Full wwPDB EM Validation Report

Nov 16, 2022 – 12:02 PM JST

PDB ID	:	6LU8
EMDB ID	:	EMD-0978
Title	:	Cryo-EM structure of a human pre-60S ribosomal subunit - state A
Authors	:	Liang, X.; Zuo, M.; Zhang, Y.; Li, N.; Ma, C.; Dong, M.; Gao, N.
Deposited on	:	2020-01-26
Resolution	:	3.13 Å(reported)

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:

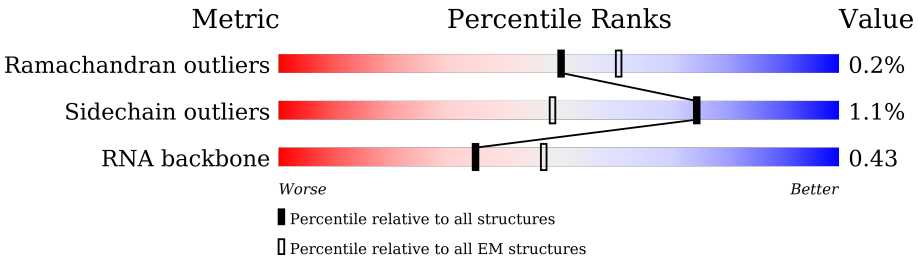
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.13 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	1	731	97%
2	2	5070	6% 24% 36% 9% 31%
3	3	503	47% 52%
4	4	634	19% 91% 5%
5	5	120	42% 47% 11%
6	6	245	7% 97%
7	7	163	82% 17%
8	8	156	37% 53% 10%

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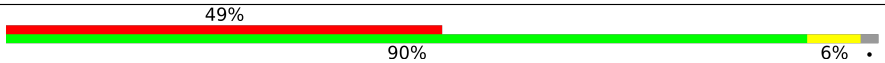
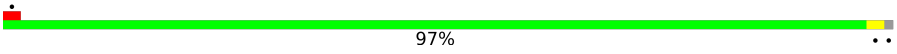
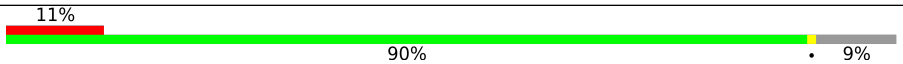
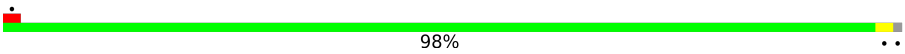
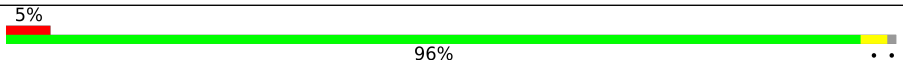
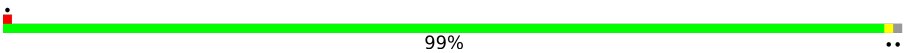
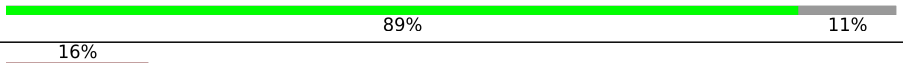
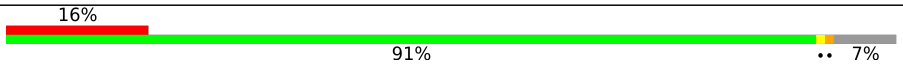
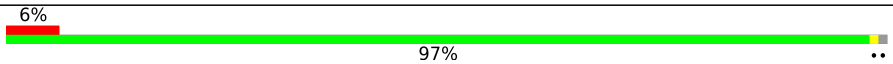
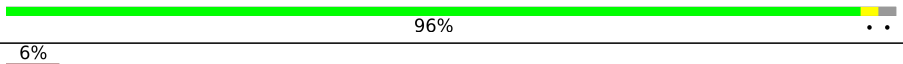
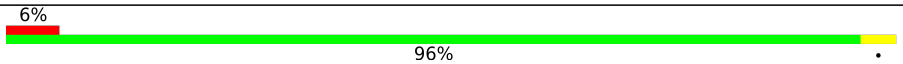
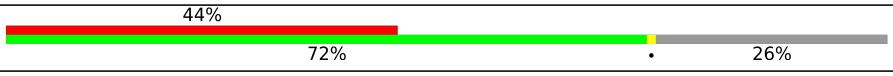
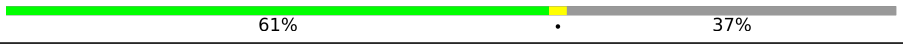
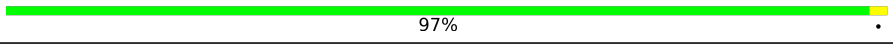
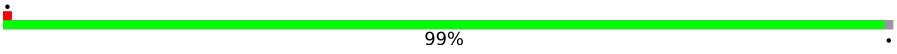
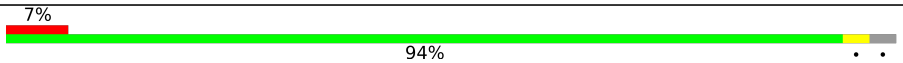
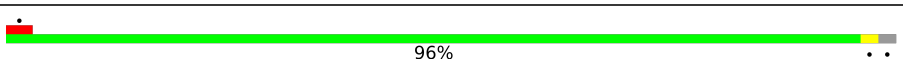
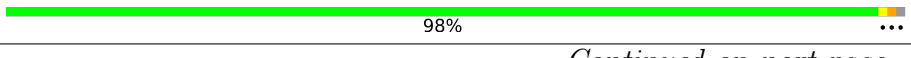
Mol	Chain	Length	Quality of chain
9	9	134	
10	A	217	
11	B	403	
12	C	159	
13	D	427	
14	E	115	
15	F	117	
16	G	266	
17	H	123	
18	I	192	
19	K	105	
20	L	148	
21	M	97	
22	N	178	
23	O	70	
24	P	51	
25	Q	211	
26	R	203	
27	S	215	
28	U	204	
29	V	203	
30	W	106	
31	X	92	
32	Y	184	
33	Z	188	

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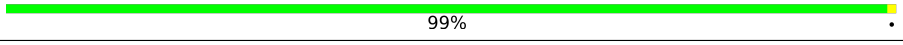
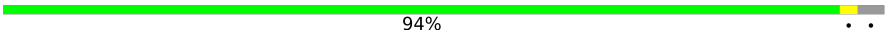
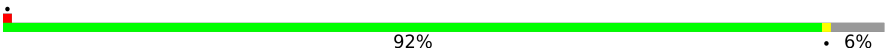
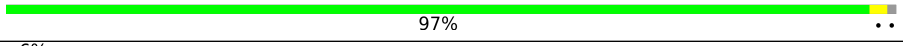
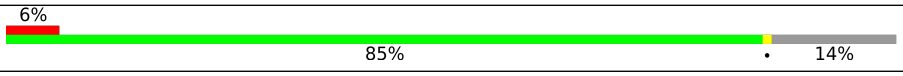
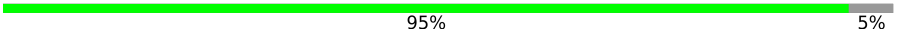
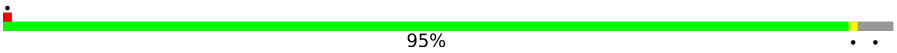
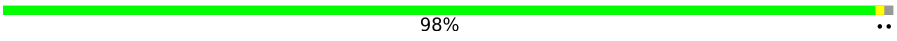
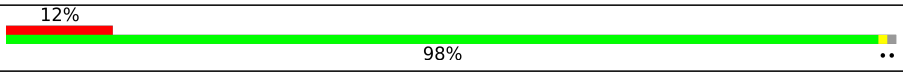
Mol	Chain	Length	Quality of chain
34	a	196	
35	b	176	
36	c	160	
37	d	128	
38	e	140	
39	g	156	
40	h	145	
41	i	136	
42	j	125	
43	k	135	
44	l	137	
45	m	257	
46	n	110	
47	o	288	
48	p	248	
49	r	297	
50	z	129	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 143909 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 protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	19	Total	C	N	O	S	0	0
			148	88	23	35	2		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3477	Total	C	N	O	P	0	0
			74680	33310	13669	24225	3476		

- Molecule 3 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	243	Total	C	N	O	S	0	0
			1951	1242	341	351	17		

- Molecule 4 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	605	Total	C	N	O	S	0	0
			4965	3124	903	911	27		

- Molecule 5 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 7 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	135	Total	C	N	O	S	0	0
			1159	737	225	187	10		

- Molecule 8 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 9 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	86	Total	C	N	O	S	0	0
			711	433	154	121	3		

- Molecule 10 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	212	Total	C	N	O	S	0	0
			1708	1092	308	300	8		

- Molecule 11 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	400	Total	C	N	O	S	1	0
			3235	2060	607	554	14		

- Molecule 12 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	90	Total	C	N	O	S	0	0
			743	462	163	114	4		

- Molecule 13 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	357	Total	C	N	O	S	0	0
			2848	1794	569	472	13		

- Molecule 14 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 15 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

- Molecule 16 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	241	Total	C	N	O	S	1	0
			1940	1236	374	326	4		

- Molecule 17 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 18 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 19 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	97	Total	C	N	O	S	0	0
			799	500	170	124	5		

- Molecule 20 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 21 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 22 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	165	Total	C	N	O	S	0	0
			1319	836	245	233	5		

- Molecule 23 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 24 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 25 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 26 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	150	Total	C	N	O	S	0	0
			1272	793	244	230	5		

- Molecule 27 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 28 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 29 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 30 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 31 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	90	Total	C	N	O	S	0	0
			698	440	134	117	7		

- Molecule 32 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 33 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 34 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	148	Total	C	N	O	S	0	0
			1239	772	266	192	9		

- Molecule 35 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 36 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	155	Total	C	N	O	S	0	0
			1264	801	248	210	5		

- Molecule 37 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 38 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 39 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 40 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 41 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 42 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 43 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 44 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 46 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 47 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	218	Total	C	N	O	S	0	0
			1750	1125	332	289	4		

- Molecule 48 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 49 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	293	Total 2386	C 1510	N 435	O 427	S 14	0	0

- Molecule 50 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	z	34	Total 284	C 179	N 61	O 43	S 1	0	0

- Molecule 51 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	2	229	Total 229	Mg 229	0
51	5	3	Total 3	Mg 3	0
51	8	6	Total 6	Mg 6	0
51	B	1	Total 1	Mg 1	0
51	D	1	Total 1	Mg 1	0
51	F	1	Total 1	Mg 1	0
51	L	1	Total 1	Mg 1	0
51	M	1	Total 1	Mg 1	0
51	k	1	Total 1	Mg 1	0
51	m	1	Total 1	Mg 1	0
51	n	1	Total 1	Mg 1	0
51	p	1	Total 1	Mg 1	0

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	2	13	Total 13	O 13	0

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Continued from previous page...

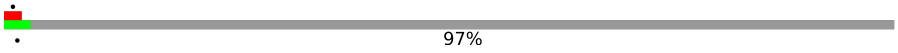
Mol	Chain	Residues	Atoms	AltConf
52	k	1	Total O 1 1	0
52	o	1	Total O 1 1	0
52	p	1	Total O 1 1	0

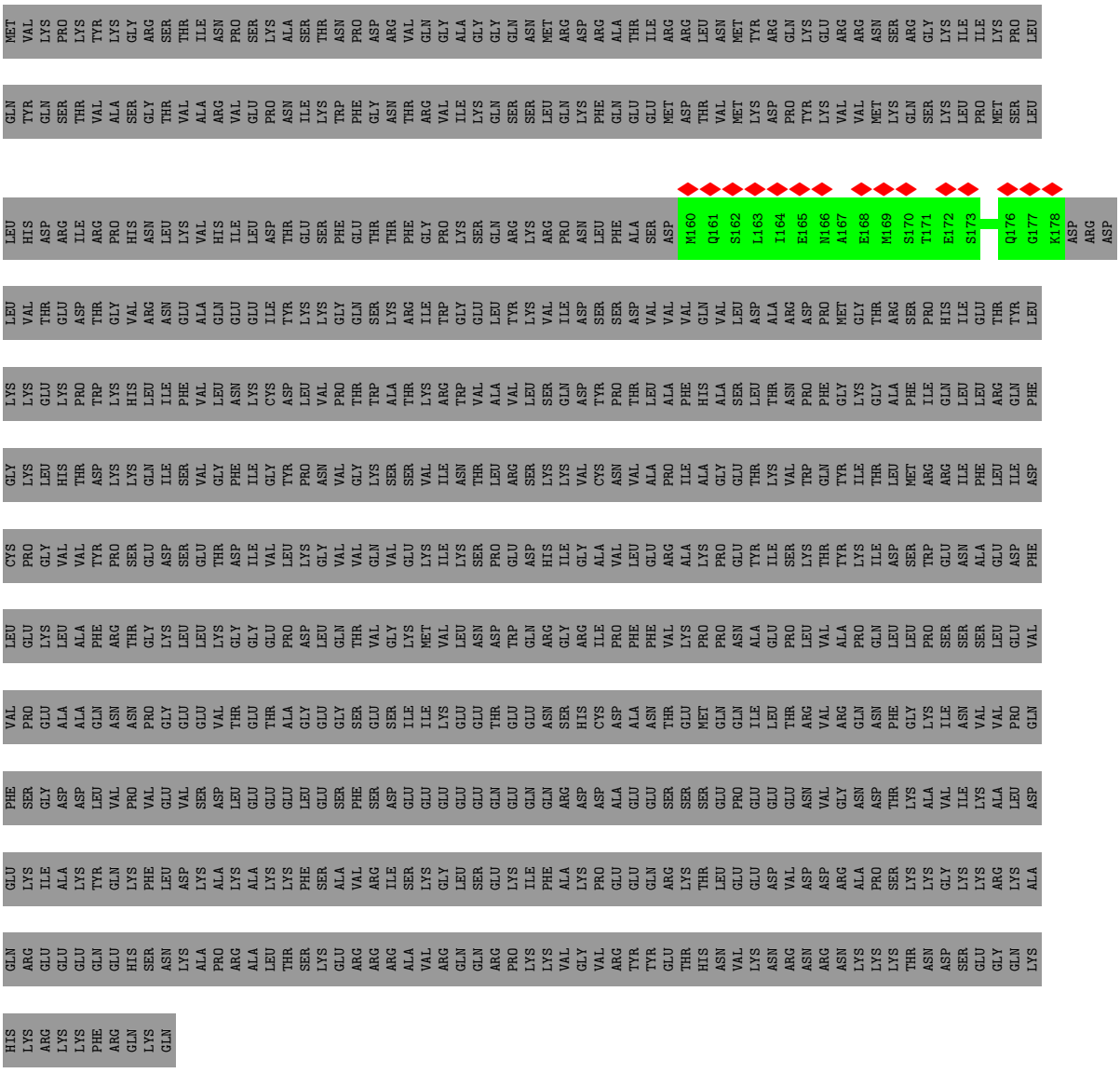
3 Residue-property plots (i)

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: Nucleolar GTP-binding protein 2

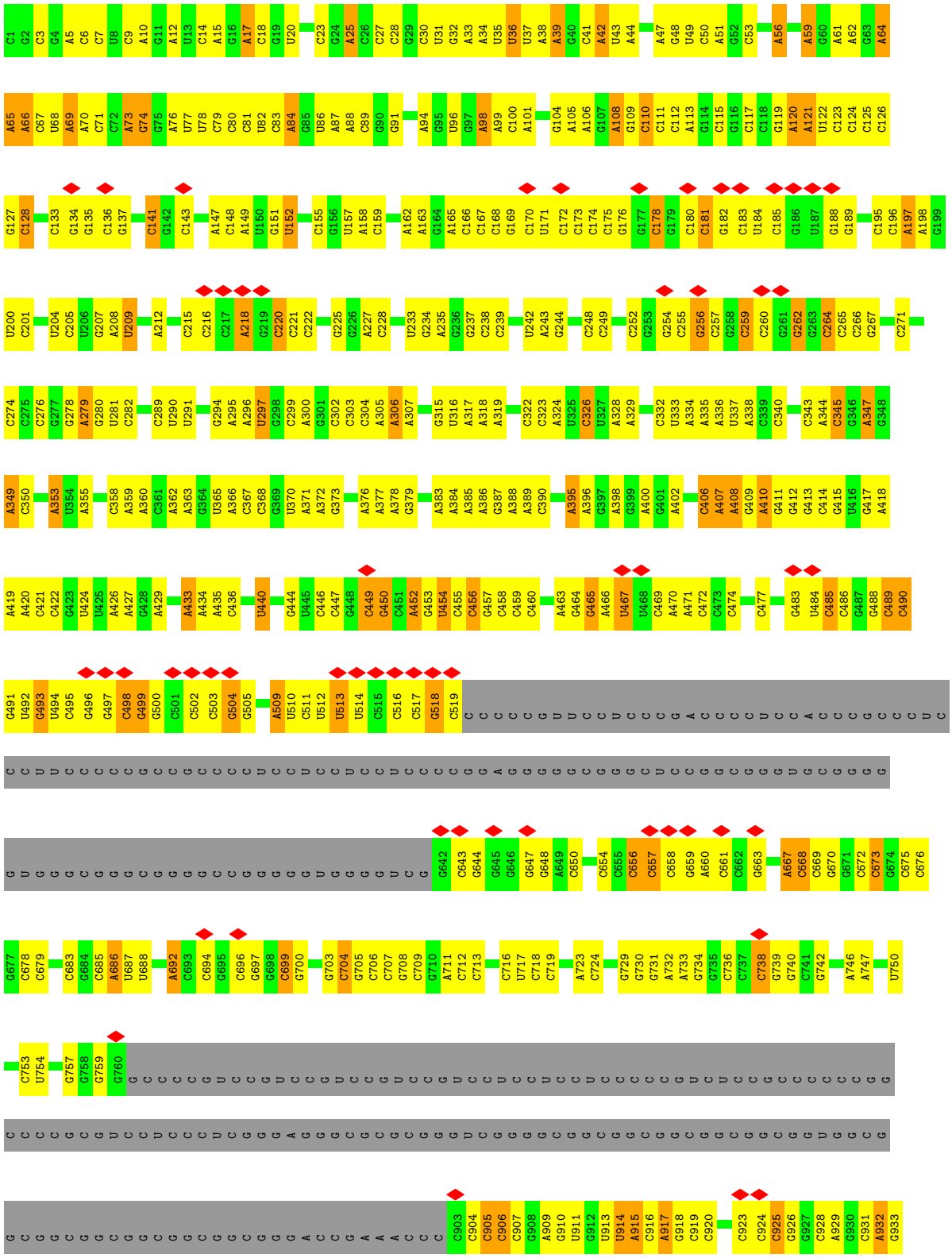
Chain 1:

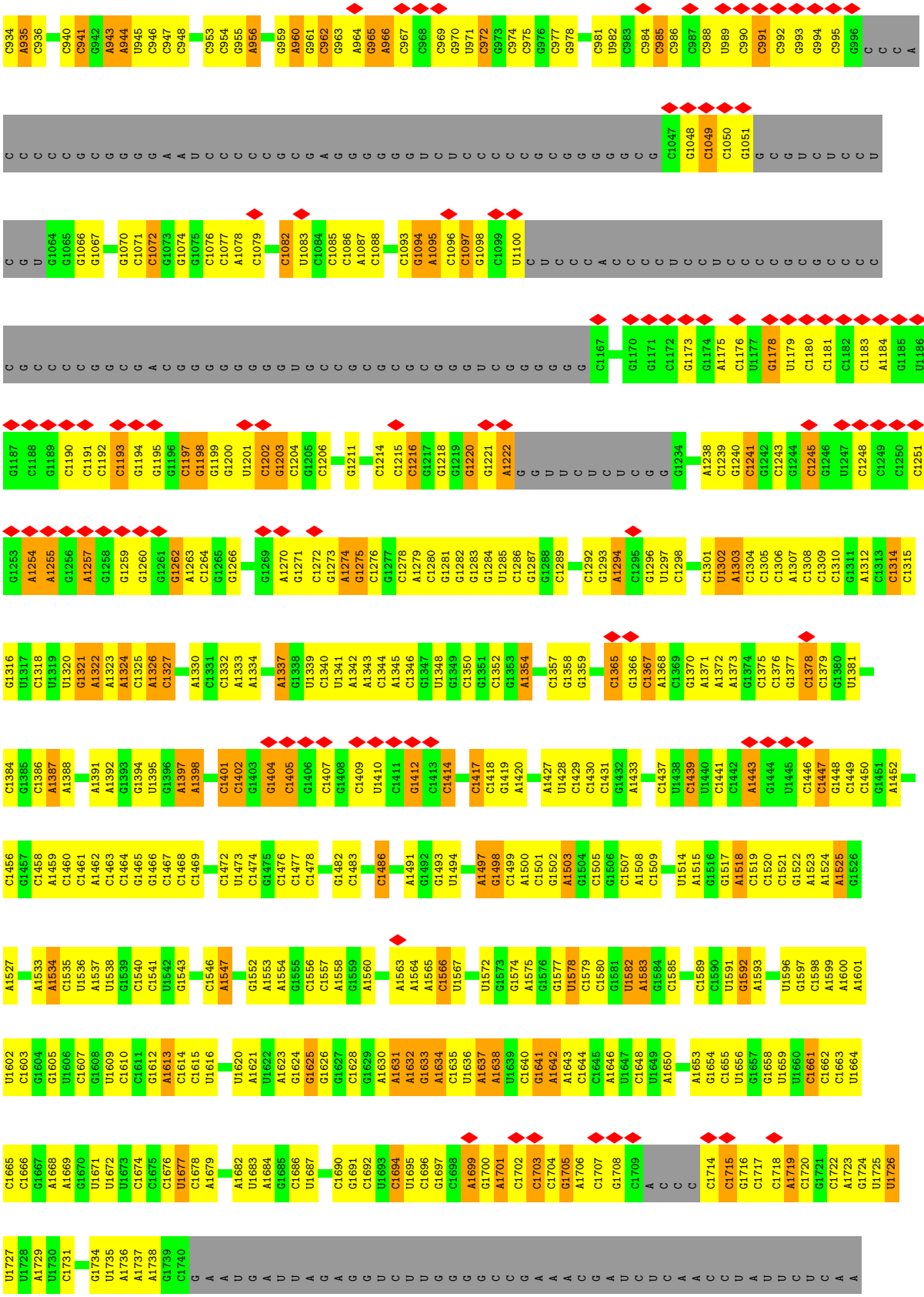


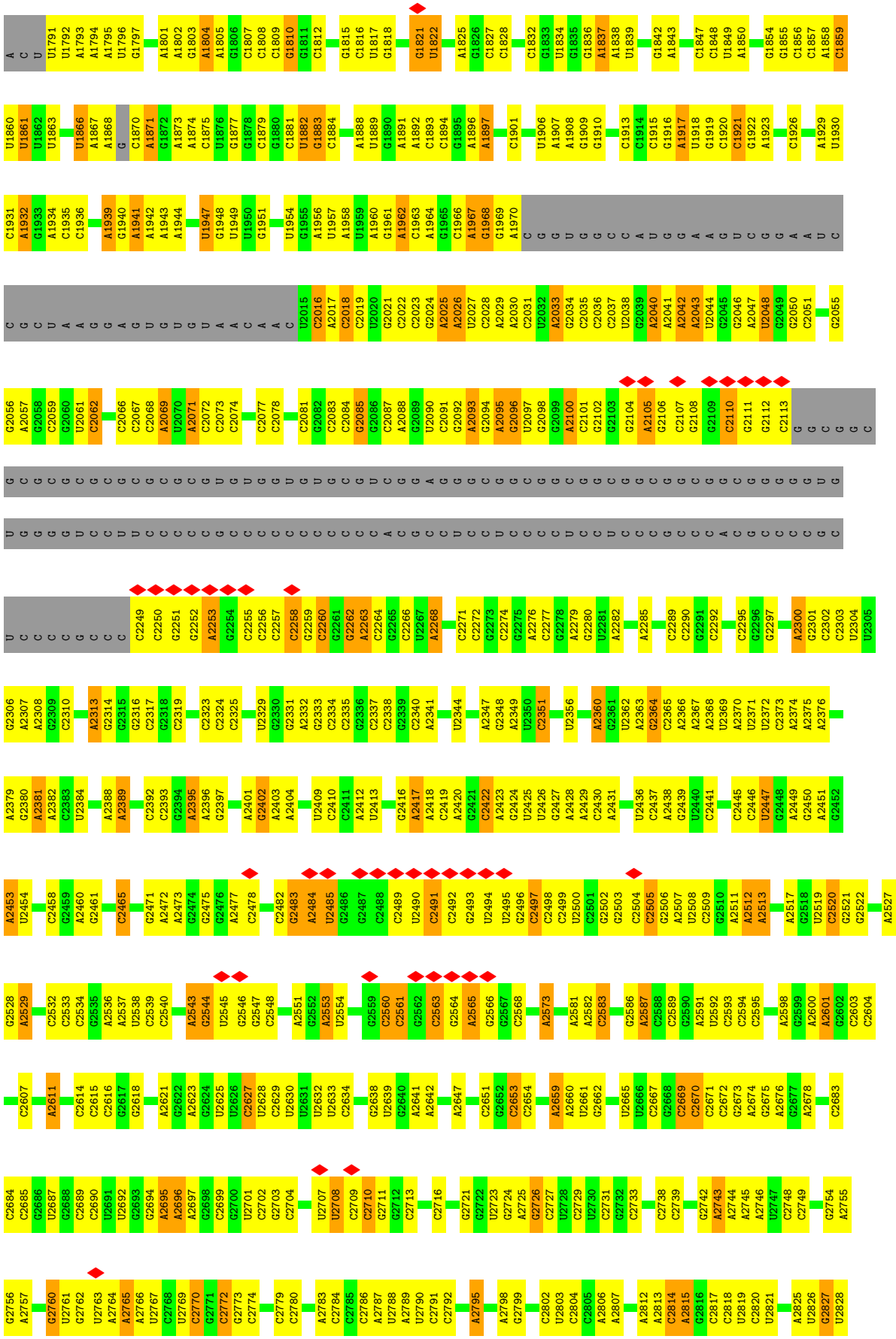


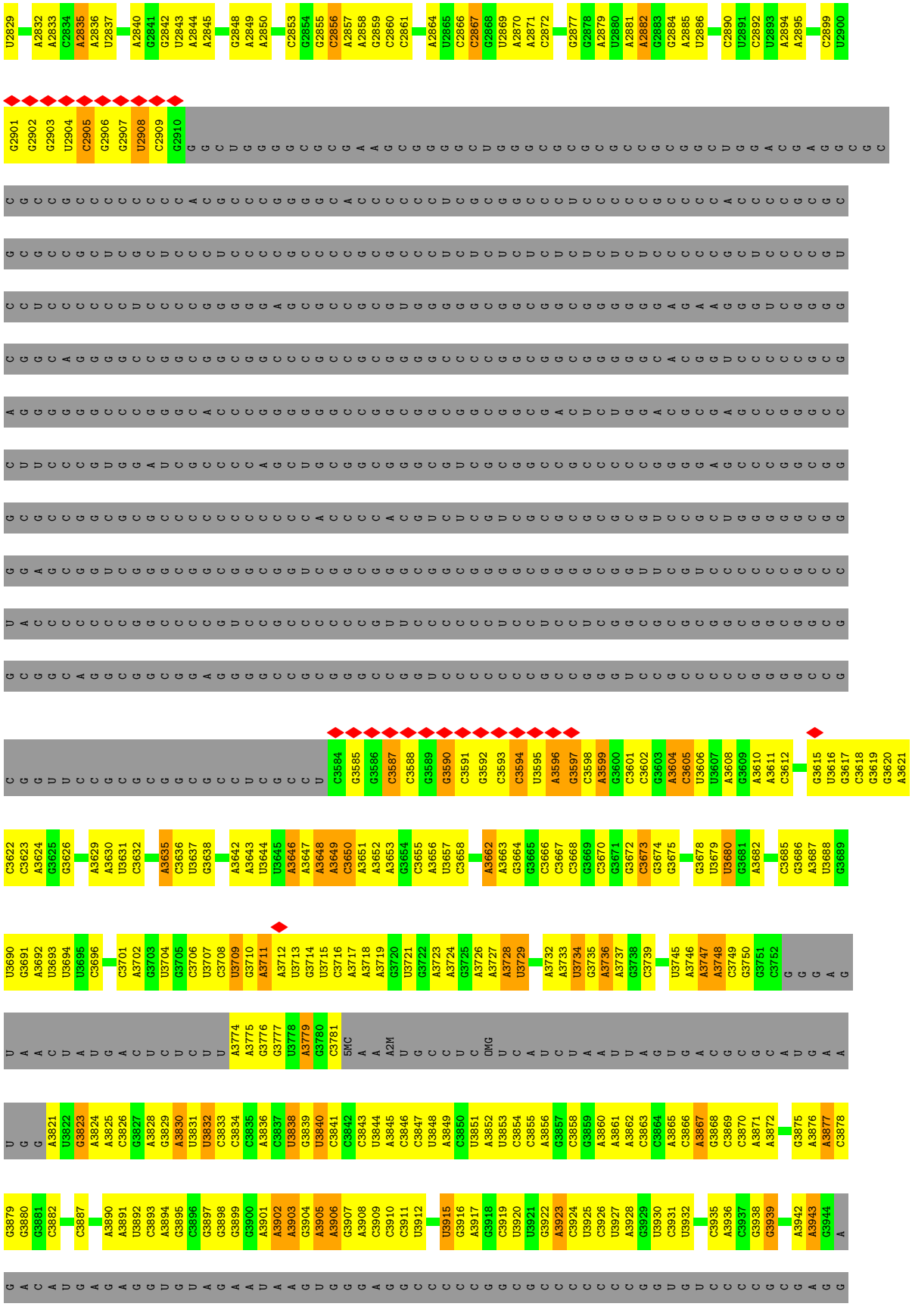
• Molecule 2: 28S rRNA

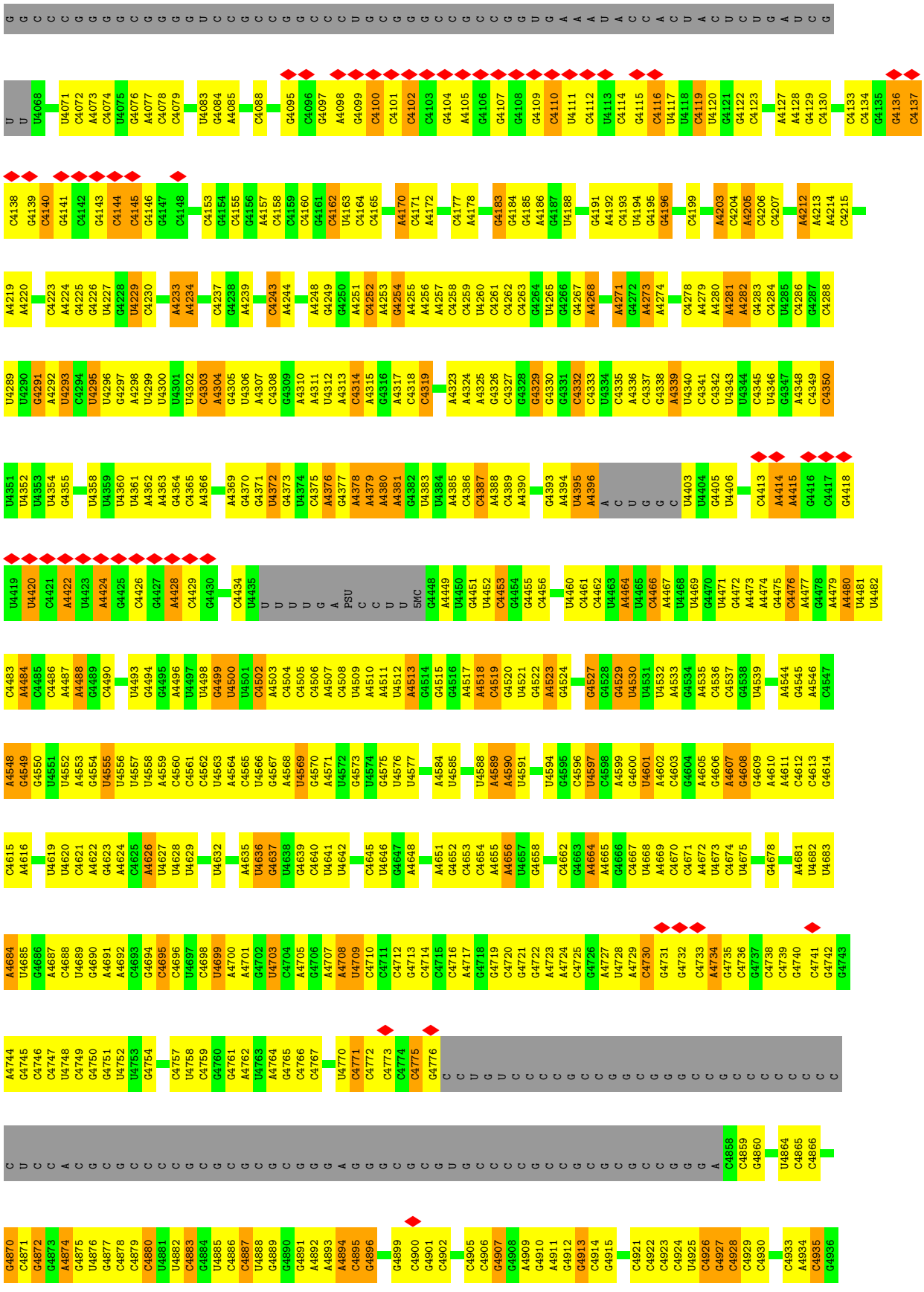
Chain 2:

