	SER	Peptide
35	m	273	GLU	Peptide
35	m	283	PRO	Peptide
35	m	47	ARG	Peptide
35	m	59	LEU	Peptide
35	m	60	ARG	Peptide
36	n	17	TYR	Peptide
36	n	37	TYR	Peptide
36	n	50	ARG	Peptide
37	o	155	ASN	Peptide
37	o	29	LEU	Peptide
37	o	3	ILE	Peptide
37	o	4	SER	Peptide
38	p	105	TYR	Peptide
38	p	134	SER	Peptide
38	p	135	HIS	Peptide
38	p	84	SER	Peptide
38	p	85	TYR	Sidechain
38	p	90	LYS	Peptide
38	p	92	LYS	Peptide
40	r	98	GLY	Peptide
41	s	104	ARG	Sidechain
41	s	132	LYS	Peptide
41	s	32	LYS	Peptide
41	s	85	ASN	Peptide
42	t	30	PRO	Peptide
42	t	37	ASP	Peptide
42	t	43	LEU	Peptide

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Mol	Chain	Res	Type	Group
42	t	70	TYR	Sidechain
42	t	86	PRO	Peptide
42	t	92	ALA	Peptide
42	t	97	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1604	0	816	0	0
2	A	37881	0	19145	0	0
3	F	635	0	327	0	0
4	P	2147	0	2191	0	0
5	G	1296	0	1374	0	0
6	H	1124	0	1193	0	0
7	I	2083	0	2189	0	0
8	J	445	0	442	0	0
9	K	1499	0	1608	0	0
10	L	1140	0	1191	0	0
11	M	288	0	269	0	0
12	O	614	0	599	0	0
13	Q	1107	0	1179	0	0
14	R	1113	0	1149	0	0
15	S	3214	0	3354	0	0
16	T	2605	0	2474	0	0
17	U	1509	0	1563	0	0
18	V	473	0	524	0	0
19	W	599	0	656	0	0
20	X	1530	0	1627	0	0
21	Y	659	0	683	0	0
22	Z	1208	0	1294	0	0
23	a	1034	0	1080	0	0
24	b	620	0	622	0	0
25	c	1743	0	1836	0	0
26	d	147	0	146	0	0
27	e	1020	0	1075	0	0
28	f	1643	0	1646	0	0
29	g	1765	0	1863	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	h	822	0	887	0	0
31	i	1742	0	1815	0	0
32	j	1016	0	1039	0	0
33	k	790	0	839	0	0
34	l	507	0	536	0	0
35	m	2437	0	2393	0	0
36	n	1061	0	1120	0	0
37	o	1680	0	1762	0	0
38	p	582	0	599	0	0
39	q	1924	0	2089	0	0
40	r	958	0	993	0	0
41	s	1065	0	1137	0	0
42	t	828	0	854	0	0
All	All	88157	0	70178	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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
4	P	264/266 (99%)	220 (83%)	26 (10%)	18 (7%)	1 14
5	G	156/158 (99%)	135 (86%)	17 (11%)	4 (3%)	5 31
6	H	139/141 (99%)	125 (90%)	7 (5%)	7 (5%)	2 20
7	I	261/263 (99%)	235 (90%)	14 (5%)	12 (5%)	2 21
8	J	51/53 (96%)	45 (88%)	4 (8%)	2 (4%)	3 23
9	K	180/182 (99%)	156 (87%)	18 (10%)	6 (3%)	4 26
10	L	135/137 (98%)	118 (87%)	11 (8%)	6 (4%)	2 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	M	36/38 (95%)	31 (86%)	5 (14%)	0	100 100
12	O	75/77 (97%)	70 (93%)	5 (7%)	0	100 100
13	Q	140/142 (99%)	119 (85%)	15 (11%)	6 (4%)	2 22
14	R	139/141 (99%)	130 (94%)	7 (5%)	2 (1%)	11 46
15	S	420/422 (100%)	364 (87%)	41 (10%)	15 (4%)	3 25
16	T	327/329 (99%)	292 (89%)	29 (9%)	6 (2%)	8 40
17	U	189/191 (99%)	169 (89%)	13 (7%)	7 (4%)	3 24
18	V	57/59 (97%)	46 (81%)	8 (14%)	3 (5%)	2 19
19	W	73/75 (97%)	61 (84%)	11 (15%)	1 (1%)	11 46
20	X	188/190 (99%)	163 (87%)	11 (6%)	14 (7%)	1 13
21	Y	82/84 (98%)	71 (87%)	5 (6%)	6 (7%)	1 13
22	Z	148/150 (99%)	137 (93%)	9 (6%)	2 (1%)	11 46
23	a	127/129 (98%)	118 (93%)	6 (5%)	3 (2%)	6 33
24	b	80/82 (98%)	65 (81%)	6 (8%)	9 (11%)	0 7
25	c	224/226 (99%)	209 (93%)	9 (4%)	6 (3%)	5 31
26	d	15/17 (88%)	15 (100%)	0	0	100 100
27	e	124/126 (98%)	110 (89%)	11 (9%)	3 (2%)	6 33
28	f	206/208 (99%)	174 (84%)	24 (12%)	8 (4%)	3 23
29	g	225/227 (99%)	203 (90%)	14 (6%)	8 (4%)	3 25
30	h	102/104 (98%)	86 (84%)	12 (12%)	4 (4%)	3 23
31	i	213/215 (99%)	188 (88%)	17 (8%)	8 (4%)	3 24
32	j	134/136 (98%)	107 (80%)	19 (14%)	8 (6%)	1 16
33	k	97/99 (98%)	87 (90%)	7 (7%)	3 (3%)	4 27
34	l	62/64 (97%)	57 (92%)	5 (8%)	0	100 100
35	m	311/313 (99%)	278 (89%)	23 (7%)	10 (3%)	4 26
36	n	125/127 (98%)	103 (82%)	10 (8%)	12 (10%)	0 9
37	o	204/206 (99%)	182 (89%)	14 (7%)	8 (4%)	3 23
38	p	69/71 (97%)	47 (68%)	14 (20%)	8 (12%)	0 6
39	q	235/237 (99%)	211 (90%)	16 (7%)	8 (3%)	3 26
40	r	122/124 (98%)	103 (84%)	12 (10%)	7 (6%)	1 17
41	s	129/131 (98%)	113 (88%)	7 (5%)	9 (7%)	1 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
42	t	96/98 (98%)	76 (79%)	10 (10%)	10 (10%)	0 8
All	All	5960/6038 (99%)	5219 (88%)	492 (8%)	249 (4%)	5 22

All (249) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	P	115	VAL
4	P	166	LEU
4	P	172	GLU
4	P	223	MET
6	H	19	ALA
7	I	2	ALA
7	I	196	THR
7	I	242	LYS
9	K	22	LYS
13	Q	128	VAL
15	S	82	PHE
15	S	194	LYS
17	U	202	SER
20	X	66	VAL
20	X	115	LYS
20	X	190	PRO
20	X	191	GLU
24	b	50	SER
24	b	65	SER
25	c	175	SER
27	e	89	SER
29	g	98	ALA
29	g	193	ASP
29	g	213	PRO
30	h	51	LYS
31	i	78	GLU
31	i	210	VAL
32	j	23	GLU
32	j	52	THR
33	k	10	ARG
35	m	47	ARG
35	m	96	THR
35	m	276	SER
37	o	133	GLU
38	p	135	HIS
39	q	33	ALA