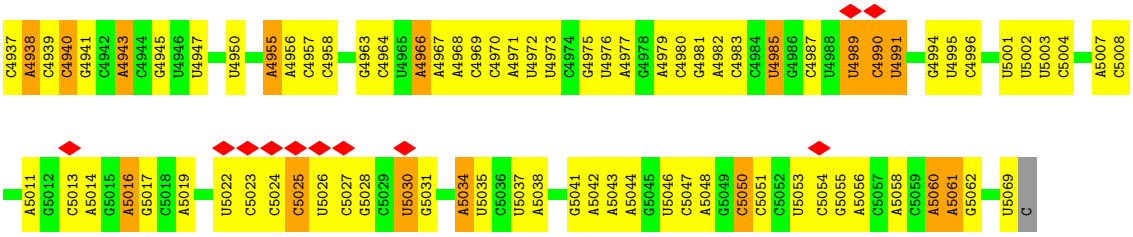






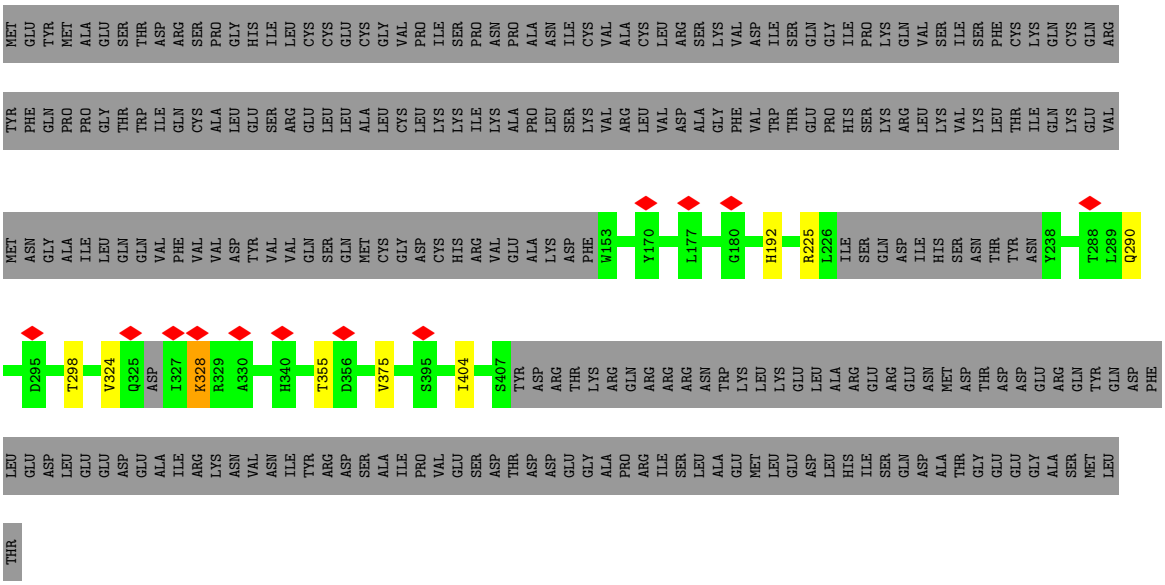






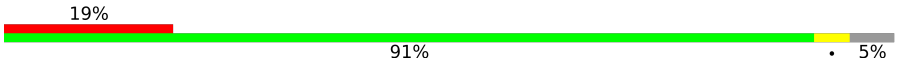
• Molecule 3: 60S ribosomal export protein NMD3

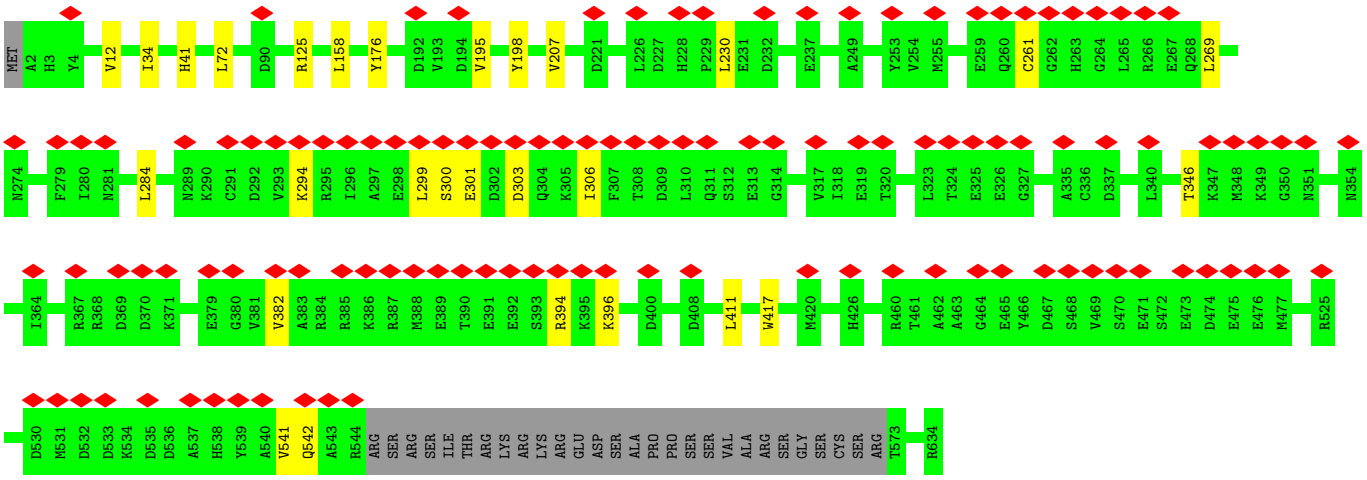
Chain 3:



• Molecule 4: Nucleolar GTP-binding protein 1

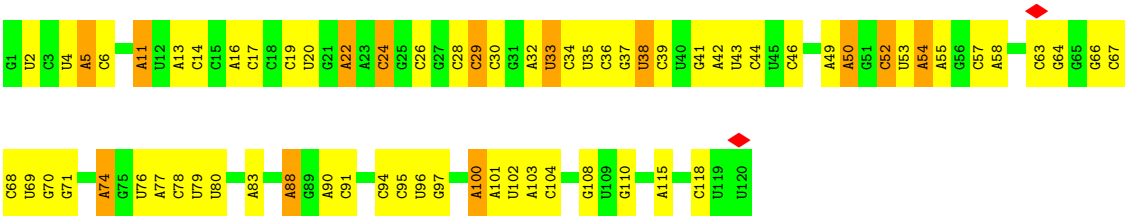
Chain 4:





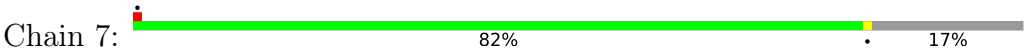
• Molecule 5: 5S rRNA

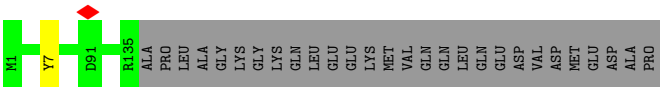
Chain 5:



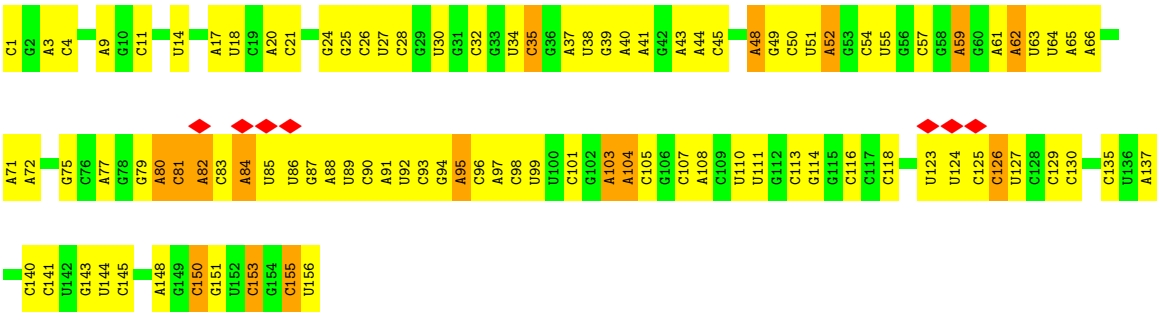
• Molecule 6: Eukaryotic translation initiation factor 6

• Molecule 7: Probable ribosome biogenesis protein RLP24

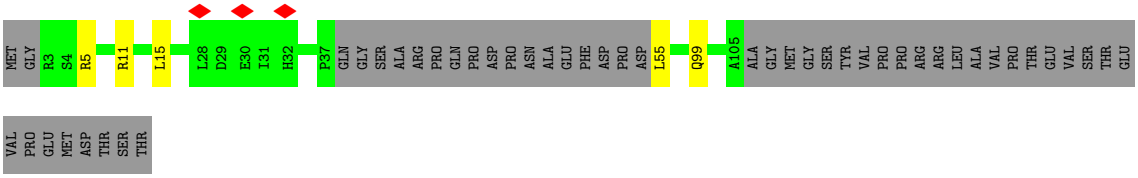




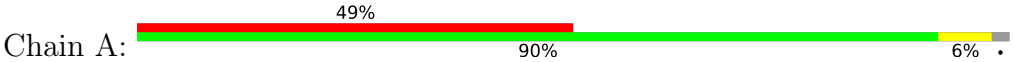
• Molecule 8: 5.8S rRNA

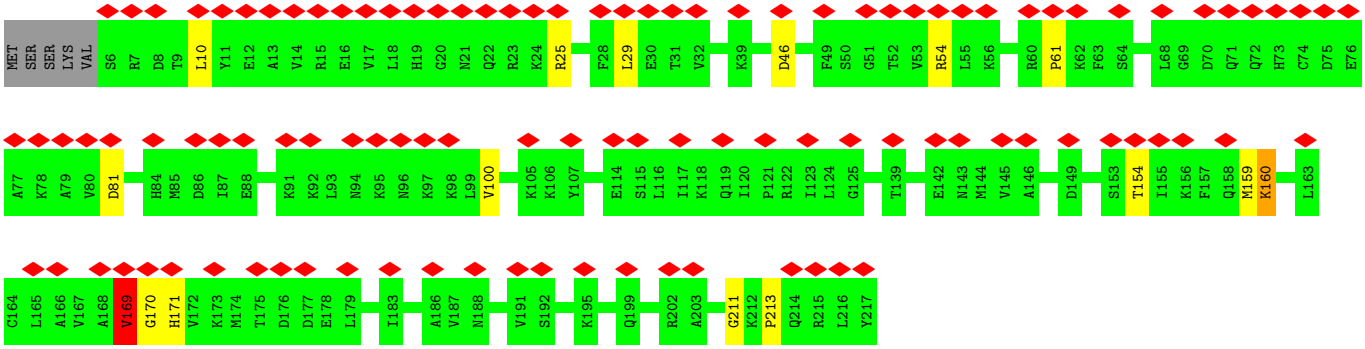


• Molecule 9: Zinc finger protein 593

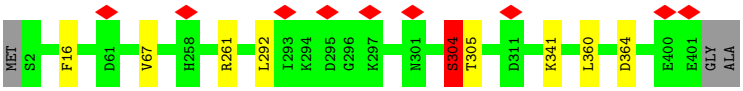


• Molecule 10: 60S ribosomal protein L10a

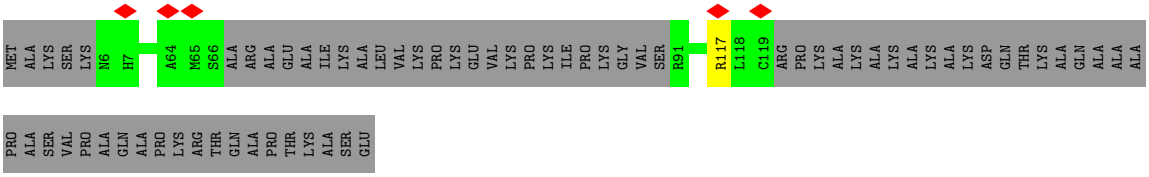




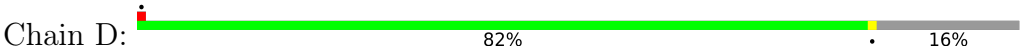
• Molecule 11: 60S ribosomal protein L3

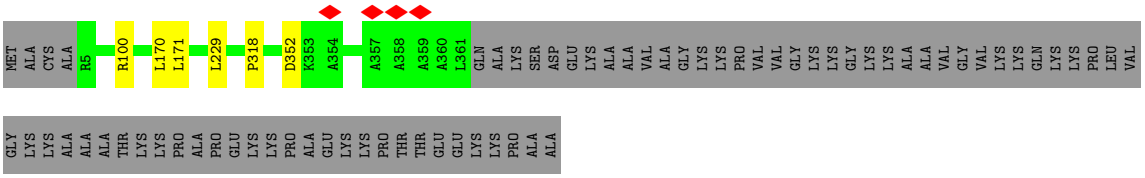


• Molecule 12: 60S ribosomal protein L29

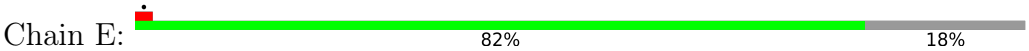


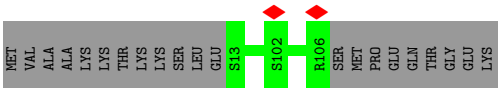
• Molecule 13: 60S ribosomal protein L4



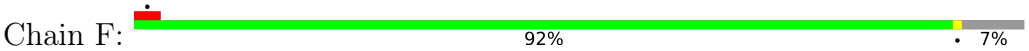


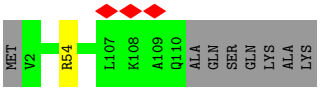
• Molecule 14: 60S ribosomal protein L30





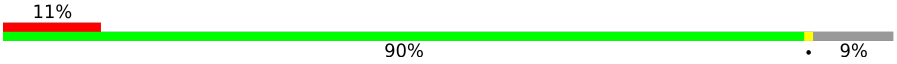
• Molecule 15: 60S ribosomal protein L34

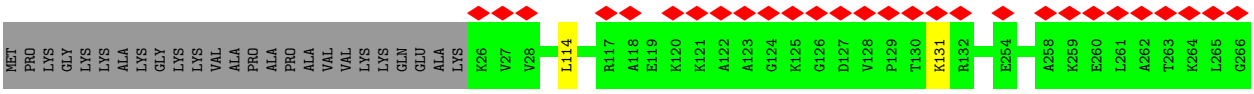




• Molecule 16: 60S ribosomal protein L7a

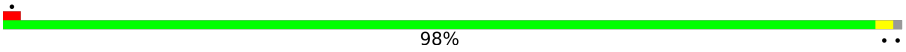
Chain G:

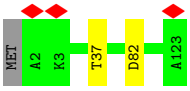




• Molecule 17: 60S ribosomal protein L35

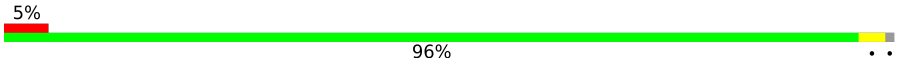
Chain H:

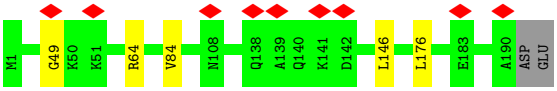




• Molecule 18: 60S ribosomal protein L9

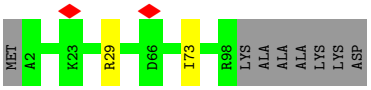
Chain I:





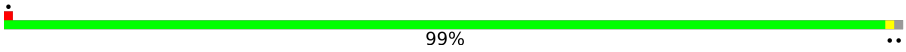
• Molecule 19: 60S ribosomal protein L36

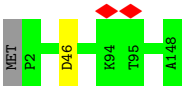
Chain K:



• Molecule 20: 60S ribosomal protein L27a

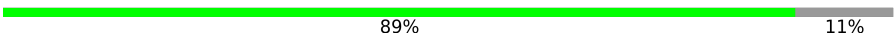
Chain L:





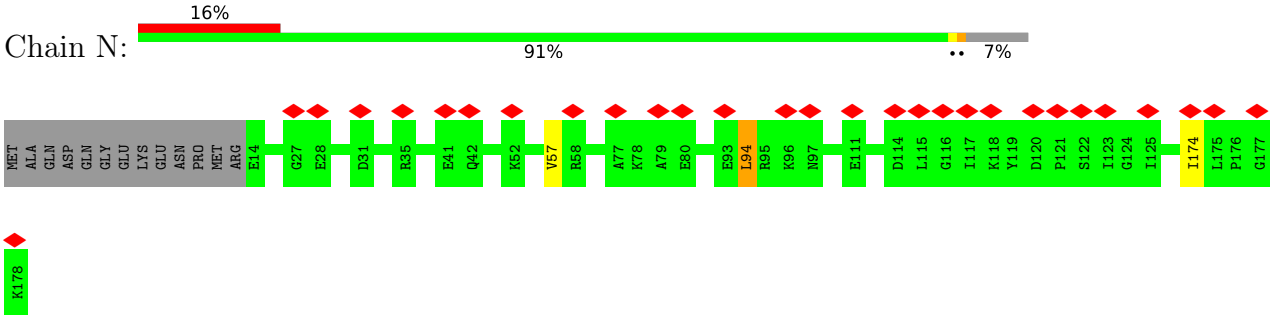
• Molecule 21: 60S ribosomal protein L37

Chain M:



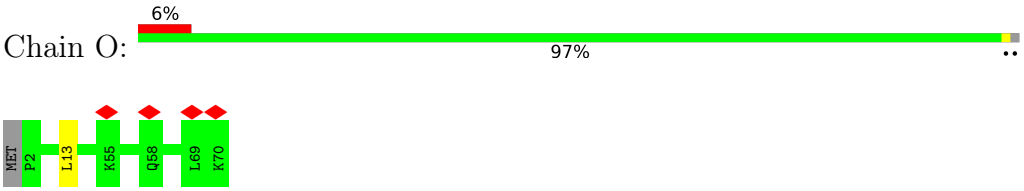
• Molecule 22: 60S ribosomal protein L11

Chain N:



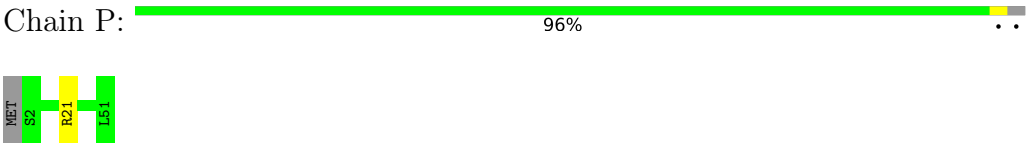
• Molecule 23: 60S ribosomal protein L38

Chain O:



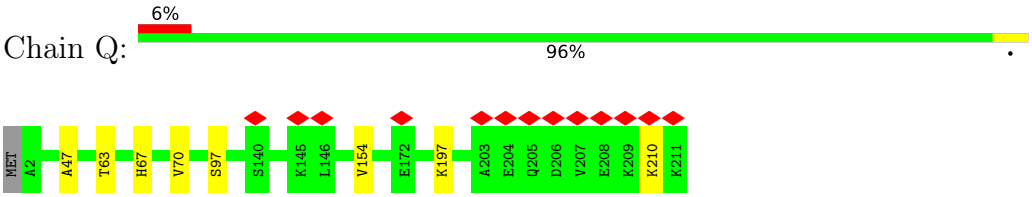
• Molecule 24: 60S ribosomal protein L39

Chain P:



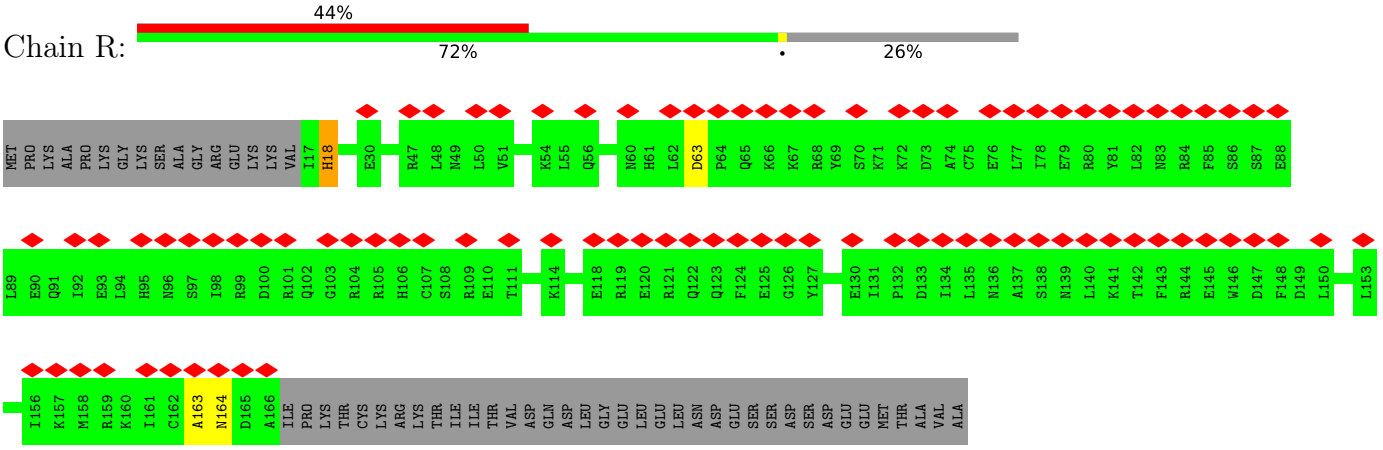
• Molecule 25: 60S ribosomal protein L13

Chain Q:



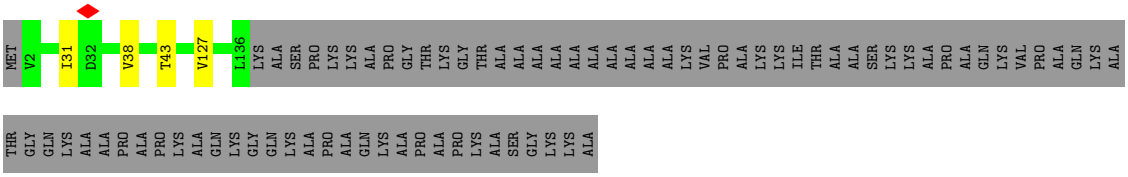
• Molecule 26: Translation machinery-associated protein 16

Chain R:



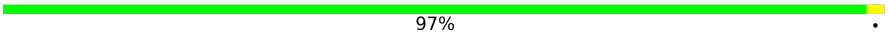
• Molecule 27: 60S ribosomal protein L14

Chain S:



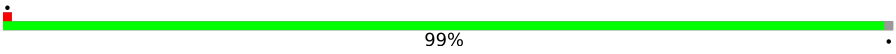
• Molecule 28: 60S ribosomal protein L15

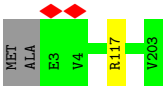
Chain U:



• Molecule 29: 60S ribosomal protein L13a

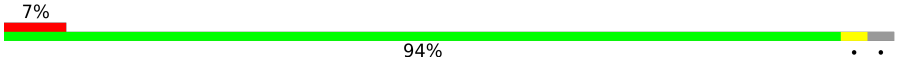
Chain V:

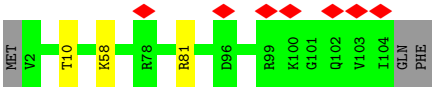




• Molecule 30: 60S ribosomal protein L36a

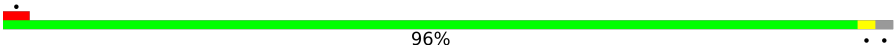
Chain W:

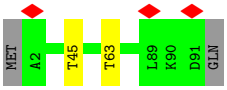




• Molecule 31: 60S ribosomal protein L37a

Chain X:



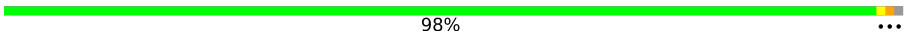


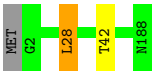
• Molecule 32: 60S ribosomal protein L17

Chain Y:

• Molecule 33: 60S ribosomal protein L18

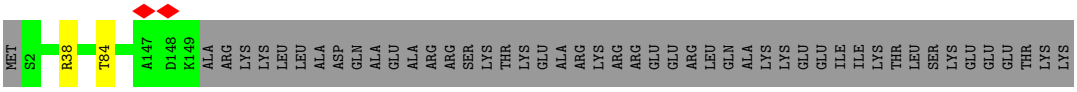
Chain Z:





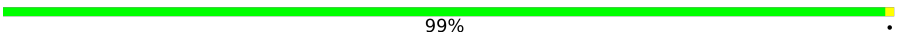
• Molecule 34: 60S ribosomal protein L19

Chain a:



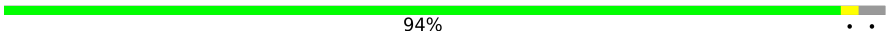
• Molecule 35: 60S ribosomal protein L18a

Chain b:



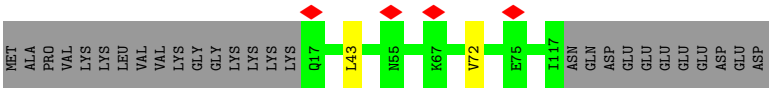
• Molecule 36: 60S ribosomal protein L21

Chain c:



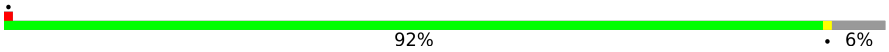
• Molecule 37: 60S ribosomal protein L22

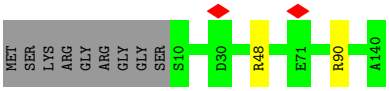
Chain d:



• Molecule 38: 60S ribosomal protein L23

Chain e:



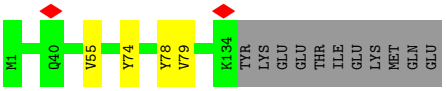


• Molecule 39: 60S ribosomal protein L23a

Chain g:

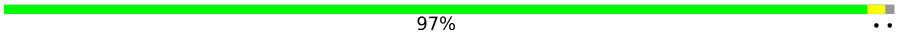
• Molecule 40: 60S ribosomal protein L26

Chain h:



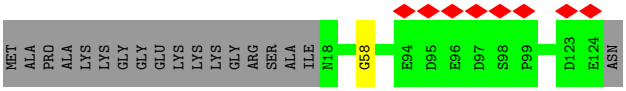
• Molecule 41: 60S ribosomal protein L27

Chain i:



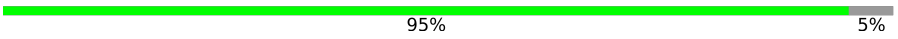
• Molecule 42: 60S ribosomal protein L31

Chain j:



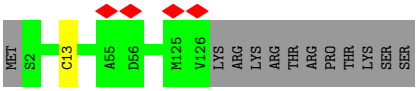
• Molecule 43: 60S ribosomal protein L32

Chain k:



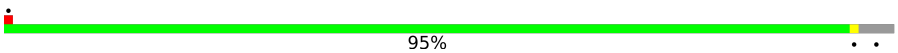
• Molecule 44: 60S ribosomal protein L28

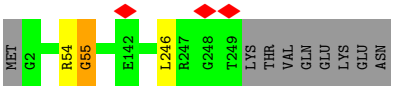
Chain l:



• Molecule 45: 60S ribosomal protein L8

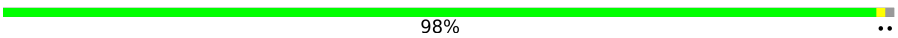
Chain m:





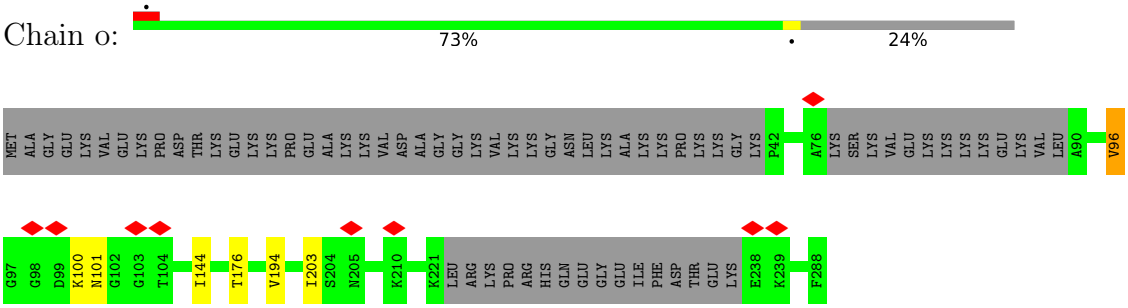
• Molecule 46: 60S ribosomal protein L35a

Chain n:



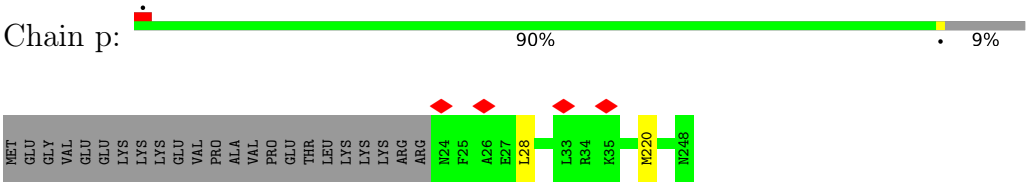
• Molecule 47: 60S ribosomal protein L6

Chain o:



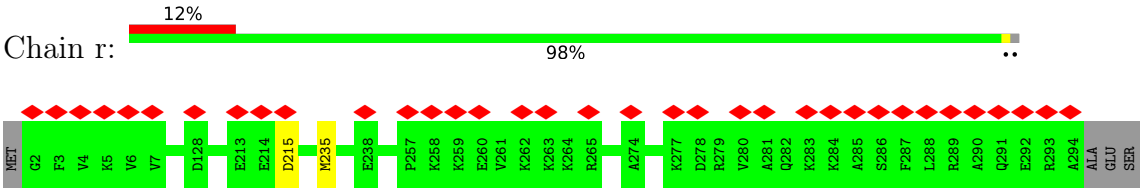
• Molecule 48: 60S ribosomal protein L7

Chain p:



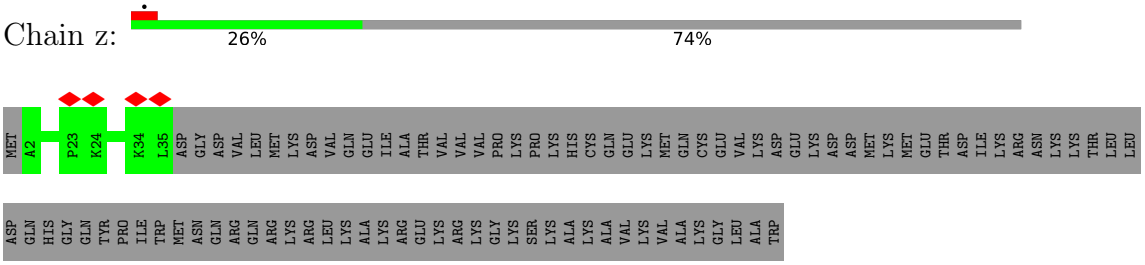
• Molecule 49: 60S ribosomal protein L5

Chain r:



• Molecule 50: Protein LLP homolog

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21489	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 ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.454	Depositor
Minimum map value	-0.187	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	507.84, 507.84, 507.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: B9H, 7MG, B8Q, B8T, B9B, P4U, MG, 6MZ, 5MC, OMG, B8H, B8K, M7A, MHG, OMU, E7G, P7G, 1MA, I4U, PSU, BGH, 5MU, B8W, OMC, E6G, A2M, 2MG, UR3

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	1	0.37	0/148	0.72	0/196
2	2	0.92	13/81168 (0.0%)	1.80	3749/126540 (3.0%)
3	3	0.42	0/1990	0.71	2/2685 (0.1%)
4	4	0.42	0/5048	0.76	12/6774 (0.2%)
5	5	0.81	0/2858	1.77	129/4455 (2.9%)
6	6	0.45	0/1877	0.74	1/2554 (0.0%)
7	7	0.45	0/1181	0.71	1/1563 (0.1%)
8	8	0.98	0/3679	1.78	161/5732 (2.8%)
9	9	0.39	0/723	0.77	2/961 (0.2%)
10	A	0.43	1/1736 (0.1%)	0.92	6/2328 (0.3%)
11	B	0.53	0/3306	0.79	7/4423 (0.2%)
12	C	0.37	0/755	0.63	0/996
13	D	0.51	0/2902	0.73	2/3898 (0.1%)
14	E	0.42	0/742	0.69	0/996
15	F	0.49	0/878	0.72	0/1170
16	G	0.47	0/1976	0.77	2/2658 (0.1%)
17	H	0.42	0/1023	0.63	0/1351
18	I	0.44	0/1537	0.69	2/2066 (0.1%)
19	K	0.39	0/810	0.65	1/1072 (0.1%)
20	L	0.51	0/1191	0.72	1/1591 (0.1%)
21	M	0.56	0/720	0.72	0/952
22	N	0.42	0/1341	0.78	2/1793 (0.1%)
23	O	0.42	0/575	0.65	1/761 (0.1%)
24	P	0.50	0/454	0.70	0/599
25	Q	0.48	0/1732	0.66	0/2315
26	R	0.38	0/1293	0.71	0/1725
27	S	0.48	0/1133	0.70	1/1516 (0.1%)
28	U	0.51	0/1746	0.71	1/2338 (0.0%)
29	V	0.49	0/1682	0.69	0/2250
30	W	0.48	0/855	0.75	2/1128 (0.2%)
31	X	0.49	0/708	0.65	0/941

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Y	0.48	0/1268	0.67	0/1701
33	Z	0.50	0/1537	0.74	1/2052 (0.0%)
34	a	0.46	0/1255	0.66	1/1662 (0.1%)
35	b	0.48	0/1501	0.65	0/2013
36	c	0.47	0/1291	0.69	0/1725
37	d	0.45	0/839	0.83	1/1126 (0.1%)
38	e	0.49	0/993	0.72	1/1332 (0.1%)
39	g	0.45	0/984	0.63	1/1323 (0.1%)
40	h	0.49	0/1132	0.68	0/1504
41	i	0.47	0/1130	0.68	0/1507
42	j	0.51	1/903 (0.1%)	0.70	0/1216
43	k	0.53	0/1071	0.69	0/1429
44	l	0.46	0/1017	0.72	1/1364 (0.1%)
45	m	0.53	0/1936	0.77	2/2596 (0.1%)
46	n	0.52	0/895	0.72	0/1198
47	o	0.42	0/1784	0.73	1/2393 (0.0%)
48	p	0.49	0/1916	0.72	2/2553 (0.1%)
49	r	0.43	0/2432	0.71	1/3256 (0.0%)
50	z	0.37	0/286	0.54	0/372
All	All	0.76	15/151937 (0.0%)	1.48	4097/222649 (1.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	3	0	2
4	4	0	6
6	6	0	1
10	A	0	7
11	B	0	2
18	I	0	1
22	N	0	1
25	Q	0	1
26	R	0	1
27	S	0	1
30	W	0	1
41	i	0	1
45	m	0	1
46	n	0	1
47	o	0	2
All	All	0	29

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	256	G	N7-C5	-7.57	1.34	1.39
2	2	2465	C	N1-C6	-7.32	1.32	1.37
2	2	1577	G	C2-N3	-7.08	1.27	1.32
2	2	4764	A	N9-C4	-6.65	1.33	1.37
2	2	1254	A	N9-C4	6.39	1.41	1.37
2	2	2484	A	N9-C4	6.38	1.41	1.37
2	2	485	C	N1-C2	6.17	1.46	1.40
2	2	2409	U	C2-O2	-5.95	1.17	1.22
2	2	256	G	C8-N7	-5.78	1.27	1.30
2	2	467	U	N1-C2	5.56	1.43	1.38
2	2	3646	A	N7-C5	-5.51	1.35	1.39
42	j	58	GLY	C-N	-5.50	1.21	1.34
2	2	2404	A	N7-C5	-5.21	1.36	1.39
10	A	170	GLY	N-CA	5.20	1.53	1.46
2	2	504	G	N9-C4	5.10	1.42	1.38