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Mol	Chain	Res	Type
40	r	103	VAL
42	t	30	PRO
42	t	31	LYS
42	t	43	LEU
4	P	47	LEU
4	P	51	LEU
4	P	59	ILE
4	P	116	ALA
4	P	156	ALA
4	P	188	ALA
4	P	225	ILE
7	I	13	ALA
7	I	194	VAL
9	K	138	ARG
10	L	23	ARG
10	L	31	THR
10	L	92	ASP
10	L	95	TYR
13	Q	59	ALA
14	R	34	VAL
15	S	63	VAL
15	S	224	VAL
15	S	229	ALA
15	S	398	ARG
15	S	452	GLU
16	T	177	SER
17	U	41	VAL
18	V	104	GLY
21	Y	51	GLN
23	a	58	ALA
24	b	27	LYS
24	b	42	VAL
25	c	158	LYS
28	f	46	ILE
28	f	202	TYR
29	g	201	LYS
29	g	211	VAL
30	h	98	VAL
32	j	43	HIS
32	j	53	ILE
33	k	27	ALA
36	n	9	LYS

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Mol	Chain	Res	Type
36	n	18	ARG
36	n	49	LEU
36	n	75	VAL
37	o	5	ARG
37	o	10	LYS
38	p	91	ASN
38	p	98	VAL
38	p	102	VAL
38	p	148	TYR
39	q	104	ALA
41	s	96	LEU
42	t	38	LYS
42	t	44	HIS
42	t	63	ALA
42	t	89	ILE
42	t	94	LEU
4	P	91	SER
6	H	117	ARG
7	I	30	ARG
7	I	152	PRO
8	J	8	TRP
9	K	124	HIS
9	K	183	GLY
10	L	12	ILE
13	Q	99	GLU
13	Q	106	GLY
14	R	35	ASP
15	S	81	ARG
15	S	135	GLY
15	S	179	PRO
15	S	378	PRO
16	T	8	GLY
16	T	64	THR
16	T	74	ASN
16	T	176	LYS
17	U	51	HIS
17	U	79	HIS
18	V	78	GLY
20	X	12	ASN
20	X	36	LEU
20	X	135	PHE
21	Y	3	LEU

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Mol	Chain	Res	Type
21	Y	61	THR
22	Z	26	LEU
24	b	6	GLY
24	b	28	ASP
24	b	33	PRO
24	b	48	GLY
25	c	156	GLY
25	c	261	THR
30	h	107	GLU
31	i	24	PRO
31	i	209	ASP
32	j	66	ARG
35	m	37	ASP
35	m	181	ASN
36	n	12	PHE
36	n	54	HIS
36	n	100	LYS
36	n	126	VAL
38	p	93	HIS
39	q	68	LEU
41	s	31	GLY
41	s	33	ALA
41	s	60	PHE
41	s	97	TYR
4	P	94	GLU
5	G	8	ARG
5	G	28	THR
5	G	148	ALA
6	H	41	MET
6	H	42	ILE
6	H	43	GLU
6	H	100	VAL
7	I	22	LYS
7	I	153	LEU
7	I	245	ARG
15	S	279	LYS
16	T	264	LYS
17	U	42	LYS
18	V	119	VAL
19	W	114	LYS
20	X	8	ILE
20	X	39	GLN

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Mol	Chain	Res	Type
20	X	76	GLN
20	X	108	SER
21	Y	4	ALA
21	Y	63	LEU
24	b	20	SER
28	f	104	THR
28	f	159	ILE
28	f	163	CYS
28	f	206	ASP
29	g	194	PRO
29	g	202	LYS
32	j	24	GLY
32	j	140	THR
33	k	61	ALA
35	m	103	GLY
35	m	161	SER
36	n	6	GLN
36	n	50	ARG
37	o	59	ARG
37	o	143	LYS
38	p	99	LYS
39	q	26	THR
39	q	69	THR
39	q	156	TYR
40	r	30	GLY
40	r	73	GLN
40	r	81	ASP
40	r	113	ASP
41	s	34	THR
41	s	100	LYS
41	s	104	ARG
42	t	90	VAL
4	P	29	GLU
4	P	266	ARG
7	I	12	VAL
9	K	148	ILE
10	L	17	ASN
13	Q	129	SER
15	S	196	LYS
15	S	461	GLU
17	U	44	LYS
17	U	53	ALA

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Mol	Chain	Res	Type
20	X	100	ILE
22	Z	25	TRP
23	a	30	CYS
23	a	71	LYS
25	c	249	SER
27	e	86	PRO
31	i	26	SER
35	m	107	ASP
35	m	144	ASP
35	m	150	TRP
37	o	24	LYS
37	o	192	GLY
39	q	88	ARG
40	r	118	SER
41	s	6	THR
42	t	95	ARG
4	P	168	LEU
4	P	187	GLN
9	K	172	ARG
13	Q	63	ASN
15	S	105	ASP
20	X	18	GLU
21	Y	12	PRO
31	i	77	ASP
31	i	148	ASN
32	j	123	GLY
36	n	14	LYS
36	n	38	SER
38	p	106	TYR
39	q	122	PRO
27	e	88	VAL
28	f	98	PRO
30	h	93	SER
31	i	204	ILE
4	P	90	VAL
6	H	44	PRO
29	g	5	ILE
20	X	170	VAL
28	f	119	PRO
37	o	31	ARG
40	r	11	VAL
8	J	23	VAL

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Mol	Chain	Res	Type
25	c	161	LYS
5	G	33	LEU
7	I	195	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
4	P	238/238 (100%)	231 (97%)	7 (3%)	42	64
5	G	142/142 (100%)	139 (98%)	3 (2%)	53	72
6	H	117/117 (100%)	113 (97%)	4 (3%)	37	60
7	I	225/225 (100%)	219 (97%)	6 (3%)	44	65
8	J	47/47 (100%)	47 (100%)	0	100	100
9	K	157/157 (100%)	154 (98%)	3 (2%)	57	75
10	L	119/119 (100%)	119 (100%)	0	100	100
11	M	35/35 (100%)	34 (97%)	1 (3%)	42	64
12	O	63/63 (100%)	62 (98%)	1 (2%)	62	79
13	Q	114/114 (100%)	111 (97%)	3 (3%)	46	66
14	R	113/113 (100%)	107 (95%)	6 (5%)	22	47
15	S	354/354 (100%)	340 (96%)	14 (4%)	31	55
16	T	281/281 (100%)	273 (97%)	8 (3%)	43	64
17	U	161/161 (100%)	156 (97%)	5 (3%)	40	62
18	V	49/49 (100%)	49 (100%)	0	100	100
19	W	66/66 (100%)	64 (97%)	2 (3%)	41	63
20	X	170/170 (100%)	168 (99%)	2 (1%)	71	83
21	Y	76/76 (100%)	74 (97%)	2 (3%)	46	66
22	Z	130/130 (100%)	128 (98%)	2 (2%)	65	80
23	a	112/112 (100%)	110 (98%)	2 (2%)	59	77
24	b	67/67 (100%)	65 (97%)	2 (3%)	41	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	c	187/187 (100%)	184 (98%)	3 (2%)	62 79
26	d	17/17 (100%)	17 (100%)	0	100 100
27	e	114/114 (100%)	113 (99%)	1 (1%)	78 87
28	f	174/174 (100%)	171 (98%)	3 (2%)	60 78
29	g	190/190 (100%)	187 (98%)	3 (2%)	62 79
30	h	94/94 (100%)	91 (97%)	3 (3%)	39 62
31	i	196/196 (100%)	195 (100%)	1 (0%)	88 93
32	j	106/106 (100%)	104 (98%)	2 (2%)	57 75
33	k	87/87 (100%)	83 (95%)	4 (5%)	27 52
34	l	57/57 (100%)	55 (96%)	2 (4%)	36 59
35	m	272/272 (100%)	265 (97%)	7 (3%)	46 66
36	n	116/116 (100%)	108 (93%)	8 (7%)	15 40
37	o	177/177 (100%)	177 (100%)	0	100 100
38	p	64/64 (100%)	64 (100%)	0	100 100
39	q	207/207 (100%)	203 (98%)	4 (2%)	57 75
40	r	104/104 (100%)	100 (96%)	4 (4%)	33 57
41	s	113/113 (100%)	111 (98%)	2 (2%)	59 77
42	t	89/89 (100%)	85 (96%)	4 (4%)	27 52
All	All	5200/5200 (100%)	5076 (98%)	124 (2%)	51 69

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	P	7	ARG
4	P	30	MET
4	P	45	MET
4	P	113	ARG
4	P	147	TYR
4	P	155	HIS
4	P	179	ASN
5	G	31	GLU
5	G	58	LYS
5	G	101	ARG
6	H	51	LEU
6	H	105	LYS
6	H	131	LYS

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Mol	Chain	Res	Type
6	H	140	ARG
7	I	49	ARG
7	I	88	ASP
7	I	113	ARG
7	I	155	LYS
7	I	169	ILE
7	I	220	THR
9	K	123	ILE
9	K	165	TYR
9	K	172	ARG
11	M	109	GLU
12	O	251	ARG
13	Q	67	ARG
13	Q	105	PHE
13	Q	139	GLU
14	R	11	GLN
14	R	21	PHE
14	R	28	LEU
14	R	75	MET
14	R	123	LEU
14	R	132	ASP
15	S	102	TYR
15	S	137	PHE
15	S	210	GLU
15	S	217	TYR
15	S	230	GLU
15	S	242	LYS
15	S	261	ARG
15	S	279	LYS
15	S	319	GLU
15	S	378	PRO
15	S	400	GLU
15	S	417	LEU
15	S	453	LYS
15	S	466	LEU
16	T	34	VAL
16	T	49	MET
16	T	176	LYS
16	T	186	GLU
16	T	215	PHE
16	T	234	LEU
16	T	266	GLU

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Mol	Chain	Res	Type
16	T	306	ASP
17	U	110	GLN
17	U	130	ARG
17	U	134	VAL
17	U	194	ASP
17	U	204	ARG
19	W	50	PHE
19	W	102	LYS
20	X	27	LEU
20	X	103	LYS
21	Y	33	MET
21	Y	63	LEU
22	Z	11	LEU
22	Z	86	GLU
23	a	57	ARG
23	a	65	LEU
24	b	32	ILE
24	b	46	PHE
25	c	148	VAL
25	c	221	PHE
25	c	233	TYR
27	e	67	ARG
28	f	33	GLN
28	f	88	LEU
28	f	165	ASN
29	g	94	ARG
29	g	158	ILE
29	g	178	ARG
30	h	30	LYS
30	h	72	GLU
30	h	79	ARG
31	i	32	ASP
32	j	53	ILE
32	j	66	ARG
33	k	19	GLN
33	k	39	PHE
33	k	51	ARG
33	k	85	ARG
34	l	32	VAL
34	l	68	LEU
35	m	68	ASP
35	m	71	ILE

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Mol	Chain	Res	Type
35	m	100	ARG
35	m	113	PHE
35	m	126	ASP
35	m	140	TYR
35	m	289	LEU
36	n	17	TYR
36	n	22	LEU
36	n	30	TYR
36	n	51	ARG
36	n	64	LYS
36	n	72	LYS
36	n	79	HIS
36	n	100	LYS
39	q	13	GLN
39	q	131	ARG
39	q	186	GLN
39	q	231	ARG
40	r	49	LEU
40	r	84	LYS
40	r	85	LEU
40	r	91	LEU
41	s	17	LEU
41	s	61	ARG
42	t	30	PRO
42	t	43	LEU
42	t	46	MET
42	t	85	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	N	74/75 (98%)	16 (21%)	3 (4%)
2	A	1772/1776 (99%)	499 (28%)	113 (6%)
3	F	29/30 (96%)	11 (37%)	2 (6%)
All	All	1875/1881 (99%)	526 (28%)	118 (6%)

All (526) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	N	7	G
1	N	11	C
1	N	16	C
1	N	17	G
1	N	18	G
1	N	19	A
1	N	20	A
1	N	25	G
1	N	35	U
1	N	46	U
1	N	47	C
1	N	48	G
1	N	49	A
1	N	72	A
1	N	73	C
1	N	74	C
2	A	3	C
2	A	4	C
2	A	8	U
2	A	16	G
2	A	25	A
2	A	26	U
2	A	32	U
2	A	33	G
2	A	41	G
2	A	44	U
2	A	45	A
2	A	46	A
2	A	56	G
2	A	59	U
2	A	66	G
2	A	67	C
2	A	68	A
2	A	72	C
2	A	73	C
2	A	74	G
2	A	76	U
2	A	79	A
2	A	80	G
2	A	99	A
2	A	102	A
2	A	103	A
2	A	113	G

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Mol	Chain	Res	Type
2	A	126	G
2	A	128	U
2	A	129	C
2	A	130	G
2	A	131	C
2	A	132	U
2	A	133	C
2	A	134	C
2	A	135	U
2	A	137	U
2	A	139	C
2	A	140	U
2	A	141	A
2	A	142	C
2	A	143	U
2	A	147	A
2	A	148	U
2	A	155	G
2	A	160	U
2	A	161	U
2	A	162	C
2	A	170	A
2	A	176	U
2	A	182	C
2	A	184	G
2	A	187	C
2	A	188	U
2	A	189	G
2	A	190	A
2	A	191	C
2	A	197	U
2	A	198	U
2	A	199	G
2	A	203	G
2	A	205	G
2	A	206	A
2	A	210	G
2	A	212	G
2	A	213	C
2	A	223	A
2	A	224	U
2	A	225	C

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Mol	Chain	Res	Type
2	A	226	A
2	A	229	A
2	A	230	C
2	A	232	A
2	A	233	A
2	A	234	C
2	A	235	C
2	A	238	G
2	A	241	A
2	A	269	C
2	A	273	G
2	A	275	C
2	A	278	U
2	A	279	G
2	A	286	C
2	A	287	U
2	A	296	U
2	A	297	C
2	A	300	G
2	A	303	G
2	A	304	A
2	A	307	G
2	A	309	A
2	A	311	C
2	A	313	C
2	A	314	U
2	A	315	C
2	A	316	C
2	A	317	G
2	A	318	U
2	A	320	G
2	A	322	G
2	A	326	A
2	A	332	C
2	A	337	G
2	A	339	A
2	A	352	C
2	A	354	A
2	A	357	U
2	A	358	U
2	A	375	G
2	A	376	C