All (4097) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	516	C	N1-C2-O2	16.84	129.00	118.90
2	2	485	C	C2-N1-C1'	16.20	136.62	118.80
10	A	169	VAL	O-C-N	-15.96	96.07	123.20
2	2	4119	C	N1-C2-O2	15.50	128.20	118.90
2	2	449	C	C2-N1-C1'	15.49	135.84	118.80
2	2	467	U	N3-C2-O2	-15.22	111.55	122.20
2	2	449	C	N1-C2-O2	15.04	127.92	118.90
2	2	467	U	N1-C2-O2	14.68	133.08	122.80
2	2	485	C	N1-C2-O2	14.64	127.69	118.90
2	2	516	C	C6-N1-C2	-14.48	114.51	120.30
2	2	516	C	C2-N1-C1'	14.14	134.36	118.80
2	2	753	C	N1-C2-O2	13.93	127.26	118.90
2	2	4945	G	C5-C6-O6	-13.66	120.40	128.60
2	2	4682	U	N3-C2-O2	-13.49	112.75	122.20
2	2	516	C	N3-C2-O2	-13.46	112.48	121.90
5	5	39	C	N1-C2-O2	13.39	126.94	118.90
2	2	4502	C	N1-C2-O2	12.91	126.64	118.90
2	2	1245	C	C5-C6-N1	12.79	127.39	121.00
2	2	4119	C	N3-C2-O2	-12.79	112.95	121.90
2	2	4709	U	N3-C2-O2	-12.72	113.30	122.20
2	2	2465	C	C5-C6-N1	12.53	127.26	121.00
2	2	4887	C	N1-C2-O2	12.52	126.41	118.90
2	2	2814	C	N1-C2-O2	12.49	126.39	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4682	U	N1-C2-O2	12.44	131.50	122.80
2	2	4662	C	C6-N1-C2	-12.38	115.35	120.30
2	2	256	G	C6-C5-N7	-12.14	123.12	130.40
8	8	64	U	N3-C2-O2	-12.13	113.71	122.20
2	2	4502	C	N3-C2-O2	-12.09	113.44	121.90
2	2	467	U	C2-N1-C1'	12.07	132.18	117.70
2	2	753	C	N3-C2-O2	-12.05	113.46	121.90
2	2	656	C	N1-C2-O2	12.04	126.12	118.90
2	2	1859	C	N1-C2-O2	12.04	126.12	118.90
2	2	2783	A	N1-C2-N3	-12.02	123.29	129.30
2	2	1245	C	C6-N1-C2	-12.02	115.49	120.30
2	2	4502	C	C6-N1-C2	-12.00	115.50	120.30
2	2	516	C	C5-C6-N1	11.85	126.92	121.00
2	2	738	C	N1-C2-O2	11.81	125.99	118.90
2	2	4709	U	N1-C2-O2	11.78	131.04	122.80
2	2	2820	C	N1-C2-O2	11.72	125.93	118.90
2	2	988	C	C2-N1-C1'	11.68	131.65	118.80
2	2	220	C	N1-C2-O2	11.66	125.90	118.90
2	2	2491	C	C6-N1-C2	-11.65	115.64	120.30
2	2	4969	C	C6-N1-C2	-11.63	115.65	120.30
2	2	1417	C	C6-N1-C2	-11.61	115.66	120.30
2	2	100	C	C2-N1-C1'	11.60	131.56	118.80
2	2	4119	C	C6-N1-C2	-11.58	115.67	120.30
2	2	2255	C	N1-C2-O2	11.47	125.78	118.90
2	2	115	C	C2-N1-C1'	11.36	131.30	118.80
2	2	4730	C	C6-N1-C2	-11.33	115.77	120.30
2	2	4393	G	C5-C6-O6	11.29	135.37	128.60
2	2	489	C	N1-C2-O2	11.22	125.63	118.90
2	2	485	C	C6-N1-C1'	-11.21	107.34	120.80
2	2	4229	U	N3-C2-O2	-11.20	114.36	122.20
2	2	2410	C	C6-N1-C2	-11.19	115.83	120.30
2	2	2860	C	N1-C2-O2	11.18	125.61	118.90
2	2	3637	U	N3-C2-O2	-11.17	114.38	122.20
10	A	169	VAL	CA-C-N	11.15	138.50	116.20
2	2	753	C	C2-N1-C1'	11.15	131.06	118.80
2	2	1628	C	C6-N1-C2	-11.15	115.84	120.30
2	2	454	U	N3-C2-O2	-11.09	114.44	122.20
2	2	449	C	N3-C2-O2	-11.08	114.14	121.90
2	2	1079	C	N1-C2-O2	11.04	125.53	118.90
2	2	1472	C	C6-N1-C2	-11.03	115.89	120.30
2	2	656	C	N3-C2-O2	-11.02	114.19	121.90
2	2	115	C	N1-C2-O2	11.01	125.51	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3636	C	C6-N1-C2	-10.99	115.90	120.30
2	2	4990	C	N1-C2-O2	10.98	125.48	118.90
2	2	4199	C	N1-C2-O2	10.97	125.48	118.90
2	2	4880	C	N1-C2-O2	10.95	125.47	118.90
2	2	2560	C	C6-N1-C2	-10.94	115.92	120.30
2	2	41	C	C5-C6-N1	10.90	126.45	121.00
2	2	656	C	C6-N1-C2	-10.89	115.94	120.30
2	2	100	C	N1-C2-O2	10.87	125.42	118.90
2	2	1929	A	C2-N3-C4	10.85	116.03	110.60
2	2	738	C	C6-N1-C2	-10.84	115.96	120.30
2	2	4608	G	N7-C8-N9	10.82	118.51	113.10
2	2	4360	U	N3-C2-O2	-10.82	114.63	122.20
2	2	449	C	C6-N1-C1'	-10.81	107.83	120.80
5	5	28	C	C6-N1-C2	-10.78	115.99	120.30
2	2	77	U	N3-C2-O2	-10.77	114.66	122.20
2	2	4453	C	N1-C2-O2	10.77	125.36	118.90
2	2	485	C	C6-N1-C2	-10.77	115.99	120.30
2	2	1859	C	C6-N1-C2	-10.77	115.99	120.30
2	2	1429	C	C6-N1-C2	-10.68	116.03	120.30
2	2	1577	G	C2-N3-C4	10.59	117.19	111.90
5	5	102	U	N3-C2-O2	-10.59	114.79	122.20
2	2	4758	U	N3-C2-O2	-10.57	114.80	122.20
2	2	257	C	C6-N1-C2	-10.57	116.07	120.30
2	2	4144	C	C5-C6-N1	10.57	126.28	121.00
2	2	41	C	C6-N1-C2	-10.54	116.08	120.30
2	2	654	C	N1-C2-O2	10.53	125.22	118.90
2	2	4303	C	N1-C2-O2	10.53	125.22	118.90
2	2	4505	C	C6-N1-C2	-10.51	116.10	120.30
2	2	3926	C	N1-C2-O2	10.51	125.20	118.90
2	2	4171	C	N1-C2-O2	10.49	125.19	118.90
2	2	4303	C	N3-C2-O2	-10.48	114.56	121.90
2	2	1632	A	C2-N3-C4	10.39	115.80	110.60
2	2	454	U	N1-C2-O2	10.37	130.06	122.80
2	2	2710	C	N1-C2-O2	10.35	125.11	118.90
2	2	1386	C	C6-N1-C2	-10.35	116.16	120.30
2	2	1243	C	C6-N1-C2	-10.31	116.17	120.30
2	2	753	C	C6-N1-C2	-10.29	116.18	120.30
2	2	417	G	O4'-C1'-N9	10.28	116.42	108.20
2	2	4119	C	C2-N1-C1'	10.26	130.08	118.80
2	2	195	C	C6-N1-C2	-10.23	116.21	120.30
2	2	498	C	C6-N1-C2	-10.23	116.21	120.30
2	2	4140	C	N1-C2-O2	10.20	125.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	485	C	N3-C2-O2	-10.19	114.77	121.90
2	2	1417	C	C5-C6-N1	10.18	126.09	121.00
2	2	1731	C	C6-N1-C2	-10.17	116.23	120.30
2	2	4352	U	N3-C2-O2	-10.17	115.08	122.20
2	2	2627	C	C6-N1-C2	-10.15	116.24	120.30
2	2	3637	U	N1-C2-O2	10.15	129.91	122.80
2	2	3709	U	N3-C2-O2	-10.15	115.10	122.20
2	2	1634	A	N1-C2-N3	-10.14	124.23	129.30
2	2	988	C	C6-N1-C2	-10.14	116.24	120.30
2	2	1302	U	N3-C2-O2	-10.13	115.11	122.20
2	2	9	C	C6-N1-C2	-10.12	116.25	120.30
2	2	1686	C	N1-C2-O2	10.12	124.97	118.90
2	2	1192	C	C6-N1-C2	-10.11	116.26	120.30
2	2	4887	C	N3-C2-O2	-10.10	114.83	121.90
2	2	4945	G	C4-C5-N7	10.08	114.83	110.80
2	2	449	C	C6-N1-C2	-10.07	116.27	120.30
2	2	1726	U	N3-C2-O2	-10.07	115.15	122.20
2	2	4695	C	N1-C2-O2	10.05	124.93	118.90
2	2	2255	C	C2-N1-C1'	10.04	129.84	118.80
2	2	2022	C	N1-C2-O2	10.04	124.92	118.90
2	2	4594	U	N3-C2-O2	-10.03	115.18	122.20
2	2	112	C	C6-N1-C2	-10.03	116.29	120.30
2	2	1276	C	C6-N1-C2	-10.03	116.29	120.30
2	2	4758	U	N1-C2-O2	10.01	129.81	122.80
2	2	3870	C	C6-N1-C2	-9.99	116.31	120.30
2	2	988	C	C5-C6-N1	9.98	125.99	121.00
2	2	4601	U	N3-C2-O2	-9.98	115.21	122.20
2	2	4775	C	N1-C2-O2	9.97	124.88	118.90
2	2	988	C	N1-C2-O2	9.96	124.88	118.90
2	2	4215	C	N1-C2-O2	9.96	124.88	118.90
2	2	96	U	N3-C2-O2	-9.95	115.23	122.20
2	2	4303	C	C2-N1-C1'	9.94	129.74	118.80
2	2	3680	U	N3-C2-O2	-9.94	115.24	122.20
2	2	115	C	N3-C2-O2	-9.93	114.95	121.90
2	2	53	C	C6-N1-C2	-9.92	116.33	120.30
2	2	4508	C	C6-N1-C2	-9.91	116.33	120.30
2	2	3588	C	C6-N1-C2	-9.91	116.34	120.30
2	2	4601	U	N1-C2-O2	9.91	129.74	122.80
2	2	489	C	C6-N1-C2	-9.91	116.34	120.30
2	2	2351	C	C6-N1-C2	-9.88	116.35	120.30
2	2	704	C	N1-C2-O2	9.86	124.81	118.90
8	8	126	C	C6-N1-C2	-9.86	116.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	282	C	N1-C2-O2	9.85	124.81	118.90
2	2	2410	C	C5-C6-N1	9.84	125.92	121.00
5	5	39	C	N3-C2-O2	-9.84	115.02	121.90
8	8	103	A	N1-C2-N3	-9.82	124.39	129.30
2	2	1302	U	N1-C2-O2	9.81	129.67	122.80
2	2	4887	C	C6-N1-C2	-9.81	116.38	120.30
2	2	2603	C	C6-N1-C2	-9.81	116.38	120.30
2	2	456	C	O4'-C1'-N1	9.80	116.04	108.20
2	2	4608	G	C8-N9-C4	-9.80	102.48	106.40
2	2	1816	C	C6-N1-C2	-9.78	116.39	120.30
2	2	3926	C	C6-N1-C2	-9.78	116.39	120.30
2	2	180	C	C5-C6-N1	9.77	125.88	121.00
45	m	246	LEU	CA-CB-CG	9.76	137.75	115.30
2	2	485	C	C5-C6-N1	9.76	125.88	121.00
2	2	654	C	N3-C2-O2	-9.74	115.08	121.90
2	2	3657	U	N3-C2-O2	-9.74	115.39	122.20
2	2	1191	C	C6-N1-C2	-9.71	116.42	120.30
30	W	81	ARG	NE-CZ-NH1	9.71	125.15	120.30
2	2	4453	C	C2-N1-C1'	9.71	129.48	118.80
2	2	209	U	N1-C2-O2	9.70	129.59	122.80
2	2	3588	C	C5-C6-N1	9.70	125.85	121.00
2	2	3870	C	C5-C6-N1	9.69	125.84	121.00
2	2	1352	C	C6-N1-C2	-9.68	116.43	120.30
2	2	1607	C	C6-N1-C2	-9.68	116.43	120.30
2	2	1254	A	C2-N3-C4	9.67	115.44	110.60
2	2	2814	C	N3-C2-O2	-9.67	115.13	121.90
2	2	4476	C	N1-C2-O2	9.67	124.70	118.90
2	2	4532	U	N3-C2-O2	-9.66	115.44	122.20
2	2	1686	C	C6-N1-C2	-9.66	116.44	120.30
2	2	2814	C	C2-N1-C1'	9.66	129.42	118.80
2	2	972	C	N1-C2-O2	9.65	124.69	118.90
2	2	1340	C	C5-C6-N1	9.65	125.82	121.00
2	2	2803	U	N3-C2-O2	-9.64	115.45	122.20
2	2	449	C	C5-C6-N1	9.64	125.82	121.00
2	2	77	U	N1-C2-O2	9.64	129.54	122.80
2	2	1384	C	C6-N1-C2	-9.63	116.45	120.30
2	2	972	C	C6-N1-C2	-9.63	116.45	120.30
2	2	738	C	N3-C2-O2	-9.63	115.16	121.90
2	2	2627	C	C5-C6-N1	9.62	125.81	121.00
2	2	1637	A	N1-C2-N3	-9.62	124.49	129.30
2	2	4144	C	C6-N1-C2	-9.62	116.45	120.30
2	2	3598	C	N1-C2-O2	9.61	124.67	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	14	C	C6-N1-C2	-9.61	116.46	120.30
2	2	2603	C	C5-C6-N1	9.59	125.80	121.00
2	2	256	G	C4-C5-N7	9.59	114.64	110.80
2	2	4766	C	C6-N1-C2	-9.59	116.46	120.30
2	2	209	U	N3-C2-O2	-9.59	115.49	122.20
2	2	4775	C	C2-N1-C1'	9.59	129.34	118.80
2	2	985	C	C6-N1-C2	-9.58	116.47	120.30
2	2	489	C	C2-N1-C1'	9.57	129.33	118.80
2	2	4206	C	C6-N1-C2	-9.57	116.47	120.30
2	2	1241	C	N1-C2-O2	9.56	124.64	118.90
2	2	2302	C	C6-N1-C2	-9.56	116.48	120.30
2	2	925	C	C6-N1-C2	-9.55	116.48	120.30
2	2	4243	C	C6-N1-C2	-9.54	116.48	120.30
2	2	100	C	N3-C2-O2	-9.53	115.23	121.90
2	2	948	C	C6-N1-C2	-9.52	116.49	120.30
2	2	4273	A	N1-C6-N6	-9.52	112.89	118.60
2	2	2820	C	C6-N1-C2	-9.51	116.50	120.30
2	2	1302	U	C2-N1-C1'	9.49	129.09	117.70
5	5	78	C	C6-N1-C2	-9.49	116.50	120.30
2	2	1458	C	N1-C2-O2	9.48	124.59	118.90
2	2	1344	C	C6-N1-C2	-9.48	116.51	120.30
2	2	1467	C	C6-N1-C2	-9.48	116.51	120.30
2	2	148	C	C6-N1-C2	-9.47	116.51	120.30
2	2	2710	C	C2-N1-C1'	9.47	129.21	118.80
2	2	499	G	C4-N9-C1'	9.46	138.80	126.50
2	2	1191	C	N3-C2-O2	-9.45	115.28	121.90
2	2	2362	U	N3-C2-O2	-9.45	115.58	122.20
2	2	3650	C	C6-N1-C2	-9.45	116.52	120.30
2	2	4758	U	C2-N1-C1'	9.45	129.04	117.70
2	2	1848	C	C6-N1-C2	-9.44	116.52	120.30
2	2	2373	C	C5-C6-N1	9.43	125.72	121.00
2	2	4700	A	N1-C2-N3	-9.43	124.58	129.30
2	2	2856	C	N1-C2-O2	9.43	124.56	118.90
2	2	2593	C	C6-N1-C2	-9.43	116.53	120.30
2	2	4471	U	N3-C2-O2	-9.43	115.60	122.20
2	2	2568	C	N1-C2-O2	9.42	124.55	118.90
2	2	2803	U	N1-C2-O2	9.41	129.39	122.80
2	2	2560	C	C5-C6-N1	9.40	125.70	121.00
2	2	4996	C	C6-N1-C2	-9.39	116.54	120.30
2	2	4342	C	C6-N1-C2	-9.39	116.54	120.30
2	2	2373	C	C6-N1-C2	-9.38	116.55	120.30
2	2	257	C	C5-C6-N1	9.37	125.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1859	C	N3-C2-O2	-9.36	115.34	121.90
2	2	3598	C	N3-C2-O2	-9.36	115.35	121.90
2	2	654	C	C6-N1-C2	-9.35	116.56	120.30
2	2	282	C	N3-C2-O2	-9.34	115.36	121.90
2	2	2048	U	N3-C2-O2	-9.34	115.66	122.20
2	2	1889	U	N3-C2-O2	-9.32	115.67	122.20
2	2	2802	C	C6-N1-C2	-9.32	116.57	120.30
2	2	50	C	N1-C2-O2	9.32	124.49	118.90
2	2	1472	C	C5-C6-N1	9.32	125.66	121.00
8	8	126	C	N1-C2-O2	9.32	124.49	118.90
2	2	4703	U	N3-C2-O2	-9.31	115.68	122.20
2	2	2783	A	C6-N1-C2	9.31	124.19	118.60
2	2	2022	C	C6-N1-C2	-9.30	116.58	120.30
5	5	28	C	N1-C2-O2	9.30	124.48	118.90
2	2	2048	U	N1-C2-O2	9.30	129.31	122.80
2	2	2410	C	N1-C2-O2	9.29	124.48	118.90
2	2	1859	C	C5-C6-N1	9.29	125.64	121.00
2	2	256	G	N3-C4-N9	9.29	131.57	126.00
2	2	4945	G	N3-C4-N9	9.28	131.57	126.00
2	2	2257	C	N1-C2-O2	9.26	124.46	118.90
2	2	2820	C	N3-C2-O2	-9.25	115.42	121.90
2	2	504	G	C4-N9-C1'	9.25	138.52	126.50
2	2	1429	C	C5-C6-N1	9.24	125.62	121.00
2	2	1969	G	N1-C6-O6	-9.23	114.36	119.90
5	5	39	C	C6-N1-C2	-9.23	116.61	120.30
2	2	2560	C	C2-N1-C1'	9.22	128.94	118.80
2	2	2094	G	N3-C4-C5	-9.20	124.00	128.60
2	2	673	C	C6-N1-C2	-9.20	116.62	120.30
2	2	2262	G	C4-N9-C1'	9.19	138.45	126.50
2	2	2484	A	C2-N3-C4	9.17	115.18	110.60
2	2	4508	C	N1-C2-O2	9.16	124.40	118.90
2	2	738	C	C2-N1-C1'	9.16	128.88	118.80
2	2	110	C	C6-N1-C2	-9.16	116.64	120.30
2	2	322	C	N1-C2-O2	9.15	124.39	118.90
2	2	3882	C	N1-C2-O2	9.14	124.39	118.90
2	2	3587	C	N1-C2-O2	9.13	124.38	118.90
2	2	4199	C	N3-C2-O2	-9.13	115.51	121.90
2	2	504	G	N3-C4-C5	-9.13	124.03	128.60
2	2	2802	C	C5-C6-N1	9.13	125.56	121.00
2	2	4213	A	N1-C2-N3	-9.12	124.74	129.30
2	2	3709	U	N1-C2-O2	9.12	129.18	122.80
8	8	82	A	C2-N3-C4	9.11	115.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	256	G	N3-C2-N2	9.11	126.28	119.90
2	2	2867	C	C6-N1-C2	-9.11	116.66	120.30
2	2	4655	A	N1-C2-N3	-9.11	124.75	129.30
2	2	1241	C	C2-N1-C1'	9.10	128.81	118.80
2	2	4921	C	C6-N1-C2	-9.09	116.66	120.30
8	8	107	C	C6-N1-C2	-9.09	116.67	120.30
2	2	2729	C	C6-N1-C2	-9.08	116.67	120.30
2	2	4880	C	N3-C2-O2	-9.08	115.55	121.90
8	8	140	C	C6-N1-C2	-9.08	116.67	120.30
2	2	4559	A	N1-C2-N3	-9.07	124.76	129.30
2	2	716	C	C6-N1-C2	-9.07	116.67	120.30
2	2	2505	C	C6-N1-C2	-9.07	116.67	120.30
5	5	102	U	N1-C2-O2	9.07	129.15	122.80
2	2	1395	U	N3-C2-O2	-9.06	115.86	122.20
2	2	1666	C	C6-N1-C2	-9.06	116.67	120.30
8	8	99	U	N3-C2-O2	-9.05	115.86	122.20
2	2	4945	G	N1-C6-O6	9.05	125.33	119.90
2	2	2499	C	N1-C2-O2	9.04	124.33	118.90
2	2	4714	C	C6-N1-C2	-9.04	116.68	120.30
2	2	220	C	N3-C2-O2	-9.04	115.57	121.90
2	2	4771	C	C5-C6-N1	9.04	125.52	121.00
2	2	4969	C	C5-C6-N1	9.03	125.52	121.00
2	2	2260	C	C6-N1-C2	-9.03	116.69	120.30
2	2	489	C	C5-C6-N1	9.03	125.51	121.00
2	2	4340	U	N3-C2-O2	-9.01	115.89	122.20
2	2	4289	U	N3-C2-O2	-9.00	115.90	122.20
2	2	1889	U	N1-C2-O2	9.00	129.10	122.80
2	2	79	C	C6-N1-C2	-8.99	116.70	120.30
2	2	4989	U	N1-C2-O2	8.99	129.09	122.80
2	2	4280	A	N1-C2-N3	-8.98	124.81	129.30
2	2	1722	C	C6-N1-C2	-8.98	116.71	120.30
2	2	2337	C	C6-N1-C2	-8.98	116.71	120.30
2	2	1192	C	N1-C2-O2	8.98	124.29	118.90
2	2	1494	U	N3-C2-O2	-8.97	115.92	122.20
2	2	1243	C	C5-C6-N1	8.97	125.48	121.00
2	2	2274	C	C6-N1-C2	-8.96	116.72	120.30
2	2	4764	A	N1-C2-N3	-8.96	124.82	129.30
2	2	2351	C	C5-C6-N1	8.96	125.48	121.00
2	2	2410	C	C2-N1-C1'	8.94	128.63	118.80
2	2	2653	C	C6-N1-C2	-8.94	116.72	120.30
2	2	1663	C	C5-C6-N1	8.93	125.47	121.00
2	2	390	C	C6-N1-C2	-8.93	116.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1674	C	C6-N1-C2	-8.93	116.73	120.30
2	2	2465	C	C6-N1-C2	-8.91	116.74	120.30
2	2	2860	C	N3-C2-O2	-8.91	115.66	121.90
2	2	4360	U	N1-C2-O2	8.91	129.04	122.80
2	2	4972	U	N3-C2-O2	-8.91	115.96	122.20
2	2	205	C	C6-N1-C2	-8.90	116.74	120.30
2	2	738	C	C5-C6-N1	8.89	125.45	121.00
2	2	4989	U	N3-C2-O2	-8.89	115.98	122.20
2	2	1722	C	C5-C6-N1	8.89	125.44	121.00
2	2	1893	C	C6-N1-C2	-8.89	116.75	120.30
2	2	1906	U	N3-C2-O2	-8.89	115.98	122.20
2	2	4505	C	C5-C6-N1	8.89	125.44	121.00
2	2	390	C	C5-C6-N1	8.88	125.44	121.00
2	2	4505	C	N1-C2-O2	8.88	124.23	118.90
2	2	4990	C	N3-C2-O2	-8.87	115.69	121.90
2	2	4365	C	C5-C6-N1	8.87	125.44	121.00
2	2	4171	C	N3-C2-O2	-8.86	115.70	121.90
2	2	2667	C	N1-C2-O2	8.85	124.21	118.90
2	2	4958	C	C5-C6-N1	8.85	125.42	121.00
2	2	3926	C	N3-C2-O2	-8.84	115.71	121.90
2	2	5025	C	C6-N1-C2	-8.84	116.76	120.30
2	2	1342	A	N1-C2-N3	-8.83	124.88	129.30
2	2	4119	C	C5-C6-N1	8.82	125.41	121.00
2	2	4140	C	N3-C2-O2	-8.82	115.72	121.90
5	5	78	C	C5-C6-N1	8.81	125.41	121.00
2	2	489	C	N3-C2-O2	-8.81	115.73	121.90
2	2	3866	C	C6-N1-C2	-8.79	116.78	120.30
2	2	2303	C	N1-C2-O2	8.79	124.18	118.90
2	2	220	C	C6-N1-C2	-8.78	116.79	120.30
2	2	112	C	C5-C6-N1	8.78	125.39	121.00
2	2	1579	C	C6-N1-C2	-8.77	116.79	120.30
2	2	2362	U	N1-C2-O2	8.77	128.94	122.80
2	2	2262	G	N3-C4-N9	8.76	131.26	126.00
2	2	141	C	N1-C2-O2	8.76	124.16	118.90
2	2	4708	A	C2-N3-C4	8.76	114.98	110.60
2	2	174	C	N1-C2-O2	8.76	124.15	118.90
2	2	3919	C	C6-N1-C2	-8.75	116.80	120.30
5	5	91	C	C5-C6-N1	8.75	125.38	121.00
2	2	1720	C	C6-N1-C2	-8.75	116.80	120.30
2	2	180	C	N1-C2-O2	8.75	124.15	118.90
2	2	3655	C	C6-N1-C2	-8.74	116.80	120.30
2	2	4662	C	C5-C6-N1	8.74	125.37	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	122	U	N3-C2-O2	-8.73	116.09	122.20
2	2	4229	U	N1-C2-O2	8.72	128.91	122.80
2	2	322	C	C6-N1-C2	-8.72	116.81	120.30
2	2	4772	C	C6-N1-C2	-8.71	116.81	120.30
2	2	1897	A	C2-N3-C4	8.71	114.95	110.60
2	2	4502	C	C2-N1-C1'	8.71	128.38	118.80
2	2	4237	C	C6-N1-C2	-8.71	116.82	120.30
11	B	360	LEU	CA-CB-CG	8.70	135.32	115.30
2	2	28	C	C6-N1-C2	-8.70	116.82	120.30
2	2	504	G	N3-C4-N9	8.69	131.21	126.00
2	2	2074	C	C5-C6-N1	8.69	125.34	121.00
2	2	4508	C	C5-C6-N1	8.68	125.34	121.00
8	8	150	C	N1-C2-O2	8.67	124.10	118.90
2	2	2035	C	C6-N1-C2	-8.67	116.83	120.30
2	2	4887	C	C2-N1-C1'	8.67	128.33	118.80
2	2	180	C	C6-N1-C2	-8.66	116.83	120.30
2	2	1216	C	C2-N1-C1'	8.66	128.32	118.80
8	8	51	U	C2-N1-C1'	8.66	128.09	117.70
2	2	44	A	C2-N3-C4	8.65	114.93	110.60
2	2	2867	C	C5-C6-N1	8.65	125.33	121.00
2	2	4667	C	C6-N1-C2	-8.65	116.84	120.30
2	2	1848	C	C5-C6-N1	8.65	125.33	121.00
2	2	673	C	C5-C6-N1	8.65	125.32	121.00
2	2	1632	A	N1-C2-N3	-8.65	124.98	129.30
2	2	4259	C	C5-C6-N1	8.64	125.32	121.00
2	2	4302	U	N3-C2-O2	-8.64	116.15	122.20
2	2	1447	C	C6-N1-C2	-8.64	116.85	120.30
2	2	1893	C	C5-C6-N1	8.63	125.32	121.00
2	2	68	U	N3-C2-O2	-8.63	116.16	122.20
2	2	124	C	C6-N1-C2	-8.62	116.85	120.30
2	2	1687	U	N3-C2-O2	-8.61	116.17	122.20
2	2	3866	C	C5-C6-N1	8.61	125.31	121.00
2	2	4206	C	C5-C6-N1	8.61	125.30	121.00
2	2	3618	C	C6-N1-C2	-8.60	116.86	120.30
2	2	4281	A	N7-C8-N9	8.60	118.10	113.80
2	2	4365	C	C6-N1-C2	-8.60	116.86	120.30
2	2	2404	A	N1-C2-N3	-8.60	125.00	129.30
2	2	2022	C	C2-N1-C1'	8.60	128.26	118.80
2	2	1686	C	N3-C2-O2	-8.59	115.89	121.90
2	2	498	C	N1-C2-O2	8.59	124.06	118.90
2	2	1599	A	N1-C2-N3	-8.59	125.00	129.30
5	5	28	C	C5-C6-N1	8.59	125.30	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	14	C	N1-C2-O2	8.58	124.05	118.90
2	2	3680	U	N1-C2-O2	8.58	128.81	122.80
2	2	1702	C	N1-C2-O2	8.57	124.04	118.90
2	2	4352	U	N1-C2-O2	8.56	128.79	122.80
2	2	3901	A	C2-N3-C4	8.56	114.88	110.60
2	2	1875	C	C5-C6-N1	8.55	125.28	121.00
2	2	2271	C	C6-N1-C2	-8.55	116.88	120.30
2	2	282	C	C6-N1-C2	-8.55	116.88	120.30
8	8	52	A	N1-C2-N3	-8.55	125.03	129.30
2	2	4880	C	C6-N1-C2	-8.55	116.88	120.30
2	2	1417	C	C2-N1-C1'	8.55	128.20	118.80
2	2	281	U	N3-C2-O2	-8.54	116.22	122.20
2	2	178	C	C5-C6-N1	8.54	125.27	121.00
37	d	43	LEU	CA-CB-CG	8.54	134.94	115.30
2	2	4772	C	C5-C6-N1	8.53	125.26	121.00
2	2	71	C	C6-N1-C2	-8.53	116.89	120.30
2	2	3840	U	N3-C2-O2	-8.53	116.23	122.20
5	5	67	C	C6-N1-C2	-8.52	116.89	120.30
2	2	2850	A	C2-N3-C4	8.52	114.86	110.60
2	2	14	C	C5-C6-N1	8.52	125.26	121.00
2	2	2491	C	C5-C6-N1	8.52	125.26	121.00
2	2	2349	A	N1-C2-N3	-8.50	125.05	129.30
8	8	126	C	C5-C6-N1	8.50	125.25	121.00
2	2	289	C	C6-N1-C2	-8.50	116.90	120.30
2	2	1469	C	C6-N1-C2	-8.49	116.90	120.30
2	2	4505	C	C2-N1-C1'	8.49	128.15	118.80
2	2	2073	C	C6-N1-C2	-8.49	116.90	120.30
8	8	96	C	N1-C2-O2	8.48	123.99	118.90
2	2	1731	C	C5-C6-N1	8.48	125.24	121.00
2	2	4215	C	N3-C2-O2	-8.48	115.97	121.90
5	5	24	C	C6-N1-C2	-8.47	116.91	120.30
2	2	1726	U	N1-C2-O2	8.47	128.73	122.80
2	2	2403	A	N1-C2-N3	-8.47	125.07	129.30
2	2	1847	C	C6-N1-C2	-8.46	116.91	120.30
8	8	28	C	C6-N1-C2	-8.46	116.92	120.30
8	8	64	U	N1-C2-O2	8.46	128.72	122.80
2	2	100	C	C6-N1-C1'	-8.46	110.65	120.80
2	2	1621	A	N1-C2-N3	-8.46	125.07	129.30
2	2	1921	C	N1-C2-O2	8.46	123.97	118.90
2	2	1320	U	N1-C2-O2	8.46	128.72	122.80
2	2	2729	C	C5-C6-N1	8.45	125.23	121.00
2	2	1077	C	C6-N1-C2	-8.45	116.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3856	A	N1-C2-N3	-8.45	125.08	129.30
8	8	51	U	N3-C2-O2	-8.45	116.29	122.20
2	2	4921	C	N1-C2-O2	8.45	123.97	118.90
2	2	4958	C	N1-C2-O2	8.44	123.97	118.90
8	8	111	U	C2-N1-C1'	8.44	127.83	117.70
2	2	4171	C	C6-N1-C2	-8.44	116.92	120.30
2	2	4996	C	C5-C6-N1	8.43	125.22	121.00
2	2	5008	C	C6-N1-C2	-8.43	116.93	120.30
2	2	367	C	C6-N1-C2	-8.43	116.93	120.30
2	2	663	G	C4-C5-N7	8.42	114.17	110.80
2	2	4532	U	N1-C2-O2	8.42	128.70	122.80
2	2	4958	C	C6-N1-C2	-8.42	116.93	120.30
2	2	1599	A	C2-N3-C4	8.42	114.81	110.60
2	2	1097	C	C6-N1-C2	-8.41	116.94	120.30
2	2	1566	C	C6-N1-C2	-8.41	116.94	120.30
2	2	3863	C	C5-C6-N1	8.41	125.21	121.00
2	2	178	C	C6-N1-C2	-8.41	116.94	120.30
2	2	1352	C	C5-C6-N1	8.40	125.20	121.00
2	2	1792	U	N3-C2-O2	-8.40	116.32	122.20
5	5	26	C	C6-N1-C2	-8.40	116.94	120.30
2	2	1503	A	N1-C2-N3	-8.39	125.11	129.30
2	2	3693	U	N1-C2-O2	8.39	128.68	122.80
2	2	4614	G	C5-C6-O6	8.39	133.63	128.60
8	8	99	U	N1-C2-O2	8.39	128.67	122.80
8	8	51	U	N1-C2-O2	8.38	128.67	122.80
2	2	3693	U	N3-C2-O2	-8.38	116.34	122.20
2	2	2560	C	N1-C2-O2	8.37	123.92	118.90
2	2	98	A	N1-C2-N3	-8.36	125.12	129.30
2	2	2074	C	C6-N1-C2	-8.36	116.95	120.30
2	2	4308	C	N1-C2-O2	8.36	123.92	118.90
2	2	4662	C	N3-C2-O2	-8.36	116.05	121.90
2	2	2255	C	N3-C2-O2	-8.35	116.06	121.90
2	2	2683	C	C6-N1-C2	-8.34	116.96	120.30
2	2	4709	U	C2-N1-C1'	8.34	127.71	117.70
2	2	4278	C	C6-N1-C2	-8.34	116.96	120.30
2	2	3855	C	C6-N1-C2	-8.34	116.97	120.30
2	2	2791	C	C6-N1-C2	-8.34	116.97	120.30
2	2	4775	C	N3-C2-O2	-8.34	116.06	121.90
2	2	2262	G	N3-C4-C5	-8.33	124.44	128.60
2	2	4140	C	C6-N1-C2	-8.33	116.97	120.30
2	2	663	G	N7-C8-N9	8.32	117.26	113.10
2	2	2528	G	C4-N9-C1'	8.32	137.31	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1093	C	C6-N1-C2	-8.32	116.97	120.30
2	2	2710	C	N3-C2-O2	-8.31	116.08	121.90
2	2	4258	C	C5-C6-N1	8.31	125.16	121.00
2	2	5004	C	C5-C6-N1	8.30	125.15	121.00
2	2	1535	C	C5-C6-N1	8.30	125.15	121.00
2	2	1816	C	C5-C6-N1	8.30	125.15	121.00
2	2	2022	C	N3-C2-O2	-8.30	116.09	121.90
2	2	76	A	N1-C2-N3	-8.29	125.15	129.30
2	2	419	A	N1-C2-N3	-8.29	125.16	129.30
2	2	4928	C	C2-N1-C1'	8.29	127.92	118.80
2	2	49	U	N3-C2-O2	-8.28	116.40	122.20
2	2	9	C	C5-C6-N1	8.28	125.14	121.00
2	2	175	C	C6-N1-C2	-8.28	116.99	120.30
8	8	32	C	C6-N1-C2	-8.28	116.99	120.30
5	5	22	A	C2-N3-C4	8.28	114.74	110.60
2	2	2806	A	N1-C2-N3	-8.27	125.17	129.30
2	2	3636	C	C5-C6-N1	8.27	125.13	121.00
2	2	50	C	C6-N1-C2	-8.26	117.00	120.30
2	2	80	C	C6-N1-C2	-8.26	117.00	120.30
2	2	1458	C	N3-C2-O2	-8.26	116.12	121.90
2	2	3826	C	C6-N1-C2	-8.25	117.00	120.30
2	2	115	C	C6-N1-C2	-8.25	117.00	120.30
8	8	101	C	N1-C2-O2	8.25	123.85	118.90
2	2	27	C	C6-N1-C2	-8.24	117.00	120.30
2	2	1402	C	N1-C2-O2	8.24	123.85	118.90
2	2	2094	G	C2-N3-C4	8.24	116.02	111.90
5	5	76	U	N3-C2-O2	-8.24	116.43	122.20
2	2	2627	C	C2-N1-C1'	8.24	127.87	118.80
2	2	2716	C	C6-N1-C2	-8.24	117.00	120.30