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Mol	Chain	Res	Type
2	A	379	A
2	A	382	A
2	A	390	C
2	A	397	G
2	A	398	A
2	A	399	C
2	A	407	C
2	A	438	A
2	A	439	A
2	A	440	C
2	A	442	G
2	A	449	C
2	A	454	A
2	A	455	A
2	A	456	G
2	A	460	G
2	A	461	G
2	A	462	C
2	A	463	A
2	A	464	G
2	A	466	A
2	A	472	G
2	A	477	U
2	A	482	C
2	A	484	C
2	A	486	C
2	A	493	C
2	A	515	A
2	A	522	C
2	A	523	A
2	A	525	G
2	A	537	G
2	A	539	C
2	A	541	U
2	A	542	G
2	A	543	U
2	A	544	A
2	A	546	U
2	A	547	U
2	A	549	G
2	A	550	A
2	A	554	A

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Mol	Chain	Res	Type
2	A	555	G
2	A	566	A
2	A	574	A
2	A	577	A
2	A	578	G
2	A	580	A
2	A	582	C
2	A	583	C
2	A	586	U
2	A	590	G
2	A	595	A
2	A	596	G
2	A	597	U
2	A	598	C
2	A	600	G
2	A	604	G
2	A	609	A
2	A	617	U
2	A	619	A
2	A	624	A
2	A	631	A
2	A	633	A
2	A	634	G
2	A	645	A
2	A	658	A
2	A	659	A
2	A	661	A
2	A	662	A
2	A	669	A
2	A	678	U
2	A	684	A
2	A	685	G
2	A	686	G
2	A	687	G
2	A	731	C
2	A	734	C
2	A	735	C
2	A	745	U
2	A	748	G
2	A	749	C
2	A	750	G
2	A	751	C

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Mol	Chain	Res	Type
2	A	756	U
2	A	775	G
2	A	777	C
2	A	781	C
2	A	782	G
2	A	784	G
2	A	787	C
2	A	788	C
2	A	789	G
2	A	793	C
2	A	794	G
2	A	795	U
2	A	807	A
2	A	808	A
2	A	817	G
2	A	818	U
2	A	826	A
2	A	827	G
2	A	830	C
2	A	833	A
2	A	835	C
2	A	836	C
2	A	837	G
2	A	838	C
2	A	839	C
2	A	841	G
2	A	843	A
2	A	847	C
2	A	849	C
2	A	860	A
2	A	864	G
2	A	865	A
2	A	866	A
2	A	867	U
2	A	868	A
2	A	869	G
2	A	870	G
2	A	871	A
2	A	872	C
2	A	873	C
2	A	877	G
2	A	882	A

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Mol	Chain	Res	Type
2	A	883	U
2	A	884	U
2	A	885	U
2	A	886	U
2	A	890	G
2	A	891	G
2	A	893	U
2	A	899	A
2	A	907	C
2	A	909	A
2	A	910	U
2	A	916	A
2	A	917	G
2	A	929	G
2	A	951	A
2	A	962	U
2	A	965	U
2	A	966	G
2	A	967	G
2	A	972	G
2	A	974	G
2	A	983	A
2	A	986	A
2	A	988	A
2	A	995	G
2	A	997	A
2	A	1004	A
2	A	1012	U
2	A	1013	U
2	A	1017	U
2	A	1021	U
2	A	1027	A
2	A	1035	C
2	A	1041	U
2	A	1045	A
2	A	1046	A
2	A	1047	G
2	A	1048	A
2	A	1050	G
2	A	1056	A
2	A	1057	U
2	A	1058	A

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Mol	Chain	Res	Type
2	A	1068	U
2	A	1073	A
2	A	1074	C
2	A	1079	A
2	A	1092	G
2	A	1093	G
2	A	1105	C
2	A	1106	G
2	A	1107	U
2	A	1111	U
2	A	1112	C
2	A	1113	C
2	A	1114	C
2	A	1116	U
2	A	1117	G
2	A	1119	C
2	A	1127	G
2	A	1132	U
2	A	1134	C
2	A	1135	C
2	A	1137	G
2	A	1139	A
2	A	1144	A
2	A	1145	A
2	A	1146	A
2	A	1149	C
2	A	1150	U
2	A	1151	U
2	A	1153	G
2	A	1154	G
2	A	1157	U
2	A	1162	G
2	A	1164	G
2	A	1199	G
2	A	1202	G
2	A	1204	A
2	A	1205	A
2	A	1207	G
2	A	1208	G
2	A	1210	A
2	A	1211	C
2	A	1212	C

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Mol	Chain	Res	Type
2	A	1213	A
2	A	1217	G
2	A	1220	G
2	A	1232	G
2	A	1233	C
2	A	1238	U
2	A	1241	G
2	A	1244	U
2	A	1247	A
2	A	1249	A
2	A	1250	C
2	A	1252	G
2	A	1253	G
2	A	1255	A
2	A	1256	A
2	A	1258	C
2	A	1260	C
2	A	1270	G
2	A	1271	G
2	A	1272	A
2	A	1274	A
2	A	1279	C
2	A	1280	A
2	A	1281	G
2	A	1297	A
2	A	1299	C
2	A	1303	U
2	A	1304	U
2	A	1310	U
2	A	1312	C
2	A	1313	U
2	A	1320	G
2	A	1339	U
2	A	1341	G
2	A	1344	G
2	A	1354	U
2	A	1367	U
2	A	1368	U
2	A	1369	C
2	A	1374	A
2	A	1390	G
2	A	1391	C

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Mol	Chain	Res	Type
2	A	1392	A
2	A	1393	U
2	A	1394	G
2	A	1397	A
2	A	1398	A
2	A	1400	U
2	A	1401	A
2	A	1402	G
2	A	1403	U
2	A	1405	A
2	A	1406	C
2	A	1408	C
2	A	1412	C
2	A	1413	C
2	A	1414	C
2	A	1415	C
2	A	1422	U
2	A	1426	C
2	A	1431	C
2	A	1433	C
2	A	1445	G
2	A	1448	A
2	A	1450	A
2	A	1452	G
2	A	1455	G
2	A	1458	U
2	A	1461	A
2	A	1470	A
2	A	1471	G
2	A	1472	A
2	A	1479	A
2	A	1485	A
2	A	1486	G
2	A	1489	C
2	A	1490	U
2	A	1491	G
2	A	1493	G
2	A	1494	A
2	A	1503	G
2	A	1504	A
2	A	1506	G
2	A	1507	U

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Mol	Chain	Res	Type
2	A	1508	C
2	A	1511	G
2	A	1513	C
2	A	1514	U
2	A	1515	G
2	A	1516	C
2	A	1519	G
2	A	1528	A
2	A	1532	A
2	A	1535	G
2	A	1539	C
2	A	1540	A
2	A	1545	G
2	A	1546	U
2	A	1547	G
2	A	1548	C
2	A	1549	C
2	A	1550	U
2	A	1551	A
2	A	1552	C
2	A	1553	C
2	A	1558	G
2	A	1559	C
2	A	1565	G
2	A	1574	A
2	A	1575	A
2	A	1576	C
2	A	1577	C
2	A	1580	U
2	A	1581	U
2	A	1583	A
2	A	1593	G
2	A	1594	U
2	A	1595	G
2	A	1597	U
2	A	1599	G
2	A	1618	A
2	A	1627	G
2	A	1628	A
2	A	1632	A
2	A	1633	G
2	A	1634	G

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Mol	Chain	Res	Type
2	A	1649	G
2	A	1660	G
2	A	1675	G
2	A	1683	C
2	A	1684	C
2	A	1690	A
2	A	1696	C
2	A	1697	G
2	A	1698	C
2	A	1699	C
2	A	1716	U
2	A	1717	G
2	A	1722	G
2	A	1724	U
2	A	1741	U
2	A	1743	G
2	A	1745	C
2	A	1747	C
2	A	1748	G
2	A	1749	C
2	A	1750	C
2	A	1751	G
2	A	1757	G
2	A	1758	G
2	A	1760	C
2	A	1774	G
2	A	1775	A
2	A	1776	G
2	A	1777	C
2	A	1778	G
2	A	1779	C
2	A	1780	U
2	A	1790	G
2	A	1792	C
2	A	1799	G
2	A	1817	A
2	A	1818	A
2	A	1820	G
2	A	1822	C
2	A	1823	G
2	A	1825	A
2	A	1829	A

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Mol	Chain	Res	Type
2	A	1832	U
2	A	1833	U
2	A	1843	G
2	A	1846	C
2	A	1852	G
2	A	1855	G
2	A	1856	G
2	A	1857	A
2	A	1860	A
2	A	1863	A
3	F	8	A
3	F	9	C
3	F	10	C
3	F	11	A
3	F	14	G
3	F	18	A
3	F	19	C
3	F	21	U
3	F	27	C
3	F	29	G
3	F	30	A

All (118) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	16	C
1	N	18	G
1	N	73	C
2	A	2	A
2	A	24	C
2	A	31	U
2	A	44	U
2	A	65	C
2	A	66	G
2	A	72	C
2	A	78	C
2	A	102	A
2	A	127	C
2	A	129	C
2	A	131	C
2	A	133	C
2	A	138	C

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Mol	Chain	Res	Type
2	A	139	C
2	A	140	U
2	A	141	A
2	A	161	U
2	A	189	G
2	A	211	U
2	A	222	G
2	A	225	C
2	A	267	G
2	A	278	U
2	A	285	U
2	A	299	G
2	A	317	G
2	A	372	C
2	A	396	U
2	A	455	A
2	A	506	A
2	A	521	A
2	A	522	C
2	A	524	G
2	A	538	C
2	A	540	C
2	A	542	G
2	A	582	C
2	A	594	A
2	A	596	G
2	A	662	A
2	A	685	G
2	A	730	C
2	A	747	G
2	A	748	G
2	A	749	C
2	A	750	G
2	A	756	U
2	A	759	A
2	A	775	G
2	A	780	G
2	A	781	C
2	A	787	C
2	A	794	G
2	A	807	A
2	A	817	G

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Mol	Chain	Res	Type
2	A	829	C
2	A	865	A
2	A	869	G
2	A	876	G
2	A	882	A
2	A	966	G
2	A	1104	G
2	A	1111	U
2	A	1133	U
2	A	1153	G
2	A	1161	G
2	A	1210	A
2	A	1249	A
2	A	1279	C
2	A	1303	U
2	A	1390	G
2	A	1391	C
2	A	1392	A
2	A	1397	A
2	A	1400	U
2	A	1412	C
2	A	1414	C
2	A	1425	G
2	A	1430	C
2	A	1470	A
2	A	1471	G
2	A	1490	U
2	A	1493	G
2	A	1514	U
2	A	1538	U
2	A	1540	A
2	A	1544	U
2	A	1548	C
2	A	1551	A
2	A	1552	C
2	A	1573	U
2	A	1576	C
2	A	1593	G
2	A	1594	U
2	A	1596	A
2	A	1615	A
2	A	1627	G

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Mol	Chain	Res	Type
2	A	1632	A
2	A	1659	A
2	A	1674	A
2	A	1716	U
2	A	1750	C
2	A	1757	G
2	A	1758	G
2	A	1760	C
2	A	1763	C
2	A	1774	G
2	A	1777	C
2	A	1817	A
2	A	1819	A
2	A	1824	U
2	A	1857	A
3	F	4	A
3	F	8	A

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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
2	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	736:C	O3’	744:C	P	29.45
1	A	679:U	O3’	683:G	P	18.26
1	A	761:G	O3’	774:U	P	17.60
1	A	687:G	O3’	730:C	P	14.44
1	A	243:C	O3’	267:G	P	13.79

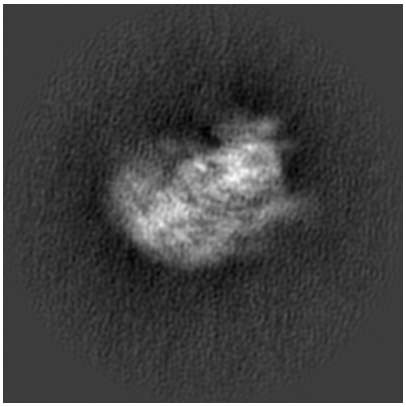
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8190. These allow visual inspection of the internal detail of the map and identification of artifacts.

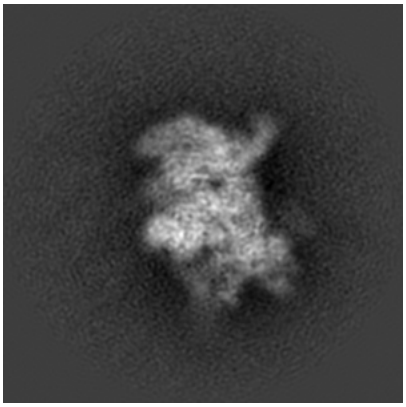
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

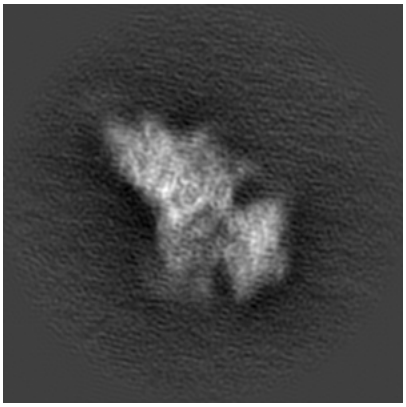
6.1.1 Primary map



X



Y

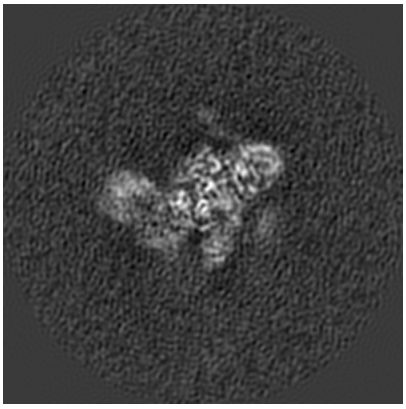


Z

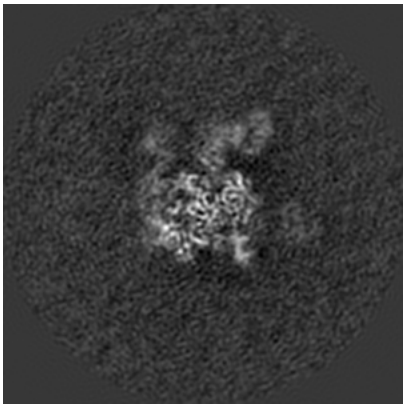
The images above show the map projected in three orthogonal directions.