2	2	4341	C	N1-C2-O2	8.24	123.84	118.90
2	2	2404	A	C2-N3-C4	8.23	114.72	110.60
2	2	1541	C	C6-N1-C2	-8.23	117.01	120.30
2	2	4674	C	C6-N1-C2	-8.23	117.01	120.30
2	2	347	A	N1-C2-N3	-8.23	125.19	129.30
2	2	4278	C	C5-C6-N1	8.23	125.11	121.00
2	2	4945	G	C6-C5-N7	-8.23	125.46	130.40
2	2	1847	C	C5-C6-N1	8.22	125.11	121.00
2	2	2890	C	C6-N1-C2	-8.22	117.01	120.30
2	2	1668	A	N1-C2-N3	-8.22	125.19	129.30
8	8	103	A	C2-N3-C4	8.21	114.71	110.60
2	2	204	U	N3-C2-O2	-8.21	116.45	122.20
5	5	4	U	N3-C2-O2	-8.21	116.45	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1859	C	C2-N1-C1'	8.21	127.83	118.80
2	2	2561	C	C6-N1-C2	-8.21	117.02	120.30
2	2	2760	G	P-O3'-C3'	8.21	129.55	119.70
2	2	4771	C	C6-N1-C2	-8.21	117.02	120.30
2	2	385	A	N1-C2-N3	-8.21	125.20	129.30
2	2	59	A	N1-C2-N3	-8.20	125.20	129.30
2	2	360	A	N1-C2-N3	-8.20	125.20	129.30
2	2	1579	C	C5-C6-N1	8.20	125.10	121.00
2	2	3696	C	N1-C2-O2	8.20	123.82	118.90
2	2	1821	G	N3-C4-C5	-8.20	124.50	128.60
2	2	1508	A	N1-C2-N3	-8.20	125.20	129.30
8	8	32	C	N1-C2-O2	8.20	123.82	118.90
2	2	1340	C	C6-N1-C2	-8.19	117.02	120.30
2	2	4714	C	N1-C2-O2	8.19	123.81	118.90
2	2	4667	C	C5-C6-N1	8.19	125.09	121.00
2	2	4672	A	N1-C2-N3	-8.19	125.21	129.30
2	2	1809	C	C6-N1-C2	-8.18	117.03	120.30
5	5	44	C	N1-C2-O2	8.18	123.81	118.90
2	2	1623	A	N1-C2-N3	-8.18	125.21	129.30
2	2	2094	G	N3-C4-N9	8.18	130.91	126.00
2	2	3748	A	N1-C2-N3	-8.18	125.21	129.30
2	2	65	A	N1-C2-N3	-8.18	125.21	129.30
8	8	59	A	N1-C2-N3	-8.18	125.21	129.30
2	2	3646	A	N1-C2-N3	-8.17	125.21	129.30
2	2	274	C	C6-N1-C2	-8.17	117.03	120.30
2	2	1308	C	C6-N1-C2	-8.17	117.03	120.30
2	2	1720	C	N1-C2-O2	8.16	123.80	118.90
2	2	2035	C	C5-C6-N1	8.16	125.08	121.00
2	2	4476	C	C2-N1-C1'	8.16	127.78	118.80
33	Z	28	LEU	CA-CB-CG	8.16	134.07	115.30
2	2	1913	C	C6-N1-C2	-8.16	117.04	120.30
2	2	472	C	C6-N1-C2	-8.15	117.04	120.30
2	2	1093	C	C5-C6-N1	8.15	125.08	121.00
2	2	3685	C	C6-N1-C2	-8.15	117.04	120.30
2	2	209	U	C2-N1-C1'	8.15	127.48	117.70
2	2	2653	C	C5-C6-N1	8.15	125.07	121.00
8	8	37	A	N1-C2-N3	-8.15	125.23	129.30
2	2	2872	C	C6-N1-C2	-8.14	117.04	120.30
2	2	372	A	N1-C2-N3	-8.14	125.23	129.30
2	2	1310	C	C5-C6-N1	8.14	125.07	121.00
2	2	1439	C	C6-N1-C2	-8.14	117.04	120.30
2	2	4286	C	C6-N1-C2	-8.14	117.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	43	U	N3-C2-O2	-8.14	116.50	122.20
2	2	279	A	N1-C2-N3	-8.13	125.23	129.30
2	2	4730	C	C5-C6-N1	8.13	125.06	121.00
2	2	4233	A	N1-C2-N3	-8.13	125.23	129.30
2	2	2598	A	C2-N3-C4	8.13	114.66	110.60
2	2	1216	C	N1-C2-O2	8.13	123.78	118.90
2	2	1097	C	N1-C2-O2	8.12	123.77	118.90
2	2	1320	U	N3-C2-O2	-8.12	116.52	122.20
2	2	1875	C	C6-N1-C2	-8.12	117.05	120.30
2	2	3926	C	C5-C6-N1	8.12	125.06	121.00
2	2	436	C	N1-C2-O2	8.12	123.77	118.90
2	2	1309	C	C5-C6-N1	8.12	125.06	121.00
2	2	2337	C	C5-C6-N1	8.12	125.06	121.00
5	5	76	U	N1-C2-O2	8.12	128.48	122.80
2	2	383	A	N1-C2-N3	-8.12	125.24	129.30
2	2	2593	C	C5-C6-N1	8.11	125.06	121.00
2	2	4426	C	N1-C2-O2	8.12	123.77	118.90
2	2	4990	C	C6-N1-C2	-8.11	117.05	120.30
2	2	208	A	N1-C2-N3	-8.11	125.24	129.30
2	2	4453	C	N3-C2-O2	-8.11	116.22	121.90
2	2	1893	C	N1-C2-O2	8.11	123.76	118.90
2	2	4102	C	N1-C2-O2	8.10	123.76	118.90
2	2	3910	C	C6-N1-C2	-8.10	117.06	120.30
2	2	4766	C	C5-C6-N1	8.10	125.05	121.00
2	2	67	C	C6-N1-C2	-8.10	117.06	120.30
2	2	4304	A	N1-C2-N3	-8.09	125.25	129.30
2	2	5043	A	N1-C2-N3	-8.09	125.25	129.30
2	2	1915	C	N1-C2-O2	8.09	123.75	118.90
2	2	516	C	C6-N1-C1'	-8.09	111.09	120.80
2	2	4327	C	C6-N1-C2	-8.09	117.06	120.30
8	8	1	C	C6-N1-C2	-8.09	117.06	120.30
2	2	1906	U	N1-C2-O2	8.09	128.46	122.80
2	2	1191	C	N1-C2-O2	8.08	123.75	118.90
5	5	39	C	C5-C6-N1	8.08	125.04	121.00
2	2	2860	C	C6-N1-C2	-8.07	117.07	120.30
2	2	4500	U	N3-C2-O2	-8.07	116.55	122.20
2	2	195	C	C5-C6-N1	8.07	125.04	121.00
2	2	4921	C	C5-C6-N1	8.07	125.04	121.00
2	2	1386	C	C5-C6-N1	8.07	125.03	121.00
2	2	4958	C	C2-N1-C1'	8.06	127.67	118.80
2	2	663	G	C6-C5-N7	-8.06	125.56	130.40
2	2	3912	U	N3-C2-O2	-8.06	116.56	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	5060	A	N1-C2-N3	-8.06	125.27	129.30
2	2	317	A	N1-C2-N3	-8.06	125.27	129.30
2	2	1197	C	C6-N1-C2	-8.06	117.08	120.30
2	2	2325	C	C6-N1-C2	-8.06	117.08	120.30
8	8	54	C	N1-C2-O2	8.06	123.73	118.90
2	2	2497	C	N1-C2-O2	8.05	123.73	118.90
2	2	44	A	N1-C2-N3	-8.05	125.27	129.30
2	2	1437	C	C6-N1-C2	-8.05	117.08	120.30
2	2	4313	A	N1-C2-N3	-8.05	125.28	129.30
2	2	1687	U	N1-C2-O2	8.05	128.43	122.80
2	2	1850	A	N1-C2-N3	-8.04	125.28	129.30
2	2	3862	A	N1-C2-N3	-8.04	125.28	129.30
2	2	4701	A	N1-C2-N3	-8.04	125.28	129.30
2	2	39	A	N1-C2-N3	-8.04	125.28	129.30
2	2	1720	C	C5-C6-N1	8.04	125.02	121.00
2	2	2697	A	N1-C2-N3	-8.04	125.28	129.30
2	2	4504	C	N1-C2-O2	8.04	123.72	118.90
2	2	657	C	N1-C2-O2	8.03	123.72	118.90
2	2	1193	C	C6-N1-C2	-8.03	117.09	120.30
2	2	1276	C	C5-C6-N1	8.03	125.01	121.00
2	2	5002	U	N3-C2-O2	-8.03	116.58	122.20
2	2	1417	C	N1-C2-O2	8.02	123.71	118.90
2	2	3911	C	C6-N1-C2	-8.02	117.09	120.30
2	2	4696	C	N1-C2-O2	8.02	123.71	118.90
2	2	683	C	C6-N1-C2	-8.01	117.09	120.30
2	2	925	C	C5-C6-N1	8.01	125.01	121.00
2	2	1420	A	C2-N3-C4	8.01	114.61	110.60
2	2	2037	C	C6-N1-C2	-8.01	117.09	120.30
2	2	4387	C	N1-C2-O2	8.01	123.71	118.90
2	2	1662	C	C6-N1-C2	-8.01	117.10	120.30
2	2	2282	A	N1-C2-N3	-8.01	125.30	129.30
8	8	101	C	C5-C6-N1	8.01	125.00	121.00
2	2	4887	C	C5-C6-N1	8.00	125.00	121.00
2	2	499	G	N3-C4-N9	8.00	130.80	126.00
5	5	28	C	N3-C2-O2	-8.00	116.30	121.90
2	2	4233	A	C2-N3-C4	7.99	114.60	110.60
2	2	1521	C	C6-N1-C2	-7.99	117.10	120.30
2	2	1333	A	N1-C2-N3	-7.99	125.31	129.30
2	2	4299	U	N3-C2-O2	-7.99	116.61	122.20
2	2	4341	C	N3-C2-O2	-7.98	116.31	121.90
2	2	1344	C	C5-C6-N1	7.98	124.99	121.00
2	2	418	A	N1-C2-N3	-7.98	125.31	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1650	A	N1-C2-N3	-7.98	125.31	129.30
2	2	1695	U	N3-C2-O2	-7.97	116.62	122.20
2	2	1289	C	N1-C2-O2	7.97	123.68	118.90
2	2	2532	C	C6-N1-C2	-7.97	117.11	120.30
2	2	2908	U	N3-C2-O2	-7.97	116.62	122.20
2	2	2268	A	N1-C2-N3	-7.97	125.32	129.30
8	8	62	A	N1-C2-N3	-7.97	125.32	129.30
2	2	941	C	C6-N1-C2	-7.96	117.11	120.30
2	2	2072	C	C6-N1-C2	-7.96	117.11	120.30
2	2	1929	A	N1-C2-N3	-7.96	125.32	129.30
2	2	3838	U	N3-C2-O2	-7.96	116.63	122.20
2	2	3860	A	N1-C2-N3	-7.96	125.32	129.30
2	2	1467	C	C5-C6-N1	7.96	124.98	121.00
2	2	3824	A	N1-C2-N3	-7.96	125.32	129.30
2	2	306	A	N1-C2-N3	-7.96	125.32	129.30
2	2	914	U	P-O3'-C3'	7.96	129.25	119.70
2	2	4302	U	N1-C2-O2	7.96	128.37	122.80
8	8	54	C	C5-C6-N1	7.96	124.98	121.00
2	2	2094	G	C4-N9-C1'	7.96	136.84	126.50
2	2	4471	U	N1-C2-O2	7.96	128.37	122.80
2	2	2062	C	C6-N1-C2	-7.95	117.12	120.30
2	2	436	C	C6-N1-C2	-7.94	117.12	120.30
2	2	4708	A	N1-C2-N3	-7.94	125.33	129.30
2	2	4945	G	N9-C4-C5	-7.94	102.22	105.40
2	2	198	A	N1-C2-N3	-7.94	125.33	129.30
2	2	1602	U	N3-C2-O2	-7.93	116.65	122.20
2	2	1832	C	N1-C2-O2	7.93	123.66	118.90
2	2	2818	C	C6-N1-C2	-7.93	117.13	120.30
2	2	4613	C	N1-C2-O2	7.92	123.66	118.90
2	2	1566	C	C5-C6-N1	7.92	124.96	121.00
2	2	1578	U	N3-C2-O2	-7.92	116.66	122.20
2	2	1837	A	N1-C2-N3	-7.92	125.34	129.30
2	2	33	A	N1-C2-N3	-7.91	125.34	129.30
2	2	1674	C	C5-C6-N1	7.91	124.95	121.00
2	2	96	U	N1-C2-O2	7.91	128.34	122.80
2	2	1668	A	C2-N3-C4	7.91	114.55	110.60
2	2	1969	G	C5-C6-O6	7.90	133.34	128.60
2	2	17	A	N1-C2-N3	-7.90	125.35	129.30
2	2	1310	C	C6-N1-C2	-7.90	117.14	120.30
2	2	3863	C	C6-N1-C2	-7.90	117.14	120.30
2	2	1395	U	C6-N1-C2	-7.90	116.26	121.00
2	2	2500	U	N3-C2-O2	-7.89	116.67	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4286	C	C5-C6-N1	7.89	124.95	121.00
2	2	4289	U	N1-C2-O2	7.89	128.32	122.80
2	2	108	A	N1-C2-N3	-7.89	125.36	129.30
2	2	1192	C	N3-C2-O2	-7.88	116.38	121.90
2	2	4476	C	N3-C2-O2	-7.88	116.38	121.90
2	2	1206	C	C6-N1-C2	-7.88	117.15	120.30
2	2	4162	C	N1-C2-O2	7.88	123.63	118.90
2	2	2683	C	C5-C6-N1	7.88	124.94	121.00
2	2	335	A	N1-C2-N3	-7.87	125.36	129.30
2	2	2627	C	N1-C2-O2	7.87	123.62	118.90
2	2	3622	C	N1-C2-O2	7.87	123.62	118.90
2	2	2263	A	N1-C2-N3	-7.87	125.37	129.30
2	2	1897	A	N1-C2-N3	-7.87	125.37	129.30
2	2	366	A	N1-C2-N3	-7.86	125.37	129.30
8	8	50	C	C6-N1-C2	-7.86	117.16	120.30
2	2	3911	C	C5-C6-N1	7.86	124.93	121.00
2	2	2749	C	C6-N1-C2	-7.86	117.16	120.30
2	2	4695	C	N3-C2-O2	-7.85	116.40	121.90
2	2	289	C	C5-C6-N1	7.85	124.93	121.00
2	2	4972	U	N1-C2-O2	7.85	128.30	122.80
2	2	1707	C	C6-N1-C2	-7.85	117.16	120.30
2	2	1535	C	C6-N1-C2	-7.85	117.16	120.30
2	2	4685	U	N3-C2-O2	-7.84	116.71	122.20
2	2	2685	C	C6-N1-C2	-7.84	117.17	120.30
2	2	3621	A	N1-C2-N3	-7.84	125.38	129.30
2	2	2837	U	N3-C2-O2	-7.83	116.72	122.20
2	2	34	A	N1-C2-N3	-7.83	125.38	129.30
2	2	2483	G	N3-C4-N9	7.83	130.70	126.00
2	2	362	A	N1-C2-N3	-7.83	125.39	129.30
2	2	4155	C	N1-C2-O2	7.83	123.60	118.90
2	2	2616	C	C6-N1-C2	-7.83	117.17	120.30
2	2	2894	A	N1-C2-N3	-7.83	125.39	129.30
2	2	4712	C	C6-N1-C2	-7.83	117.17	120.30
2	2	4300	U	N3-C2-O2	-7.82	116.72	122.20
2	2	4921	C	C2-N1-C1'	7.82	127.41	118.80
2	2	1241	C	N3-C2-O2	-7.82	116.43	121.90
2	2	1308	C	C5-C6-N1	7.82	124.91	121.00
2	2	4662	C	N1-C2-O2	7.82	123.59	118.90
2	2	2835	A	N1-C2-N3	-7.81	125.39	129.30
2	2	2583	C	C6-N1-C2	-7.81	117.18	120.30
2	2	672	C	C2-N1-C1'	7.80	127.38	118.80
2	2	4775	C	C6-N1-C2	-7.80	117.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	204	U	N1-C2-O2	7.80	128.26	122.80
2	2	1601	A	N1-C2-N3	-7.80	125.40	129.30
2	2	2395	A	N1-C2-N3	-7.80	125.40	129.30
2	2	2819	U	N3-C2-O2	-7.80	116.74	122.20
2	2	4336	A	N1-C2-N3	-7.80	125.40	129.30
2	2	4376	A	N1-C2-N3	-7.80	125.40	129.30
2	2	56	A	N1-C2-N3	-7.80	125.40	129.30
2	2	274	C	C5-C6-N1	7.80	124.90	121.00
2	2	2895	A	N1-C2-N3	-7.80	125.40	129.30
2	2	2472	A	N1-C2-N3	-7.80	125.40	129.30
2	2	1402	C	N3-C2-O2	-7.80	116.44	121.90
2	2	23	C	C6-N1-C2	-7.79	117.18	120.30
2	2	1665	C	C6-N1-C2	-7.79	117.18	120.30
2	2	345	C	C6-N1-C2	-7.79	117.18	120.30
2	2	376	A	N1-C2-N3	-7.79	125.40	129.30
2	2	972	C	C5-C6-N1	7.79	124.90	121.00
2	2	1888	A	N1-C2-N3	-7.79	125.40	129.30
2	2	1486	C	C6-N1-C2	-7.79	117.18	120.30
2	2	2908	U	N1-C2-O2	7.79	128.25	122.80
2	2	3652	A	N1-C2-N3	-7.79	125.41	129.30
2	2	2445	C	C6-N1-C2	-7.79	117.19	120.30
2	2	2845	A	N1-C2-N3	-7.79	125.41	129.30
2	2	3635	A	N1-C2-N3	-7.79	125.41	129.30
2	2	4594	U	N1-C2-O2	7.79	128.25	122.80
2	2	2532	C	C5-C6-N1	7.78	124.89	121.00
2	2	4664	A	N1-C2-N3	-7.78	125.41	129.30
20	L	46	ASP	CB-CG-OD1	7.78	125.30	118.30
2	2	345	C	C5-C6-N1	7.78	124.89	121.00
2	2	2483	G	N3-C4-C5	-7.78	124.71	128.60
2	2	679	C	C6-N1-C2	-7.78	117.19	120.30
5	5	14	C	C6-N1-C2	-7.78	117.19	120.30
2	2	349	A	N1-C2-N3	-7.77	125.41	129.30
2	2	1388	A	N1-C2-N3	-7.77	125.42	129.30
2	2	2604	C	C6-N1-C2	-7.77	117.19	120.30
2	2	1439	C	C5-C6-N1	7.77	124.88	121.00
2	2	3648	A	N1-C2-N3	-7.77	125.42	129.30
2	2	1527	A	N1-C2-N3	-7.76	125.42	129.30
2	2	471	A	N1-C2-N3	-7.76	125.42	129.30
2	2	1628	C	C5-C6-N1	7.76	124.88	121.00
2	2	4565	C	C6-N1-C2	-7.76	117.20	120.30
2	2	499	G	C8-N9-C1'	-7.76	116.92	127.00
8	8	140	C	C5-C6-N1	7.76	124.88	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1809	C	C5-C6-N1	7.76	124.88	121.00
2	2	712	C	C5-C6-N1	7.75	124.88	121.00
2	2	1585	C	C6-N1-C2	-7.75	117.20	120.30
2	2	338	A	N1-C2-N3	-7.75	125.42	129.30
2	2	709	C	C6-N1-C2	-7.75	117.20	120.30
2	2	1603	C	C6-N1-C2	-7.75	117.20	120.30
2	2	2418	A	N1-C2-N3	-7.75	125.43	129.30
2	2	1663	C	C6-N1-C2	-7.75	117.20	120.30
2	2	4237	C	C5-C6-N1	7.74	124.87	121.00
2	2	15	A	N1-C2-N3	-7.74	125.43	129.30
2	2	5051	C	C6-N1-C2	-7.74	117.20	120.30
2	2	4308	C	N3-C2-O2	-7.73	116.49	121.90
2	2	454	U	C2-N1-C1'	7.73	126.98	117.70
2	2	4626	A	N1-C2-N3	-7.73	125.43	129.30
2	2	4700	A	C2-N3-C4	7.73	114.47	110.60
2	2	281	U	N1-C2-O2	7.73	128.21	122.80
2	2	1086	C	C6-N1-C2	-7.73	117.21	120.30
2	2	2544	G	N3-C4-N9	7.73	130.64	126.00
2	2	2745	A	N1-C2-N3	-7.73	125.44	129.30
2	2	4738	C	C5-C6-N1	7.73	124.86	121.00
2	2	4342	C	C5-C6-N1	7.72	124.86	121.00
2	2	2615	C	C6-N1-C2	-7.72	117.21	120.30
2	2	88	A	N1-C2-N3	-7.72	125.44	129.30
2	2	322	C	C5-C6-N1	7.72	124.86	121.00
2	2	1686	C	C5-C6-N1	7.72	124.86	121.00
2	2	2033	A	N1-C2-N3	-7.72	125.44	129.30
2	2	1607	C	N3-C2-O2	-7.72	116.50	121.90
2	2	2073	C	C5-C6-N1	7.72	124.86	121.00
2	2	2840	A	N1-C2-N3	-7.71	125.44	129.30
2	2	4324	A	N1-C2-N3	-7.71	125.44	129.30
2	2	67	C	C5-C6-N1	7.71	124.86	121.00
2	2	228	C	C6-N1-C2	-7.71	117.22	120.30
2	2	972	C	N3-C2-O2	-7.71	116.50	121.90
2	2	4379	A	N1-C2-N3	-7.71	125.44	129.30
2	2	336	A	N1-C2-N3	-7.71	125.44	129.30
2	2	1387	A	N1-C2-N3	-7.71	125.44	129.30
2	2	2615	C	N1-C2-O2	7.71	123.53	118.90
2	2	4261	C	C6-N1-C2	-7.71	117.22	120.30
2	2	4342	C	N1-C2-O2	7.71	123.53	118.90
2	2	4612	C	C6-N1-C2	-7.71	117.22	120.30
2	2	4601	U	C2-N1-C1'	7.71	126.95	117.70
2	2	3688	U	N3-C2-O2	-7.70	116.81	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	112	C	C2-N1-C1'	7.70	127.27	118.80
2	2	499	G	N3-C4-C5	-7.70	124.75	128.60
2	2	1518	A	N1-C2-N3	-7.70	125.45	129.30
2	2	5035	U	N3-C2-O2	-7.70	116.81	122.20
2	2	4484	A	N1-C2-N3	-7.69	125.45	129.30
2	2	4563	U	N3-C2-O2	-7.69	116.82	122.20
2	2	1702	C	C2-N1-C1'	7.68	127.25	118.80
2	2	4110	C	C6-N1-C2	-7.68	117.23	120.30
2	2	220	C	C5-C6-N1	7.68	124.84	121.00
2	2	307	A	N1-C2-N3	-7.68	125.46	129.30
2	2	1049	C	C6-N1-C2	-7.68	117.23	120.30
2	2	4339	A	N1-C2-N3	-7.68	125.46	129.30
2	2	4980	C	C5-C6-N1	7.68	124.84	121.00
2	2	5016	A	O4'-C1'-N9	7.68	114.34	108.20
2	2	1405	C	N1-C2-O2	7.68	123.51	118.90
2	2	2257	C	C2-N1-C1'	7.68	127.24	118.80
2	2	4268	A	N1-C2-N3	-7.67	125.46	129.30
2	2	2787	A	N1-C2-N3	-7.67	125.46	129.30
2	2	2817	C	C6-N1-C2	-7.67	117.23	120.30
4	4	230	LEU	CA-CB-CG	7.67	132.94	115.30
2	2	2107	C	N1-C2-O2	7.66	123.50	118.90
2	2	467	U	C6-N1-C1'	-7.66	110.47	121.20
2	2	1801	A	N1-C2-N3	-7.66	125.47	129.30
2	2	2107	C	C6-N1-C2	-7.66	117.24	120.30
2	2	4964	C	C6-N1-C2	-7.66	117.24	120.30
2	2	5008	C	C5-C6-N1	7.66	124.83	121.00
2	2	1367	C	N1-C2-O2	7.66	123.50	118.90
2	2	3598	C	C6-N1-C2	-7.66	117.24	120.30
2	2	421	C	C6-N1-C2	-7.65	117.24	120.30
2	2	4281	A	C5-N7-C8	-7.65	100.07	103.90
8	8	116	C	C6-N1-C2	-7.65	117.24	120.30
2	2	4596	C	N1-C2-O2	7.65	123.49	118.90
8	8	101	C	C6-N1-C2	-7.65	117.24	120.30
2	2	3894	A	N1-C2-N3	-7.64	125.48	129.30
2	2	1577	G	N1-C6-O6	-7.64	115.32	119.90
2	2	1915	C	N3-C2-O2	-7.64	116.55	121.90
2	2	4506	C	N1-C2-O2	7.64	123.48	118.90
2	2	1381	U	N3-C2-O2	-7.63	116.86	122.20
2	2	2031	C	C6-N1-C2	-7.63	117.25	120.30
2	2	4215	C	C6-N1-C2	-7.63	117.25	120.30
8	8	81	C	C6-N1-C2	-7.63	117.25	120.30
2	2	985	C	C5-C6-N1	7.62	124.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2262	G	C8-N9-C1'	-7.62	117.09	127.00
5	5	6	C	C6-N1-C2	-7.62	117.25	120.30
5	5	4	U	N1-C2-O2	7.62	128.13	122.80
2	2	337	U	N3-C2-O2	-7.62	116.87	122.20
2	2	4703	U	N1-C2-O2	7.62	128.13	122.80
8	8	9	A	N1-C2-N3	-7.61	125.49	129.30
2	2	1607	C	N1-C2-O2	7.61	123.47	118.90
2	2	4553	A	N1-C2-N3	-7.61	125.50	129.30
2	2	115	C	C6-N1-C1'	-7.61	111.67	120.80
2	2	2071	A	C2-N3-C4	7.61	114.40	110.60
2	2	365	U	N3-C2-O2	-7.61	116.88	122.20
2	2	2499	C	N3-C2-O2	-7.61	116.58	121.90
2	2	1921	C	C6-N1-C2	-7.60	117.26	120.30
2	2	3936	A	N1-C2-N3	-7.60	125.50	129.30
2	2	946	C	C6-N1-C2	-7.60	117.26	120.30
2	2	3919	C	C5-C6-N1	7.60	124.80	121.00
2	2	498	C	N3-C2-O2	-7.59	116.58	121.90
2	2	4656	A	N1-C2-N3	-7.59	125.50	129.30
2	2	4714	C	C5-C6-N1	7.59	124.80	121.00
2	2	716	C	C5-C6-N1	7.59	124.80	121.00
2	2	4682	U	C2-N1-C1'	7.59	126.81	117.70
8	8	20	A	N1-C2-N3	-7.59	125.50	129.30
2	2	661	C	C6-N1-C2	-7.59	117.26	120.30
2	2	648	G	N3-C4-N9	7.59	130.55	126.00
2	2	4979	A	N1-C2-N3	-7.59	125.51	129.30
5	5	39	C	C2-N3-C4	7.59	123.69	119.90
2	2	2695	A	N1-C2-N3	-7.59	125.51	129.30
2	2	2033	A	P-O3'-C3'	7.58	128.80	119.70
2	2	386	A	N1-C2-N3	-7.58	125.51	129.30
2	2	395	A	N1-C2-N3	-7.58	125.51	129.30
2	2	3928	A	N1-C2-N3	-7.58	125.51	129.30
2	2	733	A	N1-C2-N3	-7.58	125.51	129.30
2	2	1397	A	N1-C2-N3	-7.58	125.51	129.30
5	5	39	C	C2-N1-C1'	7.58	127.14	118.80
2	2	271	C	C5-C6-N1	7.58	124.79	121.00
2	2	1494	U	N1-C2-O2	7.57	128.10	122.80
2	2	2338	C	C6-N1-C2	-7.57	117.27	120.30
2	2	2825	A	N1-C2-N3	-7.57	125.52	129.30
2	2	2527	A	N1-C2-N3	-7.57	125.52	129.30
2	2	23	C	C5-C6-N1	7.57	124.78	121.00
2	2	163	A	N1-C2-N3	-7.57	125.52	129.30
2	2	2062	C	N1-C2-O2	7.57	123.44	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4258	C	C6-N1-C2	-7.57	117.27	120.30
2	2	1735	U	N3-C2-O2	-7.57	116.90	122.20
2	2	2303	C	C6-N1-C2	-7.57	117.27	120.30
2	2	1447	C	C5-C6-N1	7.56	124.78	121.00
2	2	39	A	C2-N3-C4	7.56	114.38	110.60
2	2	1330	A	N1-C2-N3	-7.56	125.52	129.30
2	2	2594	C	C6-N1-C2	-7.56	117.28	120.30
2	2	4764	A	C4-C5-C6	-7.56	113.22	117.00
2	2	1731	C	N1-C2-O2	7.56	123.44	118.90
2	2	3717	A	N1-C2-N3	-7.56	125.52	129.30
2	2	334	A	N1-C2-N3	-7.55	125.52	129.30
2	2	1050	C	C6-N1-C2	-7.55	117.28	120.30
2	2	1963	C	C6-N1-C2	-7.55	117.28	120.30
2	2	1870	C	C6-N1-C2	-7.55	117.28	120.30
2	2	4393	G	C6-N1-C2	7.55	129.63	125.10
2	2	2513	A	N1-C2-N3	-7.55	125.53	129.30
2	2	4546	A	N1-C2-N3	-7.55	125.53	129.30
2	2	2528	G	N3-C4-N9	7.55	130.53	126.00
2	2	4206	C	N1-C2-O2	7.55	123.43	118.90
2	2	123	C	C6-N1-C2	-7.54	117.28	120.30
2	2	152	U	N3-C2-O2	-7.54	116.92	122.20
2	2	3861	A	N1-C2-N3	-7.54	125.53	129.30
2	2	2351	C	N1-C2-O2	7.54	123.42	118.90
5	5	91	C	C6-N1-C2	-7.54	117.28	120.30
2	2	672	C	C5-C6-N1	7.54	124.77	121.00
2	2	672	C	N1-C2-O2	7.54	123.42	118.90
2	2	2820	C	C5-C6-N1	7.54	124.77	121.00
2	2	4565	C	C5-C6-N1	7.54	124.77	121.00
5	5	24	C	N1-C2-O2	7.54	123.42	118.90
2	2	30	C	C6-N1-C2	-7.53	117.29	120.30
2	2	98	A	C2-N3-C4	7.53	114.37	110.60
2	2	326	C	C6-N1-C2	-7.53	117.29	120.30
2	2	2038	U	N3-C2-O2	-7.53	116.93	122.20
2	2	2382	A	N1-C2-N3	-7.53	125.53	129.30
2	2	2856	C	N3-C2-O2	-7.53	116.63	121.90
2	2	2676	A	N1-C2-N3	-7.53	125.53	129.30
2	2	656	C	C2-N1-C1'	7.53	127.08	118.80
2	2	1469	C	C5-C6-N1	7.53	124.76	121.00
2	2	1192	C	C5-C6-N1	7.53	124.76	121.00
2	2	2483	G	C4-N9-C1'	7.52	136.28	126.50
2	2	4500	U	N1-C2-O2	7.52	128.07	122.80
2	2	3849	A	N1-C2-N3	-7.52	125.54	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4467	A	N1-C2-N3	-7.52	125.54	129.30
2	2	984	C	C6-N1-C2	-7.52	117.29	120.30
2	2	4503	A	N1-C2-N3	-7.52	125.54	129.30
2	2	656	C	C5-C6-N1	7.52	124.76	121.00
8	8	82	A	N1-C2-N3	-7.52	125.54	129.30
2	2	1324	A	N1-C2-N3	-7.52	125.54	129.30
2	2	2611	A	N1-C2-N3	-7.52	125.54	129.30
2	2	49	U	N1-C2-O2	7.51	128.06	122.80
2	2	162	A	N1-C2-N3	-7.51	125.55	129.30
2	2	943	A	N1-C2-N3	-7.51	125.55	129.30
8	8	126	C	N3-C2-O2	-7.51	116.65	121.90
2	2	472	C	N1-C2-O2	7.50	123.40	118.90
2	2	504	G	C8-N9-C1'	-7.50	117.25	127.00
2	2	3845	A	N1-C2-N3	-7.50	125.55	129.30
2	2	1391	A	N1-C2-N3	-7.50	125.55	129.30
8	8	54	C	C6-N1-C2	-7.50	117.30	120.30
2	2	319	A	N1-C2-N3	-7.50	125.55	129.30
2	2	388	A	N1-C2-N3	-7.50	125.55	129.30
2	2	1907	A	N1-C2-N3	-7.50	125.55	129.30
2	2	988	C	C6-N1-C1'	-7.49	111.81	120.80
2	2	1378	C	C2-N1-C1'	7.49	127.04	118.80
2	2	2371	U	N3-C2-O2	-7.49	116.95	122.20
2	2	297	U	N3-C2-O2	-7.49	116.96	122.20
2	2	2701	U	N3-C2-O2	-7.49	116.96	122.20
2	2	30	C	N1-C2-O2	7.49	123.39	118.90
2	2	1580	C	C6-N1-C2	-7.49	117.31	120.30
2	2	123	C	C5-C6-N1	7.48	124.74	121.00
2	2	4490	C	C6-N1-C2	-7.48	117.31	120.30
2	2	4508	C	N3-C2-O2	-7.48	116.66	121.90
2	2	3631	U	N3-C2-O2	-7.48	116.96	122.20
2	2	79	C	C5-C6-N1	7.48	124.74	121.00
2	2	2428	A	N1-C2-N3	-7.48	125.56	129.30
2	2	355	A	N1-C2-N3	-7.48	125.56	129.30
2	2	1079	C	N3-C2-O2	-7.47	116.67	121.90
2	2	1695	U	N1-C2-O2	7.47	128.03	122.80
2	2	2460	A	N1-C2-N3	-7.47	125.56	129.30
2	2	2764	A	N1-C2-N3	-7.47	125.56	129.30
2	2	4340	U	N1-C2-O2	7.47	128.03	122.80
2	2	4343	U	N3-C2-O2	-7.47	116.97	122.20
2	2	1079	C	C5-C6-N1	7.46	124.73	121.00
2	2	2890	C	C5-C6-N1	7.46	124.73	121.00
2	2	3721	U	N3-C2-O2	-7.46	116.98	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	371	A	N1-C2-N3	-7.46	125.57	129.30
2	2	2031	C	N1-C2-O2	7.46	123.38	118.90
2	2	3935	C	C6-N1-C2	-7.46	117.32	120.30
2	2	4109	G	C4-N9-C1'	7.45	136.19	126.50
8	8	35	C	C5-C6-N1	7.45	124.73	121.00
2	2	101	A	N1-C2-N3	-7.45	125.58	129.30
2	2	2864	A	N1-C2-N3	-7.45	125.58	129.30
2	2	2473	A	N1-C2-N3	-7.45	125.58	129.30
2	2	2389	A	N1-C2-N3	-7.45	125.58	129.30
2	2	4886	C	N1-C2-O2	7.44	123.37	118.90
2	2	4319	C	N1-C2-O2	7.44	123.37	118.90
2	2	435	A	N1-C2-N3	-7.44	125.58	129.30
2	2	1671	U	N3-C2-O2	-7.44	116.99	122.20
2	2	259	C	C6-N1-C2	-7.44	117.33	120.30
2	2	944	A	N1-C2-N3	-7.43	125.58	129.30
2	2	2370	A	N1-C2-N3	-7.43	125.58	129.30
2	2	498	C	C5-C6-N1	7.43	124.72	121.00
2	2	2438	A	N1-C2-N3	-7.43	125.58	129.30
2	2	2532	C	N1-C2-O2	7.43	123.36	118.90
2	2	141	C	C6-N1-C2	-7.43	117.33	120.30
2	2	1184	A	C2-N3-C4	7.43	114.31	110.60
2	2	1472	C	C2-N1-C1'	7.43	126.97	118.80
2	2	4243	C	C5-C6-N1	7.43	124.71	121.00
2	2	2528	G	N3-C4-C5	-7.42	124.89	128.60
2	2	14	C	C2-N1-C1'	7.42	126.96	118.80
2	2	1076	C	C6-N1-C2	-7.42	117.33	120.30
2	2	1633	G	P-O3'-C3'	7.42	128.61	119.70
2	2	4911	A	N1-C2-N3	-7.42	125.59	129.30
2	2	4866	C	C6-N1-C2	-7.42	117.33	120.30
2	2	2867	C	N1-C2-O2	7.42	123.35	118.90
2	2	3739	C	C6-N1-C2	-7.42	117.33	120.30
2	2	2376	A	N1-C2-N3	-7.42	125.59	129.30
2	2	407	A	N1-C2-N3	-7.41	125.59	129.30
2	2	50	C	N3-C2-O2	-7.41	116.71	121.90
2	2	1665	C	C5-C6-N1	7.41	124.70	121.00
2	2	2096	G	N3-C4-N9	7.41	130.45	126.00
2	2	4957	C	C6-N1-C2	-7.41	117.34	120.30
2	2	2568	C	N3-C2-O2	-7.41	116.71	121.90
2	2	5007	A	N1-C2-N3	-7.41	125.60	129.30
2	2	427	A	N1-C2-N3	-7.41	125.60	129.30
2	2	3656	A	N1-C2-N3	-7.41	125.60	129.30
2	2	4461	C	C6-N1-C2	-7.41	117.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4088	C	C6-N1-C2	-7.40	117.34	120.30