6.2 Central slices

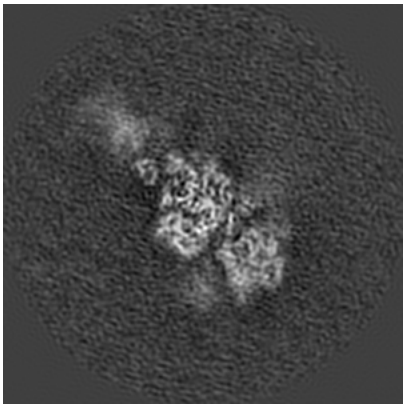
6.2.1 Primary map



X Index: 100



Y Index: 100

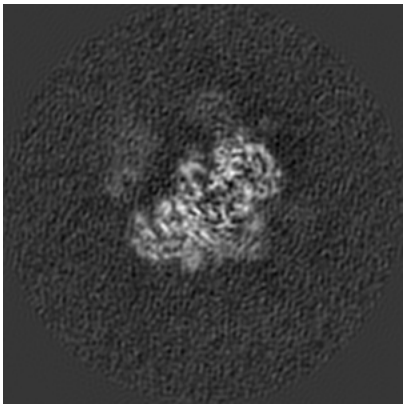


Z Index: 100

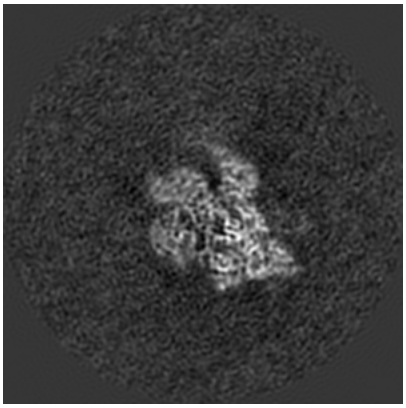
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

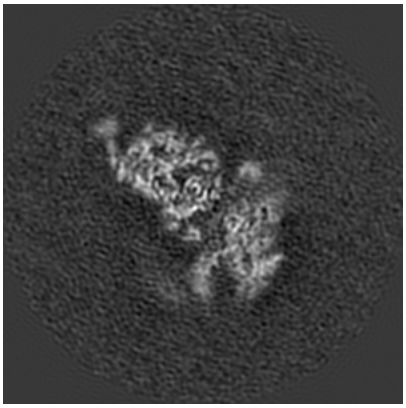
6.3.1 Primary map



X Index: 85



Y Index: 113

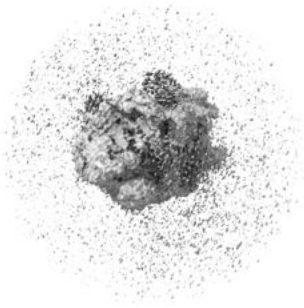


Z Index: 108

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

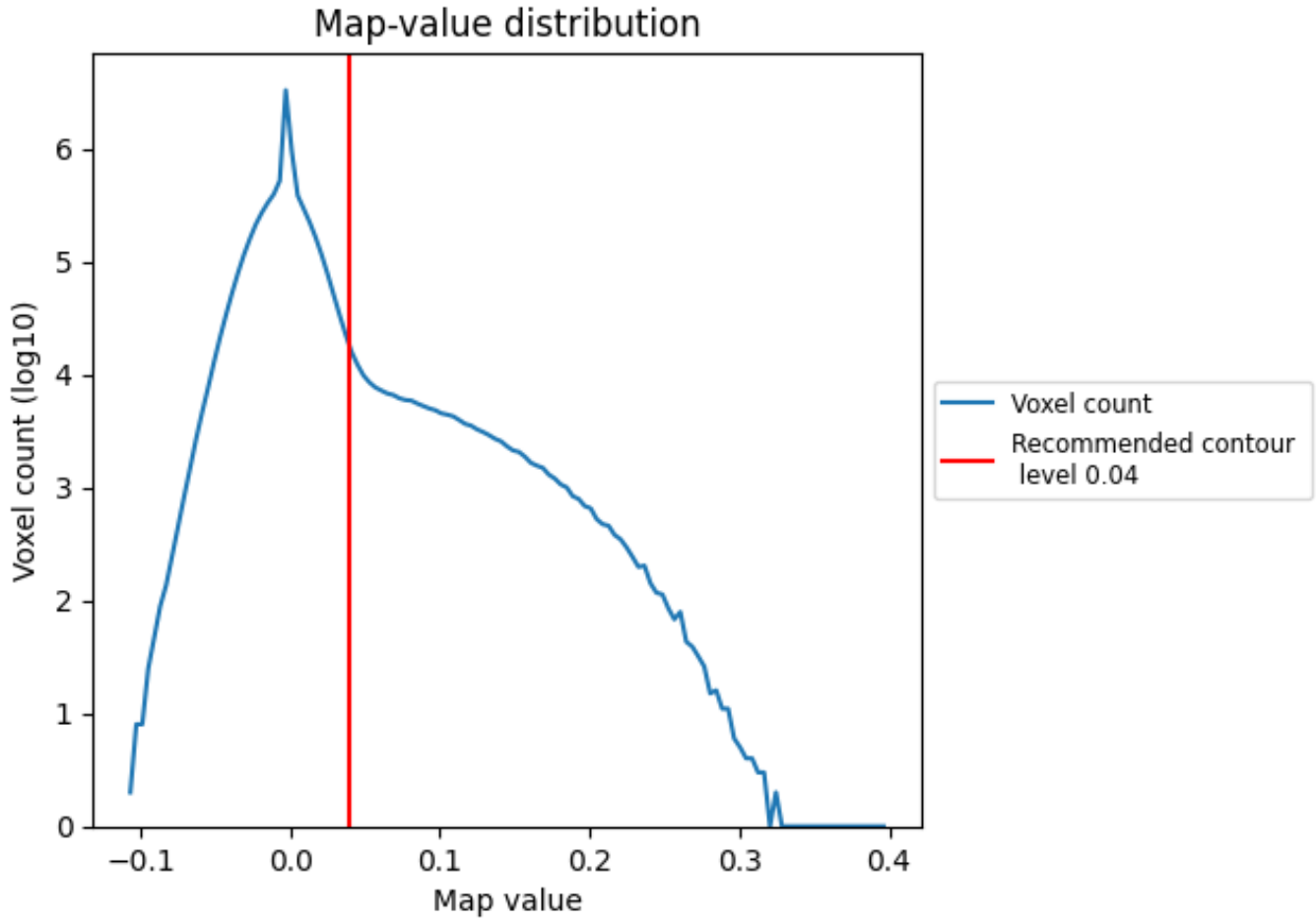
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

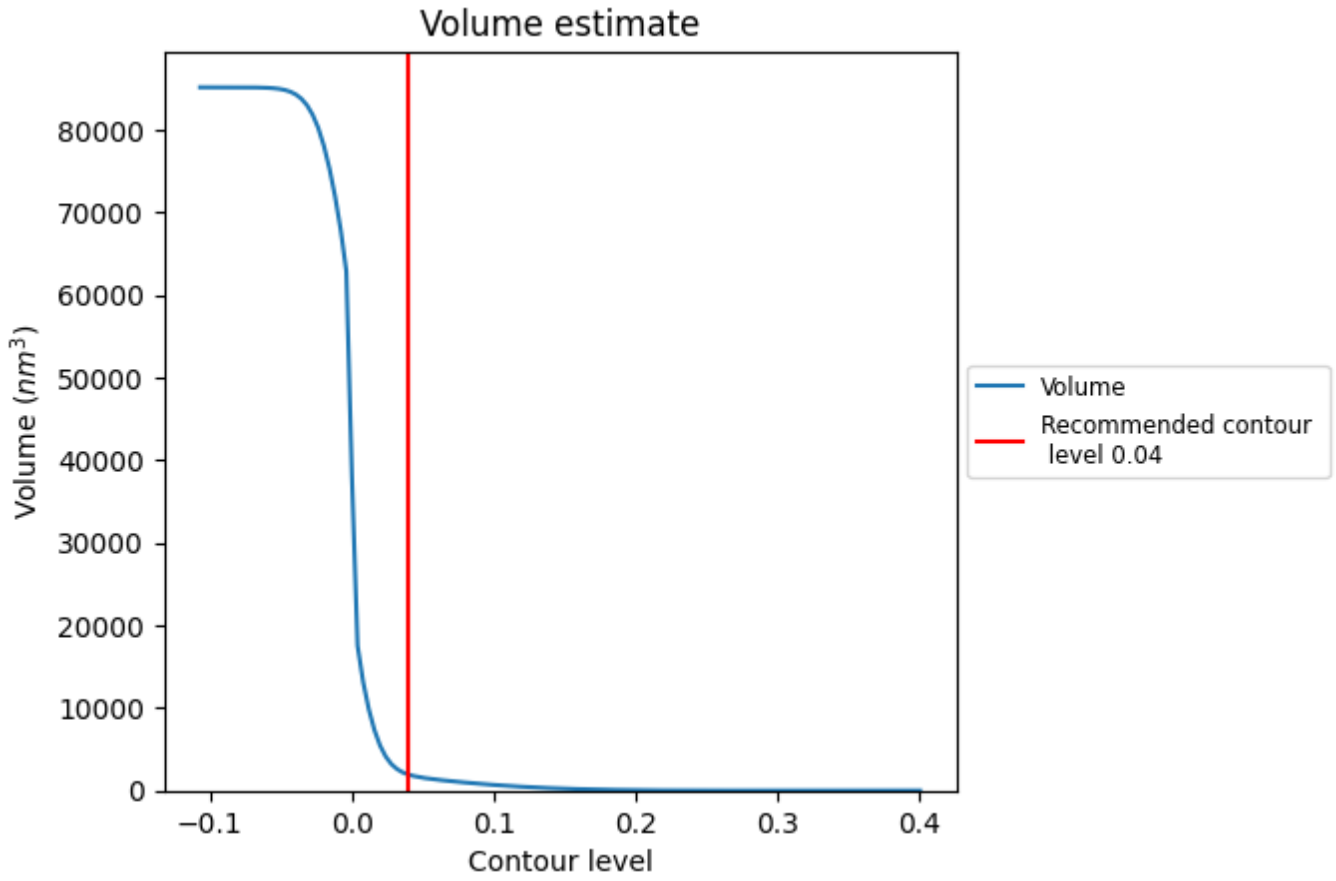
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

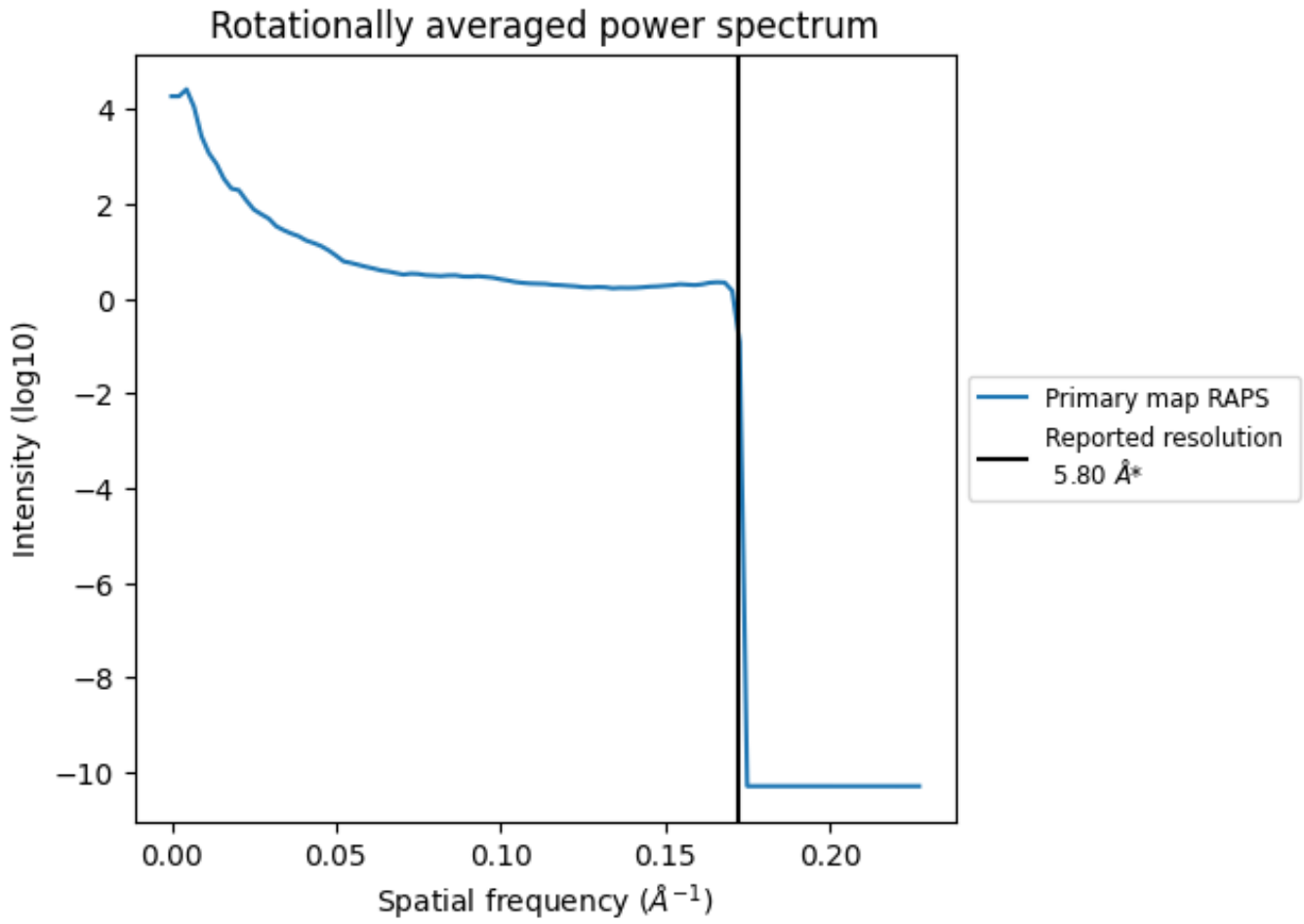
7.2 Volume estimate



The volume at the recommended contour level is 1932 nm^3; this corresponds to an approximate mass of 1746 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.172 Å^{-1}

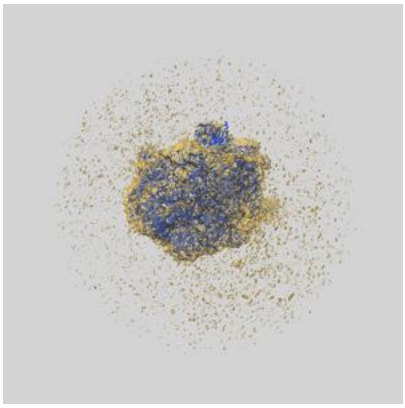
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

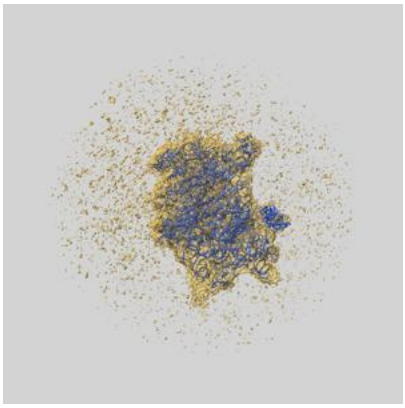
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8190 and PDB model 5K0Y. Per-residue inclusion information can be found in section 3 on page 28.