2	2	35	U	N3-C2-O2	-7.40	117.02	122.20
2	2	2807	A	N1-C2-N3	-7.40	125.60	129.30
2	2	1245	C	C2-N1-C1'	7.40	126.94	118.80
2	2	228	C	C5-C6-N1	7.40	124.70	121.00
2	2	1079	C	C6-N1-C2	-7.40	117.34	120.30
2	2	4453	C	C6-N1-C1'	-7.40	111.92	120.80
2	2	1507	C	C6-N1-C2	-7.39	117.34	120.30
2	2	2062	C	N3-C2-O2	-7.39	116.72	121.90
2	2	3872	A	N1-C2-N3	-7.39	125.60	129.30
2	2	1367	C	C2-N1-C1'	7.39	126.93	118.80
2	2	3719	A	N1-C2-N3	-7.38	125.61	129.30
2	2	3826	C	C5-C6-N1	7.38	124.69	121.00
2	2	4325	A	N1-C2-N3	-7.38	125.61	129.30
2	2	2885	A	N1-C2-N3	-7.38	125.61	129.30
2	2	4731	G	O4'-C1'-N9	7.38	114.10	108.20
5	5	43	U	N3-C2-O2	-7.38	117.04	122.20
2	2	4669	A	N1-C2-N3	-7.38	125.61	129.30
8	8	35	C	C6-N1-C2	-7.38	117.35	120.30
2	2	3935	C	C5-C6-N1	7.37	124.69	121.00
2	2	70	A	N1-C2-N3	-7.37	125.62	129.30
2	2	1477	C	C6-N1-C2	-7.37	117.35	120.30
2	2	4621	C	C6-N1-C2	-7.37	117.35	120.30
2	2	4219	A	N1-C2-N3	-7.36	125.62	129.30
2	2	47	A	N1-C2-N3	-7.36	125.62	129.30
2	2	931	C	C6-N1-C2	-7.36	117.36	120.30
2	2	977	C	N1-C2-O2	7.36	123.31	118.90
2	2	4170	A	N1-C2-N3	-7.36	125.62	129.30
2	2	68	U	N1-C2-O2	7.35	127.95	122.80
2	2	1894	C	C6-N1-C2	-7.35	117.36	120.30
2	2	663	G	N3-C4-N9	7.35	130.41	126.00
2	2	3728	A	N1-C2-N3	-7.35	125.63	129.30
2	2	2512	A	N1-C2-N3	-7.35	125.63	129.30
2	2	4199	C	C6-N1-C2	-7.35	117.36	120.30
47	o	144	ILE	C-N-CA	7.35	140.07	121.70
2	2	4308	C	C6-N1-C2	-7.35	117.36	120.30
2	2	1558	A	N1-C2-N3	-7.34	125.63	129.30
2	2	2022	C	C5-C6-N1	7.34	124.67	121.00
2	2	963	G	C4-N9-C1'	7.34	136.04	126.50
2	2	2078	C	N1-C2-O2	7.34	123.30	118.90
2	2	3727	A	N1-C2-N3	-7.34	125.63	129.30
2	2	1616	U	N3-C2-O2	-7.34	117.06	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	974	C	C6-N1-C2	-7.34	117.37	120.30
2	2	4589	A	N1-C2-N3	-7.34	125.63	129.30
2	2	1967	A	N1-C2-N3	-7.33	125.63	129.30
2	2	4307	A	N1-C2-N3	-7.33	125.63	129.30
5	5	100	A	N1-C2-N3	-7.33	125.63	129.30
2	2	1817	U	N3-C2-O2	-7.33	117.07	122.20
2	2	1197	C	C5-C6-N1	7.33	124.67	121.00
5	5	29	C	C6-N1-C2	-7.33	117.37	120.30
2	2	81	C	C6-N1-C2	-7.33	117.37	120.30
2	2	384	A	N1-C2-N3	-7.33	125.64	129.30
2	2	4640	C	N1-C2-O2	7.33	123.30	118.90
8	8	32	C	C5-C6-N1	7.33	124.66	121.00
2	2	329	A	N1-C2-N3	-7.32	125.64	129.30
5	5	38	U	N3-C2-O2	-7.32	117.08	122.20
2	2	322	C	N3-C2-O2	-7.32	116.78	121.90
2	2	1736	A	N1-C2-N3	-7.32	125.64	129.30
2	2	3892	U	N3-C2-O2	-7.32	117.08	122.20
2	2	4913	G	P-O3'-C3'	7.32	128.48	119.70
2	2	2583	C	C5-C6-N1	7.31	124.66	121.00
8	8	141	C	C5-C6-N1	7.31	124.66	121.00
2	2	3747	A	N1-C2-N3	-7.31	125.64	129.30
2	2	1794	A	N1-C2-N3	-7.31	125.64	129.30
2	2	2561	C	N1-C2-O2	7.31	123.29	118.90
2	2	1638	A	N1-C2-N3	-7.31	125.64	129.30
2	2	1934	A	N1-C2-N3	-7.31	125.64	129.30
5	5	29	C	N1-C2-O2	7.31	123.28	118.90
2	2	1963	C	N1-C2-O2	7.31	123.28	118.90
2	2	2815	A	N1-C2-N3	-7.31	125.65	129.30
2	2	4607	A	O4'-C1'-N9	7.31	114.05	108.20
2	2	2451	A	N1-C2-N3	-7.30	125.65	129.30
2	2	3923	A	N1-C2-N3	-7.30	125.65	129.30
2	2	2536	A	N1-C2-N3	-7.30	125.65	129.30
2	2	2582	A	N1-C2-N3	-7.30	125.65	129.30
2	2	2837	U	N1-C2-O2	7.30	127.91	122.80
2	2	4205	A	N1-C2-N3	-7.30	125.65	129.30
2	2	4612	C	N1-C2-O2	7.30	123.28	118.90
2	2	2791	C	C5-C6-N1	7.30	124.65	121.00
2	2	1323	A	N1-C2-N3	-7.29	125.66	129.30
2	2	1663	C	N1-C2-O2	7.29	123.27	118.90
2	2	2844	A	N1-C2-N3	-7.29	125.66	129.30
2	2	4259	C	C6-N1-C2	-7.29	117.39	120.30
2	2	488	G	C6-C5-N7	-7.29	126.03	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1547	A	N1-C2-N3	-7.29	125.66	129.30
2	2	259	C	N1-C2-O2	7.28	123.27	118.90
2	2	1427	A	N1-C2-N3	-7.28	125.66	129.30
2	2	2381	A	N1-C2-N3	-7.28	125.66	129.30
2	2	1176	C	C6-N1-C2	-7.28	117.39	120.30
2	2	3647	A	N1-C2-N3	-7.28	125.66	129.30
2	2	455	C	C6-N1-C2	-7.27	117.39	120.30
2	2	1289	C	C6-N1-C2	-7.27	117.39	120.30
2	2	1392	A	N1-C2-N3	-7.27	125.66	129.30
2	2	2511	A	N1-C2-N3	-7.27	125.66	129.30
2	2	227	A	N1-C2-N3	-7.27	125.67	129.30
2	2	1077	C	C5-C6-N1	7.27	124.64	121.00
2	2	36	U	N3-C2-O2	-7.27	117.11	122.20
2	2	2307	A	N1-C2-N3	-7.27	125.67	129.30
2	2	3924	C	C6-N1-C2	-7.27	117.39	120.30
2	2	4885	U	N3-C2-O2	-7.27	117.11	122.20
2	2	4310	A	N1-C2-N3	-7.27	125.67	129.30
8	8	155	C	C6-N1-C2	-7.27	117.39	120.30
2	2	1381	U	N1-C2-O2	7.26	127.89	122.80
2	2	124	C	C5-C6-N1	7.26	124.63	121.00
2	2	1738	A	N1-C2-N3	-7.26	125.67	129.30
2	2	4605	A	N1-C2-N3	-7.26	125.67	129.30
2	2	4622	A	N1-C2-N3	-7.26	125.67	129.30
5	5	77	A	N1-C2-N3	-7.26	125.67	129.30
2	2	2447	U	N3-C2-O2	-7.26	117.12	122.20
2	2	377	A	N1-C2-N3	-7.26	125.67	129.30
2	2	1540	C	C6-N1-C2	-7.26	117.40	120.30
2	2	1450	C	C6-N1-C2	-7.26	117.40	120.30
2	2	2368	A	N1-C2-N3	-7.26	125.67	129.30
2	2	3871	A	N1-C2-N3	-7.26	125.67	129.30
2	2	4665	A	N1-C2-N3	-7.25	125.67	129.30
2	2	1418	C	C6-N1-C2	-7.25	117.40	120.30
2	2	1384	C	C5-C6-N1	7.25	124.62	121.00
2	2	4707	A	N1-C2-N3	-7.25	125.68	129.30
2	2	1515	A	N1-C2-N3	-7.25	125.68	129.30
2	2	2625	U	N3-C2-O2	-7.25	117.13	122.20
2	2	2641	A	N1-C2-N3	-7.25	125.68	129.30
2	2	4601	U	C6-N1-C2	-7.25	116.65	121.00
2	2	1499	C	C6-N1-C2	-7.24	117.40	120.30
8	8	40	A	N1-C2-N3	-7.24	125.68	129.30
2	2	4926	C	C2-N1-C1'	7.24	126.77	118.80
2	2	50	C	C5-C6-N1	7.24	124.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2789	A	N1-C2-N3	-7.24	125.68	129.30
2	2	2892	C	N1-C2-O2	7.24	123.24	118.90
2	2	4705	A	N1-C2-N3	-7.24	125.68	129.30
2	2	1821	G	N3-C4-N9	7.24	130.34	126.00
2	2	2303	C	N3-C2-O2	-7.24	116.83	121.90
2	2	4361	U	N3-C2-O2	-7.24	117.14	122.20
2	2	1615	C	C6-N1-C2	-7.23	117.41	120.30
2	2	1646	A	N1-C2-N3	-7.23	125.68	129.30
2	2	3838	U	N1-C2-O2	7.23	127.86	122.80
2	2	4716	C	C6-N1-C2	-7.23	117.41	120.30
8	8	104	A	N1-C2-N3	-7.23	125.69	129.30
2	2	1193	C	C5-C6-N1	7.22	124.61	121.00
2	2	2505	C	C5-C6-N1	7.22	124.61	121.00
2	2	4466	C	C6-N1-C2	-7.22	117.41	120.30
2	2	4098	A	N1-C2-N3	-7.22	125.69	129.30
2	2	4214	A	N1-C2-N3	-7.22	125.69	129.30
2	2	5042	A	N1-C2-N3	-7.22	125.69	129.30
2	2	932	A	N1-C2-N3	-7.22	125.69	129.30
2	2	947	C	C6-N1-C2	-7.22	117.41	120.30
2	2	1585	C	C5-C6-N1	7.22	124.61	121.00
8	8	107	C	C5-C6-N1	7.22	124.61	121.00
2	2	276	C	C6-N1-C2	-7.21	117.41	120.30
2	2	2072	C	C5-C6-N1	7.21	124.61	121.00
2	2	3746	A	N1-C2-N3	-7.21	125.69	129.30
2	2	3870	C	N1-C2-O2	7.21	123.23	118.90
2	2	4183	G	N3-C4-N9	7.21	130.33	126.00
2	2	1087	A	N1-C2-N3	-7.21	125.70	129.30
2	2	2051	C	C6-N1-C2	-7.21	117.42	120.30
2	2	3917	A	N1-C2-N3	-7.21	125.70	129.30
2	2	4482	U	N3-C2-O2	-7.21	117.16	122.20
2	2	328	A	N1-C2-N3	-7.20	125.70	129.30
5	5	26	C	C5-C6-N1	7.20	124.60	121.00
8	8	41	A	N1-C2-N3	-7.20	125.70	129.30
2	2	4507	A	N1-C2-N3	-7.20	125.70	129.30
2	2	1472	C	N1-C2-O2	7.20	123.22	118.90
28	U	134	LEU	CA-CB-CG	7.20	131.86	115.30
2	2	2629	C	C6-N1-C2	-7.20	117.42	120.30
2	2	5011	A	N1-C2-N3	-7.20	125.70	129.30
2	2	1354	A	N1-C2-N3	-7.20	125.70	129.30
2	2	5019	A	C4-C5-C6	-7.20	113.40	117.00
2	2	3903	A	N1-C2-N3	-7.19	125.70	129.30
2	2	80	C	C5-C6-N1	7.19	124.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3891	A	N1-C2-N3	-7.19	125.70	129.30
2	2	4314	C	N1-C2-O2	7.19	123.21	118.90
2	2	359	A	N1-C2-N3	-7.18	125.71	129.30
2	2	1085	C	C6-N1-C2	-7.18	117.43	120.30
2	2	4078	C	C6-N1-C2	-7.18	117.43	120.30
2	2	4133	C	C6-N1-C2	-7.18	117.43	120.30
2	2	2689	C	C6-N1-C2	-7.18	117.43	120.30
5	5	11	A	N1-C2-N3	-7.18	125.71	129.30
2	2	1923	A	N1-C2-N3	-7.18	125.71	129.30
2	2	2815	A	C2-N3-C4	7.17	114.19	110.60
2	2	3844	U	N3-C2-O2	-7.17	117.18	122.20
2	2	4224	A	N1-C2-N3	-7.17	125.71	129.30
2	2	4362	A	N1-C2-N3	-7.17	125.71	129.30
2	2	4773	C	C6-N1-C2	-7.17	117.43	120.30
2	2	4464	A	C2-N3-C4	7.17	114.19	110.60
2	2	4263	C	C6-N1-C2	-7.17	117.43	120.30
2	2	1795	A	N1-C2-N3	-7.17	125.72	129.30
2	2	4350	C	N1-C2-O2	7.17	123.20	118.90
2	2	53	C	C5-C6-N1	7.17	124.58	121.00
2	2	2517	A	N1-C2-N3	-7.16	125.72	129.30
2	2	2509	C	N1-C2-O2	7.16	123.20	118.90
2	2	2818	C	C5-C6-N1	7.16	124.58	121.00
2	2	753	C	C5-C6-N1	7.16	124.58	121.00
2	2	1929	A	C4-N9-C1'	7.16	139.18	126.30
2	2	2047	A	N1-C2-N3	-7.16	125.72	129.30
2	2	112	C	N1-C2-O2	7.15	123.19	118.90
2	2	477	C	C6-N1-C2	-7.15	117.44	120.30
5	5	101	A	N1-C2-N3	-7.15	125.72	129.30
2	2	1936	C	C6-N1-C2	-7.15	117.44	120.30
2	2	2594	C	C5-C6-N1	7.15	124.58	121.00
2	2	3847	C	C6-N1-C2	-7.15	117.44	120.30
2	2	4588	U	N3-C2-O2	-7.15	117.19	122.20
2	2	4261	C	C5-C6-N1	7.15	124.57	121.00
2	2	4977	A	N1-C2-N3	-7.15	125.73	129.30
2	2	87	A	N1-C2-N3	-7.14	125.73	129.30
2	2	2337	C	N1-C2-O2	7.14	123.19	118.90
2	2	2308	A	N1-C2-N3	-7.14	125.73	129.30
2	2	205	C	C5-C6-N1	7.14	124.57	121.00
2	2	4387	C	C6-N1-C2	-7.14	117.44	120.30
2	2	493	G	C4-N9-C1'	7.14	135.78	126.50
2	2	99	A	N1-C2-N3	-7.13	125.73	129.30
2	2	3939	G	N3-C4-C5	-7.13	125.03	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	509	A	N1-C2-N3	-7.13	125.73	129.30
2	2	3650	C	C5-C6-N1	7.13	124.56	121.00
2	2	4177	C	C6-N1-C2	-7.13	117.45	120.30
2	2	4983	C	C6-N1-C2	-7.13	117.45	120.30
2	2	1956	A	N1-C2-N3	-7.12	125.74	129.30
2	2	5023	C	C6-N1-C2	-7.12	117.45	120.30
2	2	963	G	N3-C4-N9	7.12	130.27	126.00
2	2	5	A	N1-C2-N3	-7.12	125.74	129.30
2	2	2375	A	N1-C2-N3	-7.12	125.74	129.30
2	2	4077	A	N1-C2-N3	-7.12	125.74	129.30
2	2	4548	A	N1-C2-N3	-7.12	125.74	129.30
2	2	1554	A	N1-C2-N3	-7.11	125.74	129.30
8	8	104	A	C4-C5-C6	-7.11	113.44	117.00
2	2	974	C	N1-C2-O2	7.11	123.17	118.90
2	2	3673	C	P-O3'-C3'	7.11	128.23	119.70
2	2	2360	A	N1-C2-N3	-7.11	125.74	129.30
2	2	4127	A	N1-C2-N3	-7.11	125.75	129.30
2	2	4970	C	C6-N1-C2	-7.11	117.46	120.30
2	2	2341	A	N1-C2-N3	-7.11	125.75	129.30
2	2	4602	A	N1-C2-N3	-7.11	125.75	129.30
2	2	4642	U	N3-C2-O2	-7.11	117.22	122.20
2	2	4687	A	N1-C2-N3	-7.11	125.75	129.30
5	5	68	C	C6-N1-C2	-7.11	117.46	120.30
8	8	44	A	N1-C2-N3	-7.11	125.75	129.30
2	2	436	C	N3-C2-O2	-7.11	116.93	121.90
2	2	4627	U	N1-C2-O2	7.11	127.77	122.80
49	r	235	MET	CA-CB-CG	7.11	125.38	113.30
2	2	1607	C	C5-C6-N1	7.10	124.55	121.00
2	2	1825	A	N1-C2-N3	-7.10	125.75	129.30
2	2	1583	A	N1-C2-N3	-7.10	125.75	129.30
2	2	3629	A	N1-C2-N3	-7.10	125.75	129.30
2	2	909	A	N1-C2-N3	-7.10	125.75	129.30
2	2	1694	C	C6-N1-C2	-7.10	117.46	120.30
2	2	4585	U	N3-C2-O2	-7.10	117.23	122.20
2	2	5048	A	N1-C2-N3	-7.10	125.75	129.30
2	2	106	A	N1-C2-N3	-7.09	125.75	129.30
2	2	368	C	N1-C2-O2	7.09	123.16	118.90
2	2	975	C	C6-N1-C2	-7.09	117.46	120.30
2	2	1960	A	N1-C2-N3	-7.09	125.75	129.30
2	2	4502	C	C5-C6-N1	7.09	124.55	121.00
10	A	10	LEU	CA-CB-CG	7.09	131.62	115.30
2	2	1447	C	N1-C2-O2	7.09	123.16	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1729	A	N1-C2-N3	-7.09	125.75	129.30
2	2	4385	A	N1-C2-N3	-7.09	125.76	129.30
2	2	4562	C	N1-C2-O2	7.09	123.15	118.90
2	2	1577	G	C8-N9-C4	-7.08	103.57	106.40
2	2	4506	C	C6-N1-C2	-7.08	117.47	120.30
2	2	455	C	C5-C6-N1	7.08	124.54	121.00
2	2	2069	A	N1-C2-N3	-7.08	125.76	129.30
2	2	2317	C	C6-N1-C2	-7.08	117.47	120.30
2	2	4565	C	N1-C2-O2	7.08	123.15	118.90
2	2	1690	C	C6-N1-C2	-7.08	117.47	120.30
2	2	4935	C	N1-C2-O2	7.08	123.15	118.90
2	2	429	A	N1-C2-N3	-7.08	125.76	129.30
2	2	2300	A	N1-C2-N3	-7.08	125.76	129.30
2	2	289	C	N1-C2-O2	7.08	123.15	118.90
2	2	2095	A	N1-C2-N3	-7.08	125.76	129.30
8	8	118	C	C6-N1-C2	-7.08	117.47	120.30
2	2	233	U	N3-C2-O2	-7.08	117.25	122.20
8	8	88	A	N1-C2-N3	-7.08	125.76	129.30
2	2	2016	C	C6-N1-C2	-7.07	117.47	120.30
2	2	2595	C	C6-N1-C2	-7.07	117.47	120.30
2	2	4286	C	N1-C2-O2	7.07	123.14	118.90
2	2	2821	U	N3-C2-O2	-7.07	117.25	122.20
5	5	74	A	N1-C2-N3	-7.07	125.77	129.30
2	2	4692	A	N1-C2-N3	-7.07	125.77	129.30
2	2	5008	C	N1-C2-O2	7.06	123.14	118.90
8	8	48	A	N1-C2-N3	-7.06	125.77	129.30
2	2	242	U	N3-C2-O2	-7.06	117.26	122.20
2	2	1737	A	N1-C2-N3	-7.06	125.77	129.30
2	2	3604	A	N1-C2-N3	-7.06	125.77	129.30
2	2	3915	U	N3-C2-O2	-7.06	117.26	122.20
2	2	1372	A	N1-C2-N3	-7.06	125.77	129.30
2	2	3702	A	C2-N3-C4	7.06	114.13	110.60
2	2	4487	A	N1-C2-N3	-7.06	125.77	129.30
2	2	4535	A	N1-C2-N3	-7.06	125.77	129.30
2	2	2833	A	N1-C2-N3	-7.06	125.77	129.30
2	2	337	U	N1-C2-O2	7.05	127.74	122.80
2	2	1458	C	C6-N1-C2	-7.05	117.48	120.30
2	2	1597	G	N1-C6-O6	-7.05	115.67	119.90
2	2	353	A	N1-C2-N3	-7.05	125.77	129.30
2	2	2367	A	N1-C2-N3	-7.05	125.78	129.30
2	2	3905	A	P-O3'-C3'	7.05	128.16	119.70
8	8	95	A	N1-C2-N3	-7.05	125.77	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	719	C	C6-N1-C2	-7.05	117.48	120.30
2	2	1079	C	C2-N1-C1'	7.05	126.55	118.80
2	2	3670	C	N1-C2-O2	7.05	123.13	118.90
2	2	4348	A	N1-C2-N3	-7.05	125.78	129.30
2	2	148	C	C5-C6-N1	7.05	124.52	121.00
2	2	1097	C	C5-C6-N1	7.05	124.52	121.00
2	2	1621	A	C4-C5-C6	-7.05	113.48	117.00
2	2	2591	A	N1-C2-N3	-7.05	125.78	129.30
2	2	4381	A	N1-C2-N3	-7.05	125.78	129.30
2	2	4712	C	C5-C6-N1	7.05	124.52	121.00
2	2	110	C	C5-C6-N1	7.04	124.52	121.00
10	A	211	GLY	C-N-CA	7.04	139.31	121.70
2	2	1821	G	C2-N3-C4	7.04	115.42	111.90
2	2	2592	U	N3-C2-O2	-7.04	117.27	122.20
2	2	2858	A	N1-C2-N3	-7.04	125.78	129.30
2	2	3636	C	N1-C2-O2	7.04	123.12	118.90
2	2	3618	C	C5-C6-N1	7.04	124.52	121.00
8	8	135	C	N1-C2-O2	7.04	123.12	118.90
2	2	51	A	N1-C2-N3	-7.04	125.78	129.30
2	2	235	A	N1-C2-N3	-7.04	125.78	129.30
2	2	408	A	N1-C2-N3	-7.03	125.78	129.30
2	2	4464	A	N1-C2-N3	-7.03	125.78	129.30
2	2	2813	A	N1-C2-N3	-7.03	125.78	129.30
2	2	2332	A	N1-C2-N3	-7.03	125.79	129.30
2	2	1932	A	N1-C2-N3	-7.03	125.79	129.30
2	2	426	A	N1-C2-N3	-7.03	125.79	129.30
2	2	504	G	C2-N3-C4	7.03	115.41	111.90
2	2	493	G	N3-C4-N9	7.02	130.21	126.00
2	2	2615	C	N3-C2-O2	-7.02	116.98	121.90
2	2	4864	U	N1-C2-O2	7.02	127.72	122.80
2	2	654	C	C5-C6-N1	7.02	124.51	121.00
2	2	122	U	N1-C2-O2	7.02	127.71	122.80
2	2	345	C	N1-C2-O2	7.01	123.11	118.90
2	2	1943	A	N1-C2-N3	-7.01	125.79	129.30
2	2	2814	C	C6-N1-C1'	-7.01	112.39	120.80
2	2	3724	A	N1-C2-N3	-7.01	125.80	129.30
2	2	4207	C	C6-N1-C2	-7.01	117.50	120.30
2	2	4983	C	N1-C2-O2	7.01	123.11	118.90
4	4	411	LEU	CA-CB-CG	7.01	131.42	115.30
2	2	1892	A	N1-C2-N3	-7.01	125.80	129.30
2	2	2282	A	C2-N3-C4	7.01	114.10	110.60
2	2	2449	A	N1-C2-N3	-7.01	125.80	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4651	A	N1-C2-N3	-7.01	125.80	129.30
2	2	1613	A	N1-C2-N3	-7.00	125.80	129.30
2	2	2484	A	N1-C2-N3	-7.00	125.80	129.30
2	2	3890	A	N1-C2-N3	-7.00	125.80	129.30
2	2	3939	G	C2-N3-C4	7.00	115.40	111.90
2	2	711	A	N1-C2-N3	-7.00	125.80	129.30
2	2	2685	C	C5-C6-N1	7.00	124.50	121.00
8	8	28	C	C5-C6-N1	7.00	124.50	121.00
2	2	28	C	C5-C6-N1	7.00	124.50	121.00
2	2	657	C	N3-C2-O2	-7.00	117.00	121.90
2	2	1474	C	C6-N1-C2	-7.00	117.50	120.30
2	2	4691	A	N1-C2-N3	-7.00	125.80	129.30
2	2	953	C	C6-N1-C2	-7.00	117.50	120.30
2	2	2347	A	N1-C2-N3	-7.00	125.80	129.30
2	2	672	C	C6-N1-C2	-6.99	117.50	120.30
2	2	2096	G	C4-N9-C1'	6.99	135.59	126.50
2	2	3643	A	N1-C2-N3	-6.99	125.80	129.30
5	5	50	A	N1-C2-N3	-6.99	125.80	129.30
2	2	1460	C	C6-N1-C2	-6.99	117.50	120.30
2	2	299	C	C6-N1-C2	-6.99	117.50	120.30
2	2	1433	A	N1-C2-N3	-6.99	125.81	129.30
2	2	2029	A	N1-C2-N3	-6.99	125.81	129.30
8	8	150	C	C5-C6-N1	6.99	124.49	121.00
2	2	1386	C	N1-C2-O2	6.99	123.09	118.90
2	2	61	A	N1-C2-N3	-6.99	125.81	129.30
2	2	3775	A	N1-C2-N3	-6.99	125.81	129.30
2	2	4568	A	N1-C2-N3	-6.98	125.81	129.30
2	2	5002	U	N1-C2-O2	6.98	127.69	122.80
2	2	402	A	N1-C2-N3	-6.98	125.81	129.30
2	2	2850	A	N1-C2-N3	-6.98	125.81	129.30
2	2	3732	A	N1-C2-N3	-6.98	125.81	129.30
2	2	4517	A	N1-C2-N3	-6.98	125.81	129.30
2	2	2351	C	C2-N1-C1'	6.98	126.48	118.80
2	2	928	C	C6-N1-C2	-6.98	117.51	120.30
2	2	62	A	N1-C2-N3	-6.98	125.81	129.30
2	2	1334	A	N1-C2-N3	-6.98	125.81	129.30
2	2	1727	U	N3-C2-O2	-6.98	117.32	122.20
2	2	1936	C	N1-C2-O2	6.98	123.09	118.90
2	2	4212	A	N1-C2-N3	-6.97	125.81	129.30
30	W	81	ARG	NE-CZ-NH2	-6.97	116.81	120.30
2	2	3906	A	N1-C2-N3	-6.97	125.81	129.30
2	2	1838	A	N1-C2-N3	-6.97	125.82	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3649	A	N1-C2-N3	-6.97	125.81	129.30
2	2	2019	C	C6-N1-C2	-6.97	117.51	120.30
2	2	396	A	N1-C2-N3	-6.97	125.82	129.30
2	2	1655	C	C6-N1-C2	-6.97	117.51	120.30
2	2	1729	A	C2-N3-C4	6.97	114.08	110.60
2	2	4369	A	N1-C2-N3	-6.97	125.82	129.30
2	2	1564	A	N1-C2-N3	-6.96	125.82	129.30
2	2	1735	U	N1-C2-O2	6.96	127.67	122.80
2	2	2491	C	C6-N1-C1'	6.96	129.16	120.80
8	8	155	C	C5-C6-N1	6.96	124.48	121.00
2	2	1962	A	C2-N3-C4	6.96	114.08	110.60
2	2	4683	U	N3-C2-O2	-6.96	117.33	122.20
2	2	318	A	N1-C2-N3	-6.96	125.82	129.30
2	2	1870	C	C5-C6-N1	6.96	124.48	121.00
2	2	4880	C	C5-C6-N1	6.96	124.48	121.00
2	2	474	C	C6-N1-C2	-6.96	117.52	120.30
2	2	1378	C	N1-C2-O2	6.96	123.07	118.90
2	2	1796	U	N3-C2-O2	-6.96	117.33	122.20
2	2	2528	G	C8-N9-C1'	-6.96	117.96	127.00
2	2	3851	U	N3-C2-O2	-6.96	117.33	122.20
2	2	4729	A	N1-C2-N3	-6.96	125.82	129.30
2	2	1097	C	C2-N1-C1'	6.96	126.45	118.80
2	2	1486	C	C5-C6-N1	6.96	124.48	121.00
2	2	10	A	N1-C2-N3	-6.95	125.82	129.30
2	2	420	A	N1-C2-N3	-6.95	125.82	129.30
2	2	4186	A	N1-C2-N3	-6.95	125.82	129.30
2	2	2255	C	C6-N1-C1'	-6.95	112.46	120.80
2	2	4938	A	N1-C2-N3	-6.95	125.83	129.30
5	5	102	U	C2-N1-C1'	6.95	126.04	117.70
2	2	1368	A	N1-C2-N3	-6.95	125.83	129.30
2	2	4155	C	C6-N1-C2	-6.95	117.52	120.30
2	2	4279	A	N1-C2-N3	-6.95	125.83	129.30
2	2	4380	A	N1-C2-N3	-6.95	125.83	129.30
2	2	2689	C	C5-C6-N1	6.95	124.47	121.00
2	2	4282	A	N1-C2-N3	-6.95	125.83	129.30
2	2	4317	A	N1-C2-N3	-6.95	125.83	129.30
8	8	57	C	N1-C2-O2	6.95	123.07	118.90
2	2	100	C	O4'-C1'-N1	6.94	113.76	108.20
8	8	113	C	C6-N1-C2	-6.94	117.52	120.30
2	2	472	C	C5-C6-N1	6.94	124.47	121.00
2	2	4648	A	N1-C2-N3	-6.94	125.83	129.30
2	2	3912	U	N1-C2-O2	6.94	127.66	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4109	G	N3-C4-N9	6.94	130.16	126.00
2	2	1431	C	C6-N1-C2	-6.94	117.53	120.30
2	2	3821	A	N1-C2-N3	-6.94	125.83	129.30
2	2	1863	U	N3-C2-O2	-6.94	117.34	122.20
2	2	4714	C	N3-C2-O2	-6.94	117.05	121.90
2	2	2587	A	N1-C2-N3	-6.93	125.83	129.30
2	2	3649	A	C2-N3-C4	6.93	114.07	110.60
2	2	4886	C	C6-N1-C2	-6.93	117.53	120.30
2	2	2856	C	C6-N1-C2	-6.93	117.53	120.30
2	2	4762	A	N1-C2-N3	-6.93	125.83	129.30
2	2	4979	A	C2-N3-C4	6.93	114.06	110.60
8	8	43	A	C2-N3-C4	6.93	114.06	110.60
2	2	1679	A	N1-C2-N3	-6.93	125.84	129.30
2	2	2746	A	N1-C2-N3	-6.93	125.84	129.30
2	2	4229	U	C2-N1-C1'	6.93	126.01	117.70
2	2	985	C	C2-N1-C1'	6.93	126.42	118.80
2	2	1917	A	N1-C2-N3	-6.92	125.84	129.30
2	2	4234	A	N1-C2-N3	-6.92	125.84	129.30
2	2	2081	C	C6-N1-C2	-6.92	117.53	120.30
2	2	43	U	N1-C2-O2	6.92	127.64	122.80
2	2	4561	C	C6-N1-C2	-6.92	117.53	120.30
2	2	4496	A	N1-C2-N3	-6.92	125.84	129.30
2	2	1921	C	N3-C2-O2	-6.92	117.06	121.90
2	2	295	A	N1-C2-N3	-6.92	125.84	129.30
2	2	1731	C	C2-N1-C1'	6.92	126.41	118.80
2	2	2529	A	N1-C2-N3	-6.92	125.84	129.30
2	2	4584	A	N1-C2-N3	-6.92	125.84	129.30
2	2	147	A	N1-C2-N3	-6.92	125.84	129.30
2	2	2563	C	C6-N1-C2	-6.91	117.53	120.30
2	2	243	A	N1-C2-N3	-6.91	125.84	129.30
2	2	2667	C	N3-C2-O2	-6.91	117.06	121.90
2	2	101	A	C2-N3-C4	6.91	114.06	110.60
2	2	977	C	C6-N1-C2	-6.91	117.54	120.30
2	2	1656	U	N3-C2-O2	-6.91	117.36	122.20
2	2	2417	A	N1-C2-N3	-6.91	125.84	129.30
8	8	137	A	N1-C2-N3	-6.91	125.84	129.30
2	2	3901	A	N1-C2-N3	-6.91	125.85	129.30
2	2	1553	A	N1-C2-N3	-6.90	125.85	129.30
2	2	4695	C	C6-N1-C2	-6.90	117.54	120.30
2	2	71	C	C5-C6-N1	6.90	124.45	121.00
2	2	1449	C	C6-N1-C2	-6.90	117.54	120.30
2	2	2604	C	C5-C6-N1	6.90	124.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4157	A	N1-C2-N3	-6.90	125.85	129.30
2	2	1958	A	N1-C2-N3	-6.90	125.85	129.30
2	2	2412	A	N1-C2-N3	-6.90	125.85	129.30
2	2	84	A	N1-C2-N3	-6.90	125.85	129.30
2	2	1794	A	C2-N3-C4	6.90	114.05	110.60
2	2	2093	A	N1-C2-N3	-6.90	125.85	129.30
8	8	101	C	C2-N1-C1'	6.90	126.39	118.80
2	2	1631	A	N1-C2-N3	-6.90	125.85	129.30
2	2	2396	A	N1-C2-N3	-6.90	125.85	129.30
2	2	3736	A	N1-C2-N3	-6.90	125.85	129.30
2	2	4635	A	N1-C2-N3	-6.89	125.85	129.30
10	A	29	LEU	CA-CB-CG	6.89	131.16	115.30
2	2	259	C	N3-C2-O2	-6.89	117.08	121.90
2	2	1312	A	N1-C2-N3	-6.89	125.85	129.30
2	2	4576	U	N3-C2-O2	-6.89	117.38	122.20
5	5	6	C	C5-C6-N1	6.89	124.45	121.00
2	2	2882	A	N1-C2-N3	-6.89	125.86	129.30
5	5	13	A	N1-C2-N3	-6.89	125.86	129.30
5	5	22	A	N1-C2-N3	-6.89	125.86	129.30
2	2	675	C	C5-C6-N1	6.89	124.44	121.00
8	8	77	A	N1-C2-N3	-6.89	125.86	129.30
2	2	1096	C	C6-N1-C2	-6.89	117.55	120.30
2	2	1192	C	C2-N1-C1'	6.89	126.38	118.80
2	2	2379	A	N1-C2-N3	-6.89	125.86	129.30
2	2	222	C	N1-C2-O2	6.88	123.03	118.90
2	2	1580	C	C5-C6-N1	6.88	124.44	121.00
2	2	2507	A	N1-C2-N3	-6.88	125.86	129.30
5	5	14	C	C5-C6-N1	6.88	124.44	121.00
2	2	4488	A	N1-C2-N3	-6.88	125.86	129.30
2	2	165	A	N1-C2-N3	-6.88	125.86	129.30
2	2	2770	C	C6-N1-C2	-6.88	117.55	120.30
2	2	3636	C	N3-C2-O2	-6.88	117.08	121.90
2	2	5044	A	N1-C2-N3	-6.88	125.86	129.30
2	2	732	A	N1-C2-N3	-6.88	125.86	129.30
2	2	1592	G	C4-N9-C1'	6.88	135.44	126.50
2	2	2332	A	C4-C5-C6	-6.87	113.56	117.00
2	2	4303	C	C6-N1-C1'	-6.87	112.55	120.80
2	2	668	C	N1-C2-O2	6.87	123.02	118.90
2	2	2431	A	N1-C2-N3	-6.87	125.86	129.30
2	2	4883	C	C6-N1-C2	-6.87	117.55	120.30
2	2	1462	A	N1-C2-N3	-6.87	125.87	129.30
2	2	2077	C	C5-C6-N1	6.87	124.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2274	C	C5-C6-N1	6.87	124.43	121.00
2	2	2285	A	N1-C2-N3	-6.86	125.87	129.30
2	2	660	A	N1-C2-N3	-6.86	125.87	129.30
2	2	2748	C	C6-N1-C2	-6.86	117.56	120.30
2	2	663	G	C5-N7-C8	-6.86	100.87	104.30
2	2	4192	A	N1-C2-N3	-6.86	125.87	129.30
2	2	4681	A	N1-C2-N3	-6.86	125.87	129.30
2	2	516	C	C2-N3-C4	6.86	123.33	119.90
2	2	470	A	N1-C2-N3	-6.86	125.87	129.30
2	2	3908	A	N1-C2-N3	-6.85	125.87	129.30
2	2	935	A	C4-C5-C6	-6.85	113.57	117.00
2	2	1468	C	C6-N1-C2	-6.85	117.56	120.30