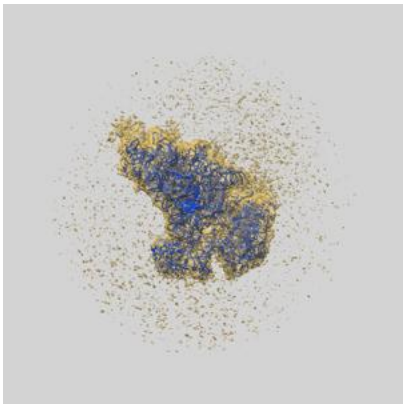
9.1 Map-model overlay



X



Y



Z

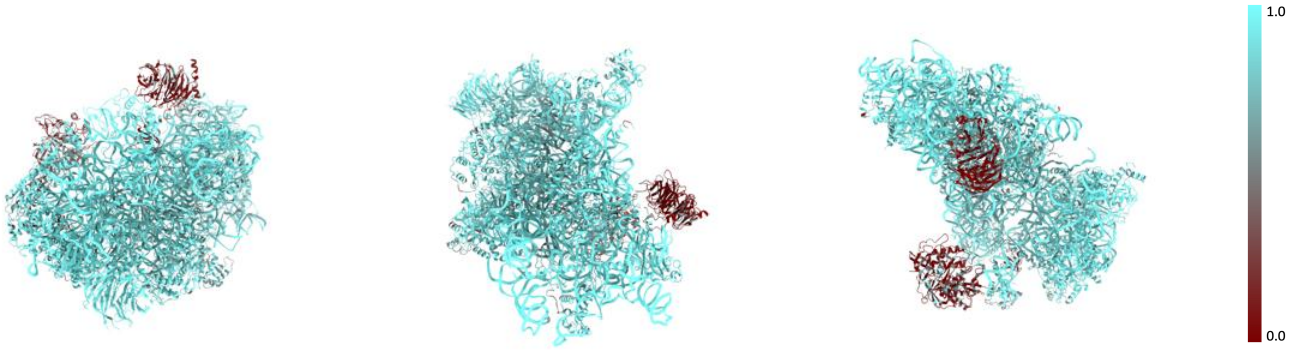
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

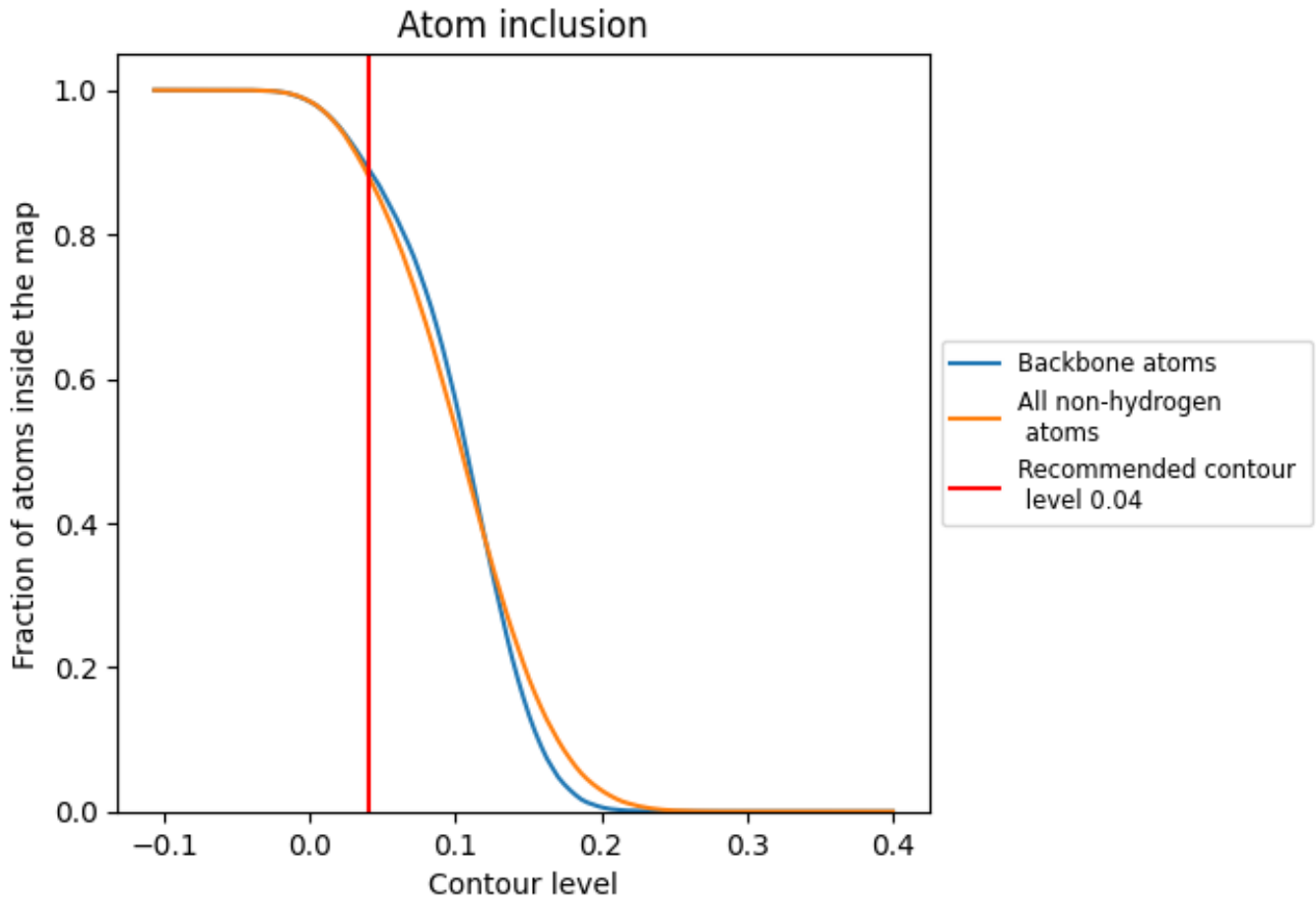
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8817	0.1410
A	0.9915	0.1880
F	0.7890	0.0970
G	0.8469	0.1270
H	0.9540	0.1200
I	0.9199	0.1450
J	0.9063	0.0990
K	0.9133	0.1380
L	0.9508	0.1050
M	0.1632	0.1060
N	0.9133	0.1420
O	0.2044	0.0100
P	0.4785	0.0450
Q	0.9093	0.1400
R	0.9603	0.1210
S	0.2385	0.0250
T	0.1134	0.0300
U	0.9285	0.1280
V	0.8706	0.1170
W	0.9469	0.1020
X	0.8021	0.1010
Y	0.9459	0.1200
Z	0.9266	0.1270
a	0.8158	0.1300
b	0.9290	0.1300
c	0.8698	0.1380
d	0.1329	0.0070
e	0.8679	0.1070
f	0.9326	0.1350
g	0.8891	0.1340
h	0.9014	0.1180
i	0.9650	0.1250
j	0.9331	0.1060
k	0.9106	0.1170
l	0.9363	0.1310

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Chain	Atom inclusion	Q-score
m	0.9645	0.1020
n	0.9474	0.0890
o	0.9372	0.1160
p	0.9718	0.0690
q	0.9628	0.1210
r	0.9025	0.0880
s	0.9364	0.1350
t	0.9566	0.1240