2	2	2071	A	N1-C2-N3	-6.85	125.87	129.30
2	2	915	A	N1-C2-N3	-6.85	125.88	129.30
2	2	2017	A	N1-C2-N3	-6.85	125.88	129.30
2	2	4608	G	C6-C5-N7	-6.85	126.29	130.40
2	2	4989	U	C2-N1-C1'	6.85	125.92	117.70
2	2	2107	C	N3-C2-O2	-6.84	117.11	121.90
2	2	4895	C	C2-N1-C1'	6.84	126.33	118.80
5	5	24	C	C5-C6-N1	6.84	124.42	121.00
2	2	1459	A	N1-C2-N3	-6.84	125.88	129.30
2	2	1793	A	N1-C2-N3	-6.84	125.88	129.30
2	2	675	C	C6-N1-C2	-6.84	117.56	120.30
2	2	948	C	C5-C6-N1	6.84	124.42	121.00
2	2	1546	C	C5-C6-N1	6.84	124.42	121.00
2	2	4257	A	N1-C2-N3	-6.84	125.88	129.30
5	5	16	A	N1-C2-N3	-6.84	125.88	129.30
2	2	4144	C	C2-N3-C4	6.83	123.32	119.90
2	2	4292	A	N1-C2-N3	-6.83	125.88	129.30
2	2	4717	A	N1-C2-N3	-6.83	125.88	129.30
8	8	97	A	N1-C2-N3	-6.83	125.88	129.30
2	2	1577	G	N3-C4-C5	-6.83	125.18	128.60
2	2	1809	C	N1-C2-O2	6.83	123.00	118.90
2	2	2335	C	C6-N1-C2	-6.83	117.57	120.30
2	2	3775	A	C2-N3-C4	6.83	114.02	110.60
2	2	4710	C	C5-C6-N1	6.83	124.42	121.00
2	2	73	A	N1-C2-N3	-6.83	125.89	129.30
2	2	1523	A	N1-C2-N3	-6.83	125.89	129.30
2	2	1540	C	N1-C2-O2	6.83	123.00	118.90
2	2	1662	C	C5-C6-N1	6.82	124.41	121.00
2	2	174	C	N3-C2-O2	-6.82	117.12	121.90
2	2	256	G	N9-C4-C5	-6.82	102.67	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	115	C	O4'-C1'-N1	6.82	113.66	108.20
2	2	141	C	N3-C2-O2	-6.82	117.13	121.90
2	2	233	U	N1-C2-O2	6.82	127.57	122.80
2	2	1541	C	C5-C6-N1	6.82	124.41	121.00
2	2	2886	U	N3-C2-O2	-6.82	117.43	122.20
2	2	4486	C	N1-C2-O2	6.82	122.99	118.90
2	2	4611	A	N1-C2-N3	-6.81	125.89	129.30
2	2	4346	U	N3-C2-O2	-6.81	117.43	122.20
2	2	274	C	N1-C2-O2	6.81	122.99	118.90
2	2	1076	C	C5-C6-N1	6.81	124.41	121.00
2	2	1703	C	N1-C2-O2	6.81	122.98	118.90
2	2	4627	U	N3-C2-O2	-6.81	117.44	122.20
2	2	1243	C	N1-C2-O2	6.80	122.98	118.90
2	2	654	C	C2-N1-C1'	6.80	126.28	118.80
2	2	2819	U	N1-C2-O2	6.80	127.56	122.80
2	2	14	C	N3-C2-O2	-6.80	117.14	121.90
2	2	1373	A	N1-C2-N3	-6.80	125.90	129.30
2	2	1949	U	N3-C2-O2	-6.80	117.44	122.20
2	2	3622	C	C6-N1-C2	-6.80	117.58	120.30
2	2	3696	C	N3-C2-O2	-6.80	117.14	121.90
2	2	42	A	N1-C2-N3	-6.80	125.90	129.30
2	2	2453	A	N1-C2-N3	-6.80	125.90	129.30
2	2	5050	C	C6-N1-C2	-6.80	117.58	120.30
2	2	469	C	C6-N1-C2	-6.79	117.58	120.30
2	2	378	A	N1-C2-N3	-6.79	125.90	129.30
2	2	1694	C	C5-C6-N1	6.79	124.40	121.00
2	2	1723	A	N1-C2-N3	-6.79	125.90	129.30
2	2	1405	C	C5-C6-N1	6.79	124.39	121.00
2	2	984	C	C5-C6-N1	6.79	124.39	121.00
2	2	985	C	N1-C2-O2	6.79	122.97	118.90
2	2	1468	C	C5-C6-N1	6.79	124.39	121.00
2	2	2581	A	N1-C2-N3	-6.79	125.91	129.30
2	2	2795	A	N1-C2-N3	-6.79	125.91	129.30
2	2	2843	U	N3-C2-O2	-6.79	117.45	122.20
2	2	1936	C	N3-C2-O2	-6.79	117.15	121.90
2	2	365	U	N1-C2-O2	6.79	127.55	122.80
2	2	467	U	C6-N1-C2	-6.79	116.93	121.00
2	2	1915	C	C2-N1-C1'	6.79	126.26	118.80
8	8	96	C	N3-C2-O2	-6.79	117.15	121.90
8	8	141	C	C6-N1-C2	-6.79	117.59	120.30
2	2	303	C	C6-N1-C2	-6.78	117.59	120.30
2	2	2313	A	N1-C2-N3	-6.78	125.91	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3630	A	N1-C2-N3	-6.78	125.91	129.30
2	2	4299	U	N1-C2-O2	6.78	127.55	122.80
2	2	4963	G	C2-N3-C4	6.78	115.29	111.90
2	2	3587	C	N3-C2-O2	-6.78	117.15	121.90
2	2	7	C	C5-C6-N1	6.78	124.39	121.00
2	2	707	C	C6-N1-C2	-6.78	117.59	120.30
2	2	1315	C	C5-C6-N1	6.78	124.39	121.00
5	5	83	A	N1-C2-N3	-6.77	125.91	129.30
2	2	220	C	C2-N1-C1'	6.77	126.25	118.80
2	2	1792	U	N1-C2-O2	6.77	127.54	122.80
2	2	4709	U	C6-N1-C2	-6.77	116.94	121.00
2	2	4767	C	C6-N1-C2	-6.77	117.59	120.30
2	2	4967	A	N1-C2-N3	-6.77	125.91	129.30
5	5	43	U	N1-C2-O2	6.77	127.54	122.80
2	2	1257	A	N1-C2-N3	-6.77	125.91	129.30
2	2	4909	A	N1-C2-N3	-6.77	125.92	129.30
8	8	11	C	C6-N1-C2	-6.77	117.59	120.30
2	2	1921	C	C2-N1-C1'	6.77	126.24	118.80
2	2	326	C	C5-C6-N1	6.76	124.38	121.00
2	2	668	C	C6-N1-C2	-6.76	117.59	120.30
2	2	1722	C	N1-C2-O2	6.76	122.96	118.90
2	2	3942	A	N1-C2-N3	-6.76	125.92	129.30
8	8	90	C	C6-N1-C2	-6.76	117.59	120.30
2	2	125	C	C6-N1-C2	-6.76	117.60	120.30
2	2	4971	A	N1-C2-N3	-6.76	125.92	129.30
2	2	1858	A	N1-C2-N3	-6.76	125.92	129.30
2	2	2716	C	C5-C6-N1	6.76	124.38	121.00
2	2	406	C	P-O3'-C3'	6.76	127.81	119.70
2	2	3893	C	C6-N1-C2	-6.76	117.60	120.30
2	2	4864	U	N3-C2-O2	-6.76	117.47	122.20
2	2	2025	A	N1-C2-N3	-6.75	125.92	129.30
2	2	4254	G	C4-N9-C1'	6.75	135.28	126.50
2	2	5051	C	C5-C6-N1	6.75	124.38	121.00
2	2	4074	C	N1-C2-O2	6.75	122.95	118.90
5	5	90	A	N1-C2-N3	-6.75	125.92	129.30
2	2	64	A	N1-C2-N3	-6.75	125.92	129.30
2	2	2077	C	C6-N1-C2	-6.75	117.60	120.30
2	2	2528	G	C2-N3-C4	6.75	115.28	111.90
2	2	4366	A	N1-C2-N3	-6.75	125.93	129.30
2	2	4426	C	N3-C2-O2	-6.75	117.18	121.90
2	2	4327	C	C5-C6-N1	6.75	124.37	121.00
2	2	4724	A	N1-C2-N3	-6.75	125.93	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	38	A	N1-C2-N3	-6.74	125.93	129.30
2	2	4608	G	C5-N7-C8	-6.74	100.93	104.30
2	2	960	A	N1-C2-N3	-6.74	125.93	129.30
8	8	111	U	N3-C2-O2	-6.74	117.48	122.20
2	2	4171	C	C5-C6-N1	6.74	124.37	121.00
5	5	35	U	N3-C2-O2	-6.74	117.48	122.20
2	2	4490	C	C5-C6-N1	6.74	124.37	121.00
2	2	4616	A	N1-C2-N3	-6.74	125.93	129.30
5	5	5	A	N1-C2-N3	-6.74	125.93	129.30
2	2	472	C	C2-N1-C1'	6.74	126.21	118.80
2	2	2040	A	N1-C2-N3	-6.73	125.93	129.30
2	2	2388	A	N1-C2-N3	-6.73	125.93	129.30
2	2	256	G	N1-C2-N2	-6.73	110.14	116.20
2	2	4696	C	N3-C2-O2	-6.73	117.19	121.90
2	2	679	C	C5-C6-N1	6.73	124.36	121.00
2	2	2856	C	C5-C6-N1	6.73	124.36	121.00
2	2	2696	A	N1-C2-N3	-6.73	125.94	129.30
2	2	753	C	C6-N1-C1'	-6.72	112.73	120.80
2	2	2833	A	C2-N3-C4	6.72	113.96	110.60
2	2	4980	C	C6-N1-C2	-6.72	117.61	120.30
2	2	2374	A	N1-C2-N3	-6.72	125.94	129.30
2	2	4244	A	N1-C2-N3	-6.72	125.94	129.30
2	2	1216	C	C6-N1-C1'	-6.72	112.73	120.80
2	2	941	C	C5-C6-N1	6.72	124.36	121.00
2	2	1540	C	C5-C6-N1	6.72	124.36	121.00
2	2	4969	C	N1-C2-O2	6.72	122.93	118.90
2	2	1603	C	C5-C6-N1	6.72	124.36	121.00
2	2	2429	A	N1-C2-N3	-6.72	125.94	129.30
2	2	2812	A	N1-C2-N3	-6.72	125.94	129.30
2	2	166	C	C6-N1-C2	-6.71	117.61	120.30
2	2	300	A	N1-C2-N3	-6.71	125.94	129.30
2	2	1939	A	N1-C2-N3	-6.71	125.94	129.30
2	2	1808	C	C6-N1-C2	-6.71	117.61	120.30
2	2	2477	A	N1-C2-N3	-6.71	125.94	129.30
8	8	80	A	N1-C2-N3	-6.71	125.94	129.30
2	2	2870	A	N1-C2-N3	-6.71	125.94	129.30
2	2	31	U	N3-C2-O2	-6.71	117.50	122.20
2	2	4562	C	C6-N1-C2	-6.71	117.62	120.30
2	2	4655	A	C5-C6-N1	6.71	121.05	117.70
2	2	4874	A	N1-C2-N3	-6.71	125.95	129.30
2	2	4640	C	C6-N1-C2	-6.71	117.62	120.30
2	2	2544	G	N3-C4-C5	-6.71	125.25	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2410	C	N3-C2-O2	-6.70	117.21	121.90
2	2	3657	U	C6-N1-C2	-6.70	116.98	121.00
2	2	141	C	C5-C6-N1	6.70	124.35	121.00
2	2	4599	A	N1-C2-N3	-6.70	125.95	129.30
2	2	1176	C	C5-C6-N1	6.70	124.35	121.00
2	2	1315	C	C6-N1-C2	-6.70	117.62	120.30
2	2	297	U	N1-C2-O2	6.70	127.49	122.80
2	2	1533	A	N1-C2-N3	-6.70	125.95	129.30
2	2	2871	A	N1-C2-N3	-6.70	125.95	129.30
2	2	4303	C	C6-N1-C2	-6.70	117.62	120.30
2	2	294	G	C2-N3-C4	6.69	115.25	111.90
2	2	2642	A	N1-C2-N3	-6.69	125.95	129.30
2	2	704	C	N3-C2-O2	-6.69	117.22	121.90
2	2	2669	C	C6-N1-C2	-6.69	117.62	120.30
2	2	3924	C	C5-C6-N1	6.69	124.35	121.00
2	2	5061	A	N1-C2-N3	-6.69	125.95	129.30
2	2	688	U	N3-C2-O2	-6.69	117.52	122.20
2	2	2670	C	C5-C6-N1	6.69	124.34	121.00
2	2	4133	C	C5-C6-N1	6.69	124.34	121.00
2	2	4878	C	C6-N1-C2	-6.69	117.62	120.30
2	2	1193	C	N1-C2-O2	6.69	122.91	118.90
2	2	1491	A	N1-C2-N3	-6.69	125.95	129.30
2	2	2600	A	N1-C2-N3	-6.69	125.96	129.30
2	2	956	A	N1-C2-N3	-6.69	125.96	129.30
2	2	4990	C	C2-N1-C1'	6.69	126.16	118.80
2	2	2684	C	C6-N1-C2	-6.69	117.63	120.30
2	2	4137	C	C5-C6-N1	6.68	124.34	121.00
2	2	5042	A	C2-N3-C4	6.68	113.94	110.60
2	2	2561	C	C5-C6-N1	6.68	124.34	121.00
2	2	201	C	N1-C2-O2	6.68	122.91	118.90
2	2	440	U	N3-C2-O2	-6.68	117.52	122.20
2	2	673	C	C2-N1-C1'	6.68	126.15	118.80
2	2	1088	C	C6-N1-C2	-6.68	117.63	120.30
2	2	4684	A	N1-C2-N3	-6.68	125.96	129.30
2	2	4716	C	C5-C6-N1	6.68	124.34	121.00
2	2	78	U	N3-C2-O2	-6.68	117.53	122.20
2	2	673	C	N1-C2-O2	6.68	122.91	118.90
2	2	4390	A	N1-C2-N3	-6.68	125.96	129.30
8	8	92	U	N3-C2-O2	-6.68	117.53	122.20
2	2	4966	A	N1-C2-N3	-6.67	125.96	129.30
2	2	4155	C	C5-C6-N1	6.67	124.34	121.00
2	2	4393	G	N1-C6-O6	-6.67	115.90	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4506	C	N3-C2-O2	-6.67	117.23	121.90
5	5	36	C	C6-N1-C2	-6.67	117.63	120.30
2	2	120	A	N1-C2-N3	-6.67	125.97	129.30
5	5	79	U	N3-C2-O2	-6.67	117.53	122.20
2	2	282	C	C5-C6-N1	6.67	124.33	121.00
2	2	2392	C	C5-C6-N1	6.67	124.33	121.00
2	2	2845	A	C2-N3-C4	6.67	113.93	110.60
5	5	44	C	N3-C2-O2	-6.67	117.23	121.90
8	8	148	A	N1-C2-N3	-6.67	125.97	129.30
2	2	2755	A	N1-C2-N3	-6.66	125.97	129.30
2	2	4621	C	N1-C2-O2	6.66	122.89	118.90
2	2	917	A	N1-C2-N3	-6.65	125.97	129.30
2	2	4413	C	N1-C2-O2	6.65	122.89	118.90
2	2	3624	A	N1-C2-N3	-6.65	125.97	129.30
2	2	386	A	C2-N3-C4	6.65	113.92	110.60
2	2	2869	U	N3-C2-O2	-6.65	117.55	122.20
2	2	434	A	N1-C2-N3	-6.65	125.98	129.30
2	2	1309	C	C6-N1-C2	-6.65	117.64	120.30
2	2	1816	C	C2-N1-C1'	6.65	126.11	118.80
2	2	3612	C	C6-N1-C2	-6.65	117.64	120.30
8	8	32	C	N3-C2-O2	-6.65	117.25	121.90
5	5	38	U	N1-C2-O2	6.65	127.45	122.80
2	2	1696	C	C5-C6-N1	6.64	124.32	121.00
2	2	4345	C	C5-C6-N1	6.64	124.32	121.00
2	2	4449	A	C2-N3-C4	6.64	113.92	110.60
2	2	27	C	C5-C6-N1	6.64	124.32	121.00
2	2	1248	C	C5-C6-N1	6.64	124.32	121.00
2	2	4906	C	C6-N1-C2	-6.64	117.64	120.30
2	2	2264	C	N1-C2-O2	6.64	122.88	118.90
8	8	3	A	N1-C2-N3	-6.64	125.98	129.30
2	2	667	A	N1-C2-N3	-6.63	125.98	129.30
2	2	1514	U	N3-C2-O2	-6.63	117.56	122.20
2	2	71	C	C6-N1-C1'	6.63	128.76	120.80
2	2	3721	U	N1-C2-O2	6.63	127.44	122.80
2	2	4533	A	N1-C2-N3	-6.63	125.98	129.30
2	2	1701	A	N1-C2-N3	-6.63	125.98	129.30
2	2	363	A	N1-C2-N3	-6.63	125.99	129.30
2	2	2699	C	C6-N1-C2	-6.63	117.65	120.30
2	2	1577	G	N3-C2-N2	-6.63	115.26	119.90
5	5	57	C	C5-C6-N1	6.63	124.31	121.00
2	2	2774	C	N1-C2-O2	6.62	122.88	118.90
2	2	385	A	OP1-P-O3'	6.62	119.77	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1556	C	C6-N1-C2	-6.62	117.65	120.30
2	2	4926	C	N1-C2-O2	6.62	122.87	118.90
2	2	294	G	C4-N9-C1'	6.62	135.11	126.50
2	2	302	C	C5-C6-N1	6.62	124.31	121.00
2	2	1222	A	N1-C2-N3	-6.62	125.99	129.30
2	2	4504	C	N3-C2-O2	-6.62	117.27	121.90
2	2	2630	U	N3-C2-O2	-6.62	117.57	122.20
2	2	4243	C	C2-N1-C1'	6.62	126.08	118.80
2	2	4653	C	C6-N1-C2	-6.61	117.66	120.30
2	2	4701	A	C2-N3-C4	6.61	113.91	110.60
2	2	2757	A	N1-C2-N3	-6.61	126.00	129.30
2	2	2043	A	N1-C2-N3	-6.61	126.00	129.30
2	2	2792	C	C6-N1-C2	-6.61	117.66	120.30
2	2	4395	U	P-O3'-C3'	6.61	127.63	119.70
2	2	1430	C	C6-N1-C2	-6.60	117.66	120.30
2	2	2255	C	C5-C6-N1	6.60	124.30	121.00
2	2	2772	C	C6-N1-C2	-6.60	117.66	120.30
2	2	3622	C	C5-C6-N1	6.60	124.30	121.00
2	2	4866	C	C5-C6-N1	6.60	124.30	121.00
5	5	91	C	N1-C2-O2	6.60	122.86	118.90
2	2	694	C	C6-N1-C2	-6.60	117.66	120.30
2	2	2302	C	C5-C6-N1	6.60	124.30	121.00
2	2	2866	C	C6-N1-C2	-6.60	117.66	120.30
2	2	4387	C	N3-C2-O2	-6.60	117.28	121.90
2	2	4655	A	C2-N3-C4	6.60	113.90	110.60
8	8	111	U	N1-C2-O2	6.60	127.42	122.80
2	2	3829	G	C2-N3-C4	6.60	115.20	111.90
2	2	2078	C	C6-N1-C2	-6.59	117.66	120.30
2	2	4341	C	C6-N1-C2	-6.59	117.66	120.30
2	2	4503	A	C2-N3-C4	6.59	113.90	110.60
2	2	4940	C	N1-C2-O2	6.59	122.86	118.90
2	2	2647	A	N1-C2-N3	-6.59	126.00	129.30
2	2	4613	C	C6-N1-C2	-6.59	117.66	120.30
2	2	4613	C	N3-C2-O2	-6.59	117.29	121.90
2	2	3658	C	C6-N1-C2	-6.59	117.67	120.30
2	2	4710	C	C6-N1-C2	-6.59	117.67	120.30
2	2	2625	U	N1-C2-O2	6.59	127.41	122.80
2	2	2016	C	N1-C2-O2	6.58	122.85	118.90
2	2	3690	U	N3-C2-O2	-6.58	117.59	122.20
2	2	4728	U	N3-C2-O2	-6.58	117.59	122.20
2	2	3840	U	N1-C2-O2	6.58	127.41	122.80
2	2	2031	C	C5-C6-N1	6.58	124.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	5046	U	N3-C2-O2	-6.58	117.60	122.20
2	2	1600	A	N1-C2-N3	-6.58	126.01	129.30
2	2	2867	C	C2-N1-C1'	6.58	126.03	118.80
2	2	3685	C	C5-C6-N1	6.58	124.29	121.00
2	2	3855	C	C5-C6-N1	6.58	124.29	121.00
2	2	2497	C	N3-C2-O2	-6.57	117.30	121.90
2	2	2872	C	C5-C6-N1	6.57	124.29	121.00
2	2	4879	C	C6-N1-C2	-6.57	117.67	120.30
2	2	282	C	C2-N1-C1'	6.57	126.03	118.80
2	2	368	C	C6-N1-C2	-6.57	117.67	120.30
2	2	4956	A	N1-C2-N3	-6.57	126.02	129.30
2	2	36	U	N1-C2-O2	6.57	127.39	122.80
2	2	227	A	C2-N3-C4	6.57	113.88	110.60
2	2	2560	C	N3-C2-O2	-6.57	117.30	121.90
2	2	4621	C	C5-C6-N1	6.57	124.28	121.00
2	2	2553	A	N1-C2-N3	-6.56	126.02	129.30
2	2	4183	G	C2-N3-C4	6.56	115.18	111.90
2	2	65	A	C4-C5-C6	-6.56	113.72	117.00
2	2	271	C	C6-N1-C2	-6.56	117.67	120.30
2	2	1289	C	C5-C6-N1	6.56	124.28	121.00
2	2	2292	C	C6-N1-C2	-6.56	117.67	120.30
2	2	2500	U	N1-C2-O2	6.56	127.39	122.80
2	2	1386	C	N3-C2-O2	-6.56	117.31	121.90
2	2	158	A	N1-C2-N3	-6.56	126.02	129.30
2	2	3662	A	C4-C5-C6	-6.56	113.72	117.00
2	2	4109	G	C8-N9-C1'	-6.56	118.47	127.00
2	2	4764	A	C6-N1-C2	6.56	122.54	118.60
2	2	1942	A	N1-C2-N3	-6.56	126.02	129.30
2	2	3892	U	N1-C2-O2	6.56	127.39	122.80
2	2	4895	C	N1-C2-O2	6.56	122.83	118.90
2	2	1609	U	N3-C2-O2	-6.55	117.61	122.20
2	2	2592	U	N1-C2-O2	6.55	127.39	122.80
8	8	55	U	N3-C2-O2	-6.55	117.61	122.20
8	8	66	A	N1-C2-N3	-6.55	126.02	129.30
2	2	17	A	C2-N3-C4	6.55	113.88	110.60
2	2	688	U	N1-C2-O2	6.55	127.39	122.80
2	2	408	A	C4-C5-C6	-6.55	113.73	117.00
2	2	2356	U	N3-C2-O2	-6.55	117.62	122.20
8	8	43	A	N1-C2-N3	-6.55	126.03	129.30
2	2	4738	C	C6-N1-C2	-6.55	117.68	120.30
2	2	238	C	C5-C6-N1	6.54	124.27	121.00
2	2	2271	C	C5-C6-N1	6.54	124.27	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4300	U	N1-C2-O2	6.54	127.38	122.80
2	2	389	A	N1-C2-N3	-6.54	126.03	129.30
2	2	1478	C	C6-N1-C2	-6.54	117.68	120.30
2	2	332	C	N1-C2-O2	6.54	122.82	118.90
2	2	657	C	C6-N1-C2	-6.54	117.68	120.30
2	2	1822	U	N3-C2-O2	-6.54	117.62	122.20
2	2	2392	C	C6-N1-C2	-6.54	117.68	120.30
8	8	50	C	C5-C6-N1	6.54	124.27	121.00
2	2	290	U	N3-C2-O2	-6.54	117.62	122.20
2	2	326	C	N1-C2-O2	6.54	122.82	118.90
2	2	2324	C	C6-N1-C2	-6.54	117.69	120.30
2	2	4626	A	C2-N3-C4	6.54	113.87	110.60
2	2	4653	C	C5-C6-N1	6.54	124.27	121.00
2	2	86	U	N3-C2-O2	-6.54	117.62	122.20
2	2	4991	U	N1-C2-O2	6.54	127.38	122.80
2	2	2037	C	C5-C6-N1	6.54	124.27	121.00
2	2	2783	A	C5-N7-C8	-6.53	100.63	103.90
2	2	2881	A	N1-C2-N3	-6.53	126.03	129.30
2	2	4420	U	N1-C2-O2	6.53	127.37	122.80
2	2	2710	C	C6-N1-C1'	-6.53	112.96	120.80
2	2	4504	C	C6-N1-C2	-6.53	117.69	120.30
2	2	935	A	N1-C2-N3	-6.53	126.03	129.30
2	2	4766	C	C2-N1-C1'	6.53	125.98	118.80
2	2	7	C	N1-C2-O2	6.53	122.82	118.90
2	2	1694	C	N1-C2-O2	6.53	122.82	118.90
2	2	488	G	N7-C8-N9	6.53	116.36	113.10
2	2	1575	A	N1-C2-N3	-6.53	126.04	129.30
2	2	1861	U	N3-C2-O2	-6.53	117.63	122.20
2	2	121	A	N1-C2-N3	-6.52	126.04	129.30
2	2	1893	C	C2-N1-C1'	6.52	125.97	118.80
2	2	3621	A	C2-N3-C4	6.52	113.86	110.60
2	2	1714	C	C6-N1-C2	-6.52	117.69	120.30
2	2	2499	C	C6-N1-C2	-6.52	117.69	120.30
2	2	1414	C	N1-C2-O2	6.51	122.81	118.90
2	2	2362	U	C2-N1-C1'	6.51	125.52	117.70
5	5	52	C	C6-N1-C2	-6.51	117.69	120.30
2	2	1450	C	C5-C6-N1	6.51	124.26	121.00
2	2	2543	A	N1-C2-N3	-6.51	126.05	129.30
2	2	3737	A	N1-C2-N3	-6.51	126.04	129.30
2	2	3919	C	N1-C2-O2	6.51	122.81	118.90
2	2	4645	C	C6-N1-C2	-6.51	117.69	120.30
2	2	5016	A	N7-C8-N9	6.51	117.05	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1653	A	N1-C2-N3	-6.51	126.05	129.30
2	2	2255	C	C6-N1-C2	-6.51	117.70	120.30
2	2	1703	C	C2-N1-C1'	6.50	125.95	118.80
2	2	2317	C	C5-C6-N1	6.50	124.25	121.00
2	2	458	C	C6-N1-C2	-6.50	117.70	120.30
2	2	2059	C	C6-N1-C2	-6.50	117.70	120.30
2	2	3610	A	N1-C2-N3	-6.50	126.05	129.30
8	8	17	A	C5-C6-N1	6.50	120.95	117.70
2	2	2674	A	N1-C2-N3	-6.50	126.05	129.30
2	2	3739	C	C5-C6-N1	6.50	124.25	121.00
2	2	4928	C	N3-C2-O2	-6.50	117.35	121.90
5	5	58	A	N1-C2-N3	-6.50	126.05	129.30
2	2	660	A	C2-N3-C4	6.50	113.85	110.60
2	2	2420	A	N1-C2-N3	-6.50	126.05	129.30
2	2	1371	A	N1-C2-N3	-6.50	126.05	129.30
2	2	1473	U	N3-C2-O2	-6.50	117.65	122.20
2	2	4500	U	C5-C6-N1	6.50	125.95	122.70
2	2	89	C	C6-N1-C2	-6.50	117.70	120.30
2	2	1404	G	N3-C4-C5	-6.50	125.35	128.60
2	2	3932	U	N3-C2-O2	-6.50	117.65	122.20
2	2	1096	C	C5-C6-N1	6.50	124.25	121.00
2	2	2621	A	N1-C2-N3	-6.50	126.05	129.30
2	2	4273	A	C4-C5-C6	-6.50	113.75	117.00
2	2	4203	A	N1-C2-N3	-6.49	126.05	129.30
2	2	1509	C	C6-N1-C2	-6.49	117.70	120.30
2	2	2659	A	C4-C5-C6	-6.49	113.76	117.00
2	2	4500	U	C2-N1-C1'	6.49	125.49	117.70
2	2	947	C	C5-C6-N1	6.49	124.24	121.00
2	2	1578	U	N1-C2-O2	6.49	127.34	122.80
2	2	3712	A	N1-C2-N3	-6.49	126.06	129.30
2	2	2743	A	N1-C2-N3	-6.48	126.06	129.30
2	2	3590	G	N3-C4-N9	6.48	129.89	126.00
2	2	3893	C	C5-C6-N1	6.48	124.24	121.00
2	2	2030	A	N1-C2-N3	-6.48	126.06	129.30
2	2	3882	C	N3-C2-O2	-6.48	117.36	121.90
2	2	4477	A	N1-C2-N3	-6.48	126.06	129.30
2	2	488	G	N3-C4-N9	6.48	129.89	126.00
2	2	712	C	C6-N1-C2	-6.48	117.71	120.30
2	2	1941	A	N1-C2-N3	-6.48	126.06	129.30
2	2	3905	A	N1-C2-N3	-6.48	126.06	129.30
2	2	4607	A	N1-C2-N3	-6.48	126.06	129.30
5	5	49	A	N1-C2-N3	-6.48	126.06	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	55	A	N1-C2-N3	-6.48	126.06	129.30
2	2	953	C	C5-C6-N1	6.48	124.24	121.00
2	2	1572	U	N3-C2-O2	-6.47	117.67	122.20
2	2	4088	C	C5-C6-N1	6.47	124.24	121.00
2	2	1822	U	N1-C2-O2	6.47	127.33	122.80
2	2	4727	A	N1-C2-N3	-6.47	126.06	129.30
2	2	2678	A	N1-C2-N3	-6.47	126.07	129.30
2	2	4372	U	N3-C2-O2	-6.47	117.67	122.20
2	2	4473	A	N1-C2-N3	-6.47	126.07	129.30
2	2	1216	C	N3-C2-O2	-6.47	117.37	121.90
2	2	2260	C	C5-C6-N1	6.47	124.23	121.00
2	2	4183	G	N3-C4-C5	-6.46	125.37	128.60
2	2	4964	C	C5-C6-N1	6.46	124.23	121.00
2	2	304	C	N1-C2-O2	6.46	122.78	118.90
2	2	2766	A	N1-C2-N3	-6.46	126.07	129.30
2	2	2856	C	C2-N1-C1'	6.46	125.91	118.80
2	2	4345	C	C6-N1-C2	-6.46	117.72	120.30
2	2	149	A	N1-C2-N3	-6.46	126.07	129.30
2	2	1589	C	C5-C6-N1	6.46	124.23	121.00
2	2	1078	A	N1-C2-N3	-6.46	126.07	129.30
2	2	1341	U	N3-C2-O2	-6.46	117.68	122.20
2	2	4510	A	N1-C2-N3	-6.46	126.07	129.30
2	2	4315	A	N1-C2-N3	-6.46	126.07	129.30
2	2	493	G	C8-N9-C1'	-6.46	118.61	127.00
2	2	4288	C	C6-N1-C2	-6.46	117.72	120.30
2	2	648	G	C4-N9-C1'	6.45	134.89	126.50
2	2	750	U	N3-C2-O2	-6.45	117.68	122.20
2	2	4079	C	C6-N1-C2	-6.45	117.72	120.30
2	2	4555	U	P-O3'-C3'	6.45	127.44	119.70
2	2	5035	U	N1-C2-O2	6.45	127.32	122.80
5	5	42	A	N1-C2-N3	-6.45	126.07	129.30
5	5	95	C	N1-C2-O2	6.45	122.77	118.90
2	2	907	C	N1-C2-O2	6.45	122.77	118.90
2	2	1298	C	C6-N1-C2	-6.45	117.72	120.30
2	2	4199	C	C2-N1-C1'	6.45	125.89	118.80
2	2	1460	C	C5-C6-N1	6.45	124.22	121.00
8	8	108	A	N1-C2-N3	-6.45	126.08	129.30
2	2	371	A	C4-C5-C6	-6.45	113.78	117.00
2	2	1964	A	N1-C2-N3	-6.45	126.08	129.30
2	2	2088	A	N1-C2-N3	-6.45	126.08	129.30
2	2	3876	A	N1-C2-N3	-6.45	126.08	129.30
2	2	4983	C	N3-C2-O2	-6.45	117.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	706	C	C6-N1-C2	-6.44	117.72	120.30
2	2	2513	A	C4-C5-C6	-6.44	113.78	117.00
2	2	4422	A	N1-C2-N3	-6.44	126.08	129.30
2	2	2817	C	C5-C6-N1	6.44	124.22	121.00
2	2	1720	C	N3-C2-O2	-6.44	117.39	121.90
2	2	2017	A	C2-N3-C4	6.44	113.82	110.60
2	2	2520	C	C6-N1-C2	-6.44	117.72	120.30
2	2	3826	C	N1-C2-O2	6.44	122.76	118.90
2	2	1494	U	C6-N1-C2	-6.44	117.14	121.00
2	2	4140	C	C5-C6-N1	6.44	124.22	121.00
2	2	4206	C	C2-N1-C1'	6.44	125.88	118.80
2	2	4239	A	N1-C2-N3	-6.44	126.08	129.30
2	2	180	C	N3-C2-O2	-6.43	117.40	121.90
2	2	1241	C	C6-N1-C2	-6.43	117.73	120.30
2	2	1500	A	N1-C2-N3	-6.43	126.08	129.30
2	2	4773	C	C5-C6-N1	6.43	124.22	121.00
2	2	2534	C	C6-N1-C2	-6.43	117.73	120.30
2	2	3910	C	C5-C6-N1	6.43	124.22	121.00
2	2	4172	A	N1-C2-N3	-6.43	126.08	129.30
2	2	41	C	N1-C2-O2	6.43	122.76	118.90
2	2	3587	C	C2-N1-C1'	6.43	125.87	118.80
2	2	4428	A	N1-C2-N3	-6.43	126.08	129.30
5	5	88	A	N1-C2-N3	-6.43	126.09	129.30
2	2	1395	U	C5-C6-N1	6.43	125.91	122.70
2	2	264	C	C5-C6-N1	6.43	124.21	121.00
2	2	4696	C	C6-N1-C2	-6.43	117.73	120.30
2	2	1635	C	C5-C6-N1	6.42	124.21	121.00
2	2	1805	A	N1-C2-N3	-6.42	126.09	129.30
2	2	4701	A	N1-C6-N6	-6.42	114.75	118.60
2	2	4654	C	C6-N1-C2	-6.42	117.73	120.30
2	2	30	C	C2-N1-C1'	6.42	125.86	118.80
2	2	513	U	C6-N1-C2	-6.42	117.15	121.00
2	2	713	C	C6-N1-C2	-6.42	117.73	120.30
2	2	1279	A	N1-C2-N3	-6.42	126.09	129.30
2	2	1305	C	C6-N1-C2	-6.42	117.73	120.30
2	2	3680	U	C2-N1-C1'	6.42	125.40	117.70
8	8	26	C	C6-N1-C2	-6.42	117.73	120.30
2	2	692	A	N1-C2-N3	-6.42	126.09	129.30
2	2	1648	C	C6-N1-C2	-6.42	117.73	120.30
2	2	2544	G	C4-N9-C1'	6.42	134.84	126.50
2	2	2744	A	N1-C2-N3	-6.42	126.09	129.30
2	2	4685	U	N1-C2-O2	6.42	127.29	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4929	C	C6-N1-C2	-6.42	117.73	120.30
2	2	238	C	C6-N1-C2	-6.42	117.73	120.30
2	2	111	C	C6-N1-C2	-6.41	117.73	120.30
2	2	759	G	N3-C4-C5	-6.41	125.39	128.60
2	2	1289	C	N3-C2-O2	-6.41	117.41	121.90
2	2	676	C	C6-N1-C2	-6.41	117.74	120.30
2	2	2708	U	C2-N1-C1'	6.41	125.39	117.70
2	2	4323	A	N1-C2-N3	-6.41	126.09	129.30
2	2	4893	A	N1-C2-N3	-6.41	126.10	129.30
2	2	2325	C	C5-C6-N1	6.41	124.20	121.00
2	2	4229	U	C6-N1-C2	-6.41	117.16	121.00
2	2	4563	U	N1-C2-O2	6.41	127.28	122.80
5	5	54	A	N1-C2-N3	-6.41	126.10	129.30
2	2	1332	C	C5-C6-N1	6.40	124.20	121.00
2	2	336	A	C2-N3-C4	6.40	113.80	110.60
2	2	324	A	N1-C2-N3	-6.40	126.10	129.30
2	2	100	C	C6-N1-C2	-6.40	117.74	120.30
2	2	2100	A	N1-C2-N3	-6.40	126.10	129.30
2	2	2843	U	O5'-P-OP1	-6.40	99.94	105.70
2	2	4164	C	C6-N1-C2	-6.40	117.74	120.30
5	5	68	C	C5-C6-N1	6.40	124.20	121.00
5	5	67	C	C5-C6-N1	6.40	124.20	121.00
2	2	2573	A	N1-C2-N3	-6.39	126.10	129.30
2	2	460	C	C5-C6-N1	6.39	124.20	121.00
2	2	2042	A	N1-C2-N3	-6.39	126.10	129.30
2	2	2338	C	C5-C6-N1	6.39	124.20	121.00
2	2	2445	C	C5-C6-N1	6.39	124.20	121.00
2	2	2533	C	C6-N1-C2	-6.39	117.74	120.30
2	2	3688	U	N1-C2-O2	6.39	127.27	122.80
2	2	30	C	C5-C6-N1	6.39	124.19	121.00
2	2	2290	C	N1-C2-O2	6.39	122.73	118.90
2	2	3702	A	N1-C2-N3	-6.39	126.10	129.30
2	2	33	A	C2-N3-C4	6.39	113.80	110.60
2	2	718	C	C5-C6-N1	6.39	124.19	121.00
2	2	1238	A	N1-C2-N3	-6.39	126.11	129.30
2	2	1593	A	N1-C2-N3	-6.39	126.11	129.30
2	2	2660	A	N1-C2-N3	-6.39	126.11	129.30
8	8	118	C	C5-C6-N1	6.39	124.19	121.00
2	2	344	A	N1-C2-N3	-6.38	126.11	129.30
5	5	103	A	N1-C2-N3	-6.38	126.11	129.30
2	2	4136	G	P-O3'-C3'	6.38	127.36	119.70
2	2	1431	C	C5-C6-N1	6.38	124.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1832	C	N3-C2-O2	-6.38	117.43	121.90
2	2	1344	C	N1-C2-O2	6.38	122.72	118.90
2	2	4683	U	N1-C2-O2	6.38	127.26	122.80
2	2	4985	U	N3-C2-O2	-6.38	117.74	122.20
2	2	4990	C	C5-C6-N1	6.38	124.19	121.00
2	2	492	U	N3-C2-O2	-6.37	117.74	122.20
2	2	1206	C	C5-C6-N1	6.37	124.19	121.00
2	2	2879	A	N1-C2-N3	-6.37	126.11	129.30
2	2	4162	C	C2-N1-C1'	6.37	125.81	118.80
2	2	991	C	N1-C2-O2	6.37	122.72	118.90
2	2	2392	C	N1-C2-O2	6.37	122.72	118.90
2	2	2832	A	N1-C2-N3	-6.37	126.11	129.30
2	2	1420	A	N1-C2-N3	-6.37	126.11	129.30
2	2	2506	G	C4-N9-C1'	6.37	134.78	126.50
2	2	946	C	C5-C6-N1	6.37	124.18	121.00
2	2	1497	A	N1-C2-N3	-6.37	126.12	129.30
2	2	4590	A	N1-C2-N3	-6.37	126.12	129.30
2	2	1428	U	N3-C2-O2	-6.37	117.74	122.20
8	8	79	G	C8-N9-C4	-6.37	103.85	106.40
2	2	167	C	C6-N1-C2	-6.37	117.75	120.30
2	2	1644	C	C5-C6-N1	6.37	124.18	121.00
2	2	4254	G	N3-C4-C5	-6.37	125.42	128.60
2	2	4262	C	C6-N1-C2	-6.37	117.75	120.30
2	2	699	C	N1-C2-O2	6.36	122.72	118.90
2	2	4284	C	C6-N1-C2	-6.36	117.75	120.30
2	2	1239	C	C6-N1-C2	-6.36	117.75	120.30
2	2	3687	A	N1-C2-N3	-6.36	126.12	129.30
2	2	1613	A	C4-C5-C6	-6.36	113.82	117.00
2	2	2565	A	N1-C2-N3	-6.36	126.12	129.30
2	2	4505	C	N3-C2-O2	-6.36	117.45	121.90
2	2	1178	G	C4-N9-C1'	6.36	134.77	126.50
2	2	3696	C	C6-N1-C2	-6.36	117.76	120.30
2	2	1635	C	C6-N1-C2	-6.35	117.76	120.30
2	2	3662	A	N1-C2-N3	-6.35	126.12	129.30
2	2	4943	A	N1-C2-N3	-6.35	126.12	129.30
2	2	686	A	N1-C2-N3	-6.35	126.12	129.30
2	2	694	C	N1-C2-O2	6.35	122.71	118.90
2	2	3642	A	N1-C2-N3	-6.35	126.12	129.30
2	2	454	U	C6-N1-C2	-6.35	117.19	121.00
8	8	65	A	N1-C2-N3	-6.35	126.13	129.30
2	2	3853	U	N3-C2-O2	-6.35	117.76	122.20
2	2	4892	A	N1-C2-N3	-6.35	126.13	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	964	A	N1-C2-N3	-6.34	126.13	129.30
2	2	2366	A	N1-C2-N3	-6.34	126.13	129.30
2	2	4116	C	OP2-P-O3'	6.34	119.16	105.20
2	2	4284	C	C5-C6-N1	6.34	124.17	121.00
2	2	4585	U	C6-N1-C2	-6.34	117.19	121.00
2	2	4767	C	C5-C6-N1	6.34	124.17	121.00
2	2	4879	C	C5-C6-N1	6.34	124.17	121.00
8	8	116	C	C5-C6-N1	6.34	124.17	121.00
2	2	909	A	C2-N3-C4	6.34	113.77	110.60
2	2	2304	U	N3-C2-O2	-6.34	117.76	122.20
2	2	1610	C	C6-N1-C2	-6.34	117.76	120.30
2	2	2532	C	C2-N1-C1'	6.34	125.77	118.80
2	2	4074	C	C6-N1-C2	-6.34	117.76	120.30
2	2	4254	G	N3-C4-N9	6.34	129.80	126.00
2	2	4100	C	N1-C2-O2	6.34	122.70	118.90
2	2	5004	C	C6-N1-C2	-6.34	117.77	120.30
2	2	1514	U	N1-C2-O2	6.33	127.23	122.80
2	2	1519	C	N1-C2-O2	6.33	122.70	118.90
2	2	3726	A	N1-C2-N3	-6.33	126.13	129.30
2	2	4518	A	N1-C2-N3	-6.33	126.13	129.30
2	2	3942	A	C2-N3-C4	6.33	113.77	110.60
2	2	4449	A	N1-C2-N3	-6.33	126.13	129.30
2	2	433	A	N1-C2-N3	-6.33	126.13	129.30
2	2	988	C	N3-C2-O2	-6.33	117.47	121.90
2	2	1191	C	C5-C6-N1	6.33	124.17	121.00
2	2	1630	A	N1-C2-N3	-6.33	126.14	129.30
2	2	1857	C	C6-N1-C2	-6.33	117.77	120.30
2	2	3594	C	N1-C2-O2	6.33	122.70	118.90
2	2	4480	A	N1-C2-N3	-6.33	126.14	129.30
2	2	1884	C	N1-C2-O2	6.33	122.70	118.90
2	2	3852	A	N1-C2-N3	-6.33	126.14	129.30
2	2	67	C	N1-C2-O2	6.33	122.70	118.90
2	2	1405	C	C6-N1-C2	-6.33	117.77	120.30
2	2	4639	G	C2-N3-C4	6.33	115.06	111.90
2	2	2551	A	N1-C2-N3	-6.33	126.14	129.30
2	2	2614	C	C6-N1-C2	-6.33	117.77	120.30
2	2	4612	C	N3-C2-O2	-6.33	117.47	121.90
2	2	4991	U	N3-C2-O2	-6.33	117.77	122.20
2	2	1666	C	C5-C6-N1	6.32	124.16	121.00
2	2	4138	C	N1-C2-O2	6.32	122.69	118.90
8	8	91	A	N1-C2-N3	-6.32	126.14	129.30
2	2	4906	C	N1-C2-O2	6.32	122.69	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3716	C	C5-C6-N1	6.32	124.16	121.00
2	2	3858	C	N1-C2-O2	6.32	122.69	118.90
16	G	114	LEU	CA-CB-CG	6.32	129.84	115.30
2	2	242	U	C6-N1-C2	-6.32	117.21	121.00
2	2	2085	G	C4-N9-C1'	6.32	134.71	126.50
2	2	1357	C	C5-C6-N1	6.32	124.16	121.00
8	8	130	C	C6-N1-C2	-6.32	117.77	120.30
2	2	4934	A	N1-C2-N3	-6.31	126.14	129.30
2	2	2684	C	C5-C6-N1	6.31	124.16	121.00
2	2	4479	A	N1-C2-N3	-6.31	126.14	129.30
2	2	113	A	N1-C2-N3	-6.31	126.14	129.30
2	2	723	A	N1-C2-N3	-6.31	126.14	129.30
2	2	1254	A	C4-N9-C1'	6.31	137.66	126.30
2	2	3870	C	C2-N1-C1'	6.31	125.74	118.80
2	2	4342	C	N3-C2-O2	-6.31	117.48	121.90
2	2	368	C	N3-C2-O2	-6.31	117.48	121.90
2	2	1097	C	N3-C2-O2	-6.31	117.48	121.90
44	l	13	CYS	CA-CB-SG	6.31	125.35	114.00
2	2	2340	C	C6-N1-C2	-6.30	117.78	120.30
2	2	3656	A	C2-N3-C4	6.30	113.75	110.60
2	2	3851	U	N1-C2-O2	6.30	127.21	122.80
2	2	1827	C	C6-N1-C2	-6.30	117.78	120.30
2	2	3590	G	N3-C4-C5	-6.30	125.45	128.60
2	2	4420	U	N3-C2-O2	-6.30	117.79	122.20
2	2	911	U	N3-C2-O2	-6.30	117.79	122.20
2	2	1404	G	N3-C4-N9	6.30	129.78	126.00
2	2	1563	A	N1-C2-N3	-6.30	126.15	129.30
2	2	2729	C	N1-C2-O2	6.30	122.68	118.90
2	2	4406	U	C2-N1-C1'	6.30	125.26	117.70
2	2	5019	A	C5-C6-N1	6.30	120.85	117.70
2	2	4698	C	C5-C6-N1	6.30	124.15	121.00
2	2	256	G	N1-C6-O6	6.30	123.68	119.90
2	2	2784	C	C5-C6-N1	6.30	124.15	121.00
2	2	4394	A	N1-C2-N3	-6.30	126.15	129.30
2	2	2483	G	C8-N9-C1'	-6.29	118.82	127.00
2	2	1583	A	C2-N3-C4	6.29	113.75	110.60
2	2	1669	A	N1-C2-N3	-6.29	126.15	129.30
2	2	2791	C	N1-C2-O2	6.29	122.68	118.90
2	2	4178	A	N1-C2-N3	-6.29	126.15	129.30
2	2	4223	C	C6-N1-C2	-6.29	117.78	120.30
8	8	72	A	N1-C2-N3	-6.29	126.15	129.30
2	2	305	A	N1-C2-N3	-6.29	126.15	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2482	C	C5-C6-N1	6.29	124.14	121.00
2	2	2628	U	N3-C2-O2	-6.29	117.80	122.20
2	2	3680	U	C6-N1-C2	-6.29	117.23	121.00
2	2	518	G	N3-C4-C5	-6.29	125.46	128.60
2	2	2670	C	C6-N1-C2	-6.29	117.78	120.30
2	2	4267	G	C2-N3-C4	6.29	115.04	111.90
2	2	4509	U	N3-C2-O2	-6.29	117.80	122.20
2	2	4929	C	C5-C6-N1	6.29	124.14	121.00
2	2	2096	G	C8-N9-C1'	-6.29	118.83	127.00
2	2	3608	A	N1-C2-N3	-6.29	126.16	129.30
2	2	1175	A	N1-C2-N3	-6.29	126.16	129.30
2	2	2303	C	C5-C6-N1	6.29	124.14	121.00
2	2	3596	A	N1-C2-N3	-6.29	126.16	129.30
2	2	4137	C	C6-N1-C2	-6.29	117.79	120.30
2	2	911	U	N1-C2-O2	6.28	127.20	122.80
2	2	2078	C	C5-C6-N1	6.28	124.14	121.00
2	2	347	A	C2-N3-C4	6.28	113.74	110.60
2	2	1726	U	C2-N1-C1'	6.28	125.24	117.70
2	2	2803	U	C5-C6-N1	6.28	125.84	122.70
2	2	209	U	C5-C6-N1	6.28	125.84	122.70
5	5	28	C	C2-N1-C1'	6.28	125.71	118.80
2	2	1642	A	N1-C2-N3	-6.28	126.16	129.30
2	2	3	C	C5-C6-N1	6.27	124.14	121.00
2	2	2710	C	C6-N1-C2	-6.27	117.79	120.30
2	2	1286	C	C6-N1-C2	-6.27	117.79	120.30
2	2	4482	U	N1-C2-O2	6.27	127.19	122.80
2	2	4982	A	N1-C2-N3	-6.27	126.17	129.30
2	2	1521	C	C5-C6-N1	6.26	124.13	121.00
5	5	94	C	N1-C2-O2	6.26	122.66	118.90
2	2	295	A	C5-C6-N1	6.26	120.83	117.70
2	2	977	C	N3-C2-O2	-6.26	117.52	121.90
2	2	3716	C	C6-N1-C2	-6.26	117.80	120.30
11	B	67	VAL	CB-CA-C	6.26	123.30	111.40
2	2	1478	C	C5-C6-N1	6.26	124.13	121.00
2	2	3655	C	C5-C6-N1	6.26	124.13	121.00
2	2	3692	A	N1-C2-N3	-6.26	126.17	129.30
2	2	1086	C	C5-C6-N1	6.26	124.13	121.00
2	2	1270	A	N1-C2-N3	-6.26	126.17	129.30
2	2	1884	C	C6-N1-C2	-6.26	117.80	120.30
2	2	2857	A	N1-C2-N3	-6.26	126.17	129.30
2	2	3865	A	N1-C2-N3	-6.26	126.17	129.30
2	2	1094	G	C4-N9-C1'	6.25	134.63	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1566	C	C2-N1-C1'	6.25	125.68	118.80
2	2	2654	C	C6-N1-C2	-6.25	117.80	120.30
2	2	23	C	N1-C2-O2	6.25	122.65	118.90
2	2	1307	A	N1-C2-N3	-6.25	126.17	129.30
2	2	1690	C	C5-C6-N1	6.25	124.13	121.00
2	2	4289	U	C2-N1-C1'	6.25	125.20	117.70
2	2	4422	A	C2-N3-C4	6.25	113.73	110.60
2	2	115	C	C5-C6-N1	6.25	124.13	121.00
2	2	410	A	N1-C2-N3	-6.25	126.17	129.30
2	2	2016	C	C5-C6-N1	6.25	124.13	121.00
2	2	4085	A	N1-C2-N3	-6.25	126.17	129.30
2	2	4673	U	N3-C2-O2	-6.25	117.82	122.20
2	2	1567	U	N3-C2-O2	-6.25	117.83	122.20
2	2	259	C	C5-C6-N1	6.24	124.12	121.00
2	2	974	C	N3-C2-O2	-6.24	117.53	121.90
2	2	1452	A	N1-C2-N3	-6.24	126.18	129.30
2	2	2439	G	N3-C4-N9	6.24	129.75	126.00
2	2	4281	A	O4'-C1'-N9	6.24	113.19	108.20
2	2	4674	C	N1-C2-O2	6.24	122.65	118.90
2	2	449	C	C2-N3-C4	6.24	123.02	119.90
2	2	2344	U	N1-C2-O2	6.24	127.17	122.80
2	2	5046	U	C6-N1-C2	-6.24	117.25	121.00
2	2	74	G	C4-N9-C1'	6.24	134.61	126.50
2	2	466	A	N1-C2-N3	-6.24	126.18	129.30
2	2	3926	C	C2-N1-C1'	6.24	125.66	118.80
2	2	2765	A	N1-C2-N3	-6.24	126.18	129.30
2	2	499	G	N7-C8-N9	6.24	116.22	113.10
2	2	1248	C	C6-N1-C2	-6.24	117.81	120.30
2	2	2257	C	N3-C2-O2	-6.24	117.54	121.90
2	2	5030	U	C4-C5-C6	6.24	123.44	119.70
2	2	1615	C	C5-C6-N1	6.23	124.12	121.00
2	2	931	C	C5-C6-N1	6.23	124.12	121.00
2	2	81	C	C5-C6-N1	6.23	124.11	121.00
2	2	294	G	N3-C4-N9	6.23	129.74	126.00
2	2	977	C	C2-N1-C1'	6.23	125.65	118.80
4	4	158	LEU	CA-CB-CG	6.23	129.63	115.30
2	2	1706	A	N1-C2-N3	-6.23	126.19	129.30
2	2	4921	C	N3-C2-O2	-6.23	117.54	121.90
2	2	1302	U	C6-N1-C1'	-6.23	112.48	121.20
2	2	3694	U	N3-C2-O2	-6.23	117.84	122.20
2	2	1096	C	N1-C2-O2	6.22	122.64	118.90
2	2	2409	U	N1-C2-N3	6.22	118.64	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4215	C	C5-C6-N1	6.22	124.11	121.00
8	8	3	A	C2-N3-C4	6.22	113.71	110.60
2	2	66	A	N1-C2-N3	-6.22	126.19	129.30
2	2	1641	G	O4'-C1'-N9	-6.22	103.22	108.20
2	2	4996	C	N1-C2-O2	6.22	122.63	118.90
2	2	1832	C	C6-N1-C2	-6.22	117.81	120.30
2	2	4744	A	N1-C2-N3	-6.22	126.19	129.30
2	2	3927	U	N3-C2-O2	-6.22	117.85	122.20
2	2	1332	C	C6-N1-C2	-6.22	117.81	120.30
2	2	1963	C	N3-C2-O2	-6.22	117.55	121.90
2	2	4987	C	N1-C2-O2	6.22	122.63	118.90
2	2	1602	U	N1-C2-O2	6.21	127.15	122.80
2	2	1804	A	N1-C2-N3	-6.21	126.19	129.30
2	2	1891	A	N1-C2-N3	-6.21	126.19	129.30
2	2	4499	G	O5'-P-OP2	-6.21	100.11	105.70
5	5	24	C	N3-C2-O2	-6.21	117.55	121.90
5	5	57	C	C6-N1-C2	-6.21	117.81	120.30
2	2	2018	C	C6-N1-C2	-6.21	117.81	120.30
2	2	178	C	N1-C2-O2	6.21	122.63	118.90
2	2	296	A	N1-C2-N3	-6.21	126.20	129.30
2	2	2540	C	C6-N1-C2	-6.21	117.82	120.30
2	2	4406	U	N3-C2-O2	-6.21	117.86	122.20
2	2	490	C	C5-C6-N1	6.21	124.10	121.00
2	2	963	G	N3-C4-C5	-6.20	125.50	128.60
2	2	966	A	C2-N3-C4	6.20	113.70	110.60
2	2	1616	U	N1-C2-O2	6.20	127.14	122.80
2	2	2094	G	C8-N9-C4	-6.20	103.92	106.40
2	2	4758	U	C6-N1-C1'	-6.20	112.52	121.20
2	2	1817	U	N1-C2-O2	6.20	127.14	122.80
2	2	5034	A	N1-C2-N3	-6.20	126.20	129.30
8	8	17	A	C2-N3-C4	6.20	113.70	110.60
2	2	1201	U	N3-C2-O2	-6.20	117.86	122.20
8	8	17	A	N1-C2-N3	-6.20	126.20	129.30
8	8	54	C	N3-C2-O2	-6.20	117.56	121.90
2	2	1620	U	N3-C2-O2	-6.20	117.86	122.20
2	2	2096	G	N3-C4-C5	-6.20	125.50	128.60
2	2	4378	A	N1-C2-N3	-6.20	126.20	129.30
2	2	4109	G	N3-C4-C5	-6.19	125.50	128.60
2	2	94	A	N1-C2-N3	-6.19	126.20	129.30
2	2	963	G	C8-N9-C1'	-6.19	118.95	127.00
2	2	2792	C	C5-C6-N1	6.19	124.10	121.00
2	2	128	C	C6-N1-C2	-6.19	117.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	8	150	C	C6-N1-C2	-6.19	117.82	120.30
2	2	4105	A	N1-C2-N3	-6.19	126.21	129.30
2	2	4624	A	N1-C2-N3	-6.19	126.21	129.30
2	2	2616	C	C5-C6-N1	6.18	124.09	121.00
2	2	2623	A	N1-C2-N3	-6.18	126.21	129.30
2	2	1375	C	N1-C2-O2	6.18	122.61	118.90
2	2	4387	C	C5-C6-N1	6.18	124.09	121.00
2	2	4981	G	C4-N9-C1'	6.18	134.54	126.50
2	2	962	C	N1-C2-O2	6.18	122.61	118.90
2	2	1184	A	N1-C2-N3	-6.18	126.21	129.30
2	2	1327	C	C6-N1-C2	-6.18	117.83	120.30
2	2	3653	A	N1-C2-N3	-6.18	126.21	129.30
2	2	2483	G	C2-N3-C4	6.18	114.99	111.90
2	2	2439	G	C4-N9-C1'	6.18	134.53	126.50
2	2	4366	A	C4-C5-C6	-6.18	113.91	117.00
2	2	367	C	C5-C6-N1	6.17	124.09	121.00
2	2	4645	C	C5-C6-N1	6.17	124.09	121.00
8	8	84	A	N1-C2-N3	-6.17	126.21	129.30
2	2	452	A	N1-C2-N3	-6.17	126.21	129.30
2	2	1521	C	N1-C2-O2	6.17	122.60	118.90
2	2	7	C	C6-N1-C2	-6.17	117.83	120.30
2	2	212	A	N1-C2-N3	-6.17	126.21	129.30
2	2	2565	A	C2-N3-C4	6.17	113.69	110.60
2	2	4605	A	C2-N3-C4	6.17	113.69	110.60
2	2	4775	C	C6-N1-C1'	-6.17	113.39	120.80
2	2	1632	A	C4-N9-C1'	6.17	137.40	126.30
2	2	2057	A	N1-C2-N3	-6.17	126.22	129.30
2	2	4291	G	C2-N3-C4	6.17	114.98	111.90
2	2	2598	A	N1-C2-N3	-6.17	126.22	129.30
2	2	1719	A	N1-C2-N3	-6.16	126.22	129.30
2	2	3882	C	C2-N1-C1'	6.16	125.58	118.80
2	2	4886	C	C5-C6-N1	6.16	124.08	121.00
2	2	474	C	C5-C6-N1	6.16	124.08	121.00
2	2	12	A	N1-C2-N3	-6.16	126.22	129.30
2	2	264	C	C6-N1-C2	-6.16	117.84	120.30
2	2	434	A	C2-N3-C4	6.16	113.68	110.60
2	2	463	A	N1-C2-N3	-6.16	126.22	129.30
2	2	1243	C	C2-N1-C1'	6.16	125.58	118.80
2	2	1449	C	C5-C6-N1	6.16	124.08	121.00
2	2	4698	C	C6-N1-C2	-6.16	117.84	120.30
2	2	69	A	N1-C2-N3	-6.16	126.22	129.30
2	2	295	A	C4-C5-C6	-6.16	113.92	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2484	A	C4-N9-C1'	6.16	137.38	126.30
2	2	3860	A	C2-N3-C4	6.15	113.68	110.60
2	2	1929	A	C8-N9-C1'	-6.15	116.62	127.70
2	2	2018	C	C5-C6-N1	6.15	124.08	121.00
2	2	3622	C	N3-C2-O2	-6.15	117.59	121.90
2	2	4562	C	C5-C6-N1	6.15	124.08	121.00
5	5	29	C	C2-N1-C1'	6.15	125.57	118.80
8	8	61	A	N1-C2-N3	-6.15	126.22	129.30
2	2	469	C	N1-C2-O2	6.15	122.59	118.90
2	2	38	A	C4-C5-C6	-6.15	113.93	117.00
2	2	1672	U	N3-C2-O2	-6.15	117.90	122.20
2	2	2749	C	C5-C6-N1	6.15	124.07	121.00
8	8	101	C	N3-C2-O2	-6.15	117.60	121.90
2	2	218	A	N1-C2-N3	-6.14	126.23	129.30
2	2	3667	C	C6-N1-C2	-6.14	117.84	120.30
3	3	324	VAL	C-N-CA	6.14	137.06	121.70
8	8	51	U	C6-N1-C1'	-6.14	112.60	121.20
2	2	3828	A	N1-C2-N3	-6.14	126.23	129.30
2	2	4957	C	C5-C6-N1	6.14	124.07	121.00
8	8	4	C	C5-C6-N1	6.14	124.07	121.00
2	2	4255	A	C2-N3-C4	6.14	113.67	110.60
5	5	19	C	C5-C6-N1	6.14	124.07	121.00
2	2	12	A	C2-N3-C4	6.14	113.67	110.60
2	2	252	C	C5-C6-N1	6.14	124.07	121.00
2	2	1669	A	C4-C5-C6	-6.14	113.93	117.00
2	2	1241	C	C6-N1-C1'	-6.14	113.44	120.80
2	2	1245	C	N1-C2-O2	6.14	122.58	118.90
2	2	1658	G	C2-N3-C4	6.14	114.97	111.90
2	2	4137	C	N1-C2-O2	6.13	122.58	118.90
2	2	2860	C	C5-C6-N1	6.13	124.07	121.00
2	2	668	C	N3-C2-O2	-6.13	117.61	121.90
2	2	757	G	C4-N9-C1'	6.13	134.47	126.50
2	2	1477	C	C5-C6-N1	6.13	124.06	121.00
2	2	3682	A	N1-C2-N3	-6.13	126.24	129.30
2	2	6	C	N1-C2-O2	6.12	122.57	118.90
2	2	1346	C	C5-C6-N1	6.12	124.06	121.00
2	2	2264	C	C6-N1-C2	-6.12	117.85	120.30
2	2	4928	C	C6-N1-C2	-6.12	117.85	120.30
2	2	4165	C	C5-C6-N1	6.12	124.06	121.00
2	2	3587	C	C6-N1-C2	-6.12	117.85	120.30
2	2	4352	U	C2-N1-C1'	6.12	125.04	117.70
2	2	4522	G	O5'-P-OP2	6.12	118.04	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	683	C	C5-C6-N1	6.12	124.06	121.00
2	2	1896	A	N1-C2-N3	-6.12	126.24	129.30
2	2	238	C	N1-C2-O2	6.12	122.57	118.90
2	2	1661	C	C5-C6-N1	6.12	124.06	121.00
2	2	1882	U	C5-C4-O4	-6.12	122.23	125.90
2	2	2497	C	C6-N1-C2	-6.11	117.86	120.30
2	2	2629	C	N1-C2-O2	6.11	122.57	118.90
2	2	1565	A	N1-C2-N3	-6.11	126.24	129.30
2	2	2272	C	C6-N1-C2	-6.11	117.86	120.30
2	2	4130	C	C6-N1-C2	-6.11	117.86	120.30
2	2	4352	U	C6-N1-C2	-6.11	117.33	121.00
2	2	3745	U	N3-C2-O2	-6.11	117.92	122.20
2	2	406	C	C6-N1-C2	-6.11	117.86	120.30
2	2	1398	A	N1-C2-N3	-6.11	126.25	129.30
2	2	2482	C	C6-N1-C2	-6.11	117.86	120.30
2	2	4165	C	C6-N1-C2	-6.11	117.86	120.30
2	2	488	G	C8-N9-C4	-6.10	103.96	106.40
2	2	2276	A	N1-C2-N3	-6.10	126.25	129.30
2	2	358	C	N1-C2-O2	6.10	122.56	118.90
2	2	1307	A	C2-N3-C4	6.10	113.65	110.60
2	2	4752	U	N1-C2-O2	6.10	127.07	122.80
2	2	1926	C	C6-N1-C2	-6.10	117.86	120.30
2	2	2038	U	N1-C2-O2	6.10	127.07	122.80
2	2	2290	C	C5-C6-N1	6.10	124.05	121.00
2	2	3891	A	C2-N3-C4	6.10	113.65	110.60
2	2	4361	U	N1-C2-O2	6.10	127.07	122.80
2	2	747	A	N1-C2-N3	-6.10	126.25	129.30
2	2	1791	U	N3-C2-O2	-6.10	117.93	122.20
2	2	1346	C	C6-N1-C2	-6.09	117.86	120.30
2	2	1696	C	C6-N1-C2	-6.09	117.86	120.30
2	2	4110	C	C5-C6-N1	6.09	124.05	121.00
2	2	4466	C	C5-C6-N1	6.09	124.05	121.00
2	2	4610	A	O4'-C1'-N9	6.09	113.08	108.20
2	2	4674	C	C5-C6-N1	6.09	124.05	121.00
2	2	4722	G	C4-N9-C1'	6.09	134.42	126.50
2	2	4955	A	N1-C2-N3	-6.09	126.25	129.30
8	8	144	U	N3-C2-O2	-6.09	117.93	122.20
2	2	385	A	C4-C5-C6	-6.09	113.95	117.00
2	2	459	C	C6-N1-C2	-6.09	117.86	120.30
2	2	4527	G	C4-C5-N7	6.09	113.24	110.80
2	2	1849	U	N3-C2-O2	-6.09	117.94	122.20
8	8	30	U	N3-C2-O2	-6.09	117.94	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	661	C	C5-C6-N1	6.08	124.04	121.00
2	2	332	C	C5-C6-N1	6.08	124.04	121.00
2	2	4133	C	C2-N1-C1'	6.08	125.49	118.80
2	2	4734	A	N1-C2-N3	-6.08	126.26	129.30
2	2	663	G	N9-C4-C5	-6.08	102.97	105.40
2	2	1430	C	C5-C6-N1	6.08	124.04	121.00
2	2	469	C	C5-C6-N1	6.08	124.04	121.00
2	2	4340	U	C6-N1-C2	-6.08	117.35	121.00
2	2	4612	C	C5-C6-N1	6.08	124.04	121.00
2	2	1564	A	C2-N3-C4	6.08	113.64	110.60
2	2	1521	C	N3-C2-O2	-6.08	117.65	121.90
2	2	1828	C	C6-N1-C2	-6.08	117.87	120.30
2	2	1894	C	C5-C6-N1	6.08	124.04	121.00
2	2	4396	A	N1-C2-N3	-6.08	126.26	129.30
2	2	2043	A	C4-C5-C6	-6.07	113.97	117.00
2	2	2820	C	C2-N1-C1'	6.07	125.48	118.80
2	2	4930	C	C6-N1-C2	-6.07	117.87	120.30
2	2	981	C	C5-C6-N1	6.07	124.03	121.00
2	2	4544	A	N1-C2-N3	-6.07	126.27	129.30
2	2	1554	A	C2-N3-C4	6.07	113.63	110.60
2	2	472	C	N3-C2-O2	-6.06	117.66	121.90
2	2	1050	C	C5-C6-N1	6.06	124.03	121.00
2	2	4639	G	N3-C4-N9	6.06	129.64	126.00
2	2	1503	A	C4-C5-C6	-6.06	113.97	117.00
2	2	2821	U	N1-C2-O2	6.06	127.04	122.80
2	2	4894	A	N1-C2-N3	-6.06	126.27	129.30
2	2	4747	C	C6-N1-C2	-6.06	117.88	120.30
2	2	4424	A	N1-C2-N3	-6.06	126.27	129.30
2	2	1702	C	N3-C2-O2	-6.06	117.66	121.90
2	2	1176	C	N1-C2-O2	6.05	122.53	118.90
2	2	1306	C	C6-N1-C2	-6.05	117.88	120.30
2	2	1341	U	N1-C2-O2	6.05	127.04	122.80
2	2	62	A	C2-N3-C4	6.05	113.62	110.60
2	2	1802	A	N1-C2-N3	-6.05	126.27	129.30
2	2	3882	C	C6-N1-C2	-6.05	117.88	120.30
2	2	4434	C	C6-N1-C2	-6.05	117.88	120.30
2	2	4500	U	C6-N1-C2	-6.05	117.37	121.00
2	2	35	U	N1-C2-O2	6.05	127.03	122.80
2	2	518	G	N3-C4-N9	6.05	129.63	126.00
5	5	115	A	N1-C2-N3	-6.05	126.28	129.30
2	2	2505	C	N1-C2-O2	6.05	122.53	118.90
2	2	4747	C	C5-C6-N1	6.05	124.02	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2344	U	N3-C2-O2	-6.04	117.97	122.20
2	2	4298	A	C2-N3-C4	6.04	113.62	110.60
2	2	4640	C	C5-C6-N1	6.04	124.02	121.00
4	4	12	VAL	CA-CB-CG1	6.04	119.96	110.90
2	2	1874	A	N1-C2-N3	-6.04	126.28	129.30
2	2	1644	C	C6-N1-C2	-6.04	117.88	120.30
2	2	4388	A	C4-C5-C6	-6.04	113.98	117.00
2	2	294	G	N3-C4-C5	-6.04	125.58	128.60
2	2	1546	C	C6-N1-C2	-6.04	117.88	120.30
2	2	2509	C	N3-C2-O2	-6.04	117.67	121.90
2	2	4766	C	N1-C2-O2	6.04	122.52	118.90
5	5	91	C	C2-N1-C1'	6.03	125.44	118.80
2	2	3	C	C6-N1-C2	-6.03	117.89	120.30
2	2	971	U	C2-N1-C1'	6.03	124.94	117.70
2	2	2731	C	C5-C6-N1	6.03	124.02	121.00
8	8	90	C	C5-C6-N1	6.03	124.02	121.00
2	2	1094	G	N3-C4-C5	-6.03	125.59	128.60
2	2	4712	C	N1-C2-O2	6.03	122.52	118.90
8	8	99	U	C2-N1-C1'	6.03	124.93	117.70
2	2	4695	C	C5-C6-N1	6.03	124.01	121.00
8	8	113	C	C5-C6-N1	6.03	124.01	121.00
2	2	518	G	C4-N9-C1'	6.02	134.33	126.50
2	2	4562	C	N3-C2-O2	-6.02	117.68	121.90
2	2	427	A	C2-N3-C4	6.02	113.61	110.60
2	2	1508	A	C4-C5-C6	-6.02	113.99	117.00
2	2	2420	A	C4-C5-C6	-6.02	113.99	117.00
2	2	4263	C	C5-C6-N1	6.02	124.01	121.00
2	2	991	C	C6-N1-C2	-6.02	117.89	120.30
2	2	709	C	N1-C2-O2	6.02	122.51	118.90
2	2	746	A	N1-C2-N3	-6.02	126.29	129.30
2	2	1889	U	C2-N1-C1'	6.02	124.92	117.70
2	2	2849	A	N1-C6-N6	-6.02	114.99	118.60
2	2	1908	A	N1-C2-N3	-6.02	126.29	129.30
2	2	1293	G	C4-N9-C1'	6.01	134.32	126.50
2	2	919	C	C6-N1-C2	-6.01	117.89	120.30
2	2	1193	C	N3-C2-O2	-6.01	117.69	121.90
2	2	83	C	C5-C6-N1	6.01	124.00	121.00
2	2	929	A	N1-C2-N3	-6.01	126.30	129.30
2	2	1566	C	N1-C2-O2	6.01	122.51	118.90
8	8	4	C	C6-N1-C2	-6.01	117.89	120.30
2	2	400	A	N1-C2-N3	-6.01	126.30	129.30
2	2	2027	U	N3-C2-O2	-6.01	117.99	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1577	G	N1-C2-N2	6.01	121.61	116.20
2	2	3877	A	N1-C2-N3	-6.00	126.30	129.30
2	2	1884	C	C5-C6-N1	6.00	124.00	121.00
2	2	2107	C	C2-N1-C1'	6.00	125.40	118.80
2	2	2323	C	C6-N1-C2	-6.00	117.90	120.30
2	2	2418	A	N7-C8-N9	6.00	116.80	113.80
2	2	3943	A	N1-C2-N3	-6.00	126.30	129.30
2	2	4164	C	C5-C6-N1	6.00	124.00	121.00
2	2	4318	C	C6-N1-C2	-6.00	117.90	120.30
2	2	4474	A	N1-C2-N3	-6.00	126.30	129.30
2	2	4928	C	N1-C2-O2	6.00	122.50	118.90
2	2	1339	U	N3-C2-O2	-6.00	118.00	122.20
5	5	19	C	C6-N1-C2	-6.00	117.90	120.30
2	2	4318	C	C5-C6-N1	6.00	124.00	121.00
2	2	4641	U	N3-C2-O2	-6.00	118.00	122.20
2	2	1367	C	N3-C2-O2	-6.00	117.70	121.90
2	2	2713	C	C6-N1-C2	-6.00	117.90	120.30
2	2	4133	C	N1-C2-O2	6.00	122.50	118.90
2	2	56	A	C4-C5-C6	-5.99	114.00	117.00
2	2	363	A	C4-C5-C6	-5.99	114.00	117.00
2	2	1305	C	C5-C6-N1	5.99	124.00	121.00
2	2	1648	C	C5-C6-N1	5.99	124.00	121.00
2	2	1966	C	C6-N1-C2	-5.99	117.90	120.30
2	2	3920	U	N3-C2-O2	-5.99	118.00	122.20
8	8	150	C	N3-C2-O2	-5.99	117.70	121.90
2	2	2072	C	N1-C2-O2	5.99	122.50	118.90
2	2	2409	U	N3-C2-O2	-5.99	118.01	122.20
2	2	4622	A	C4-C5-C6	-5.99	114.00	117.00
2	2	10	A	C2-N3-C4	5.99	113.60	110.60
2	2	125	C	C5-C6-N1	5.99	124.00	121.00
2	2	350	C	N1-C2-O2	5.99	122.49	118.90
2	2	4255	A	N1-C2-N3	-5.99	126.30	129.30
2	2	4970	C	N1-C2-O2	5.99	122.49	118.90
2	2	2371	U	N1-C2-O2	5.99	126.99	122.80
2	2	5008	C	N3-C2-O2	-5.99	117.71	121.90
2	2	460	C	C6-N1-C2	-5.99	117.91	120.30
2	2	1293	G	N3-C4-C5	-5.99	125.61	128.60
2	2	1525	A	N1-C2-N3	-5.99	126.31	129.30
2	2	2094	G	C8-N9-C1'	-5.98	119.22	127.00
2	2	2798	A	N1-C2-N3	-5.98	126.31	129.30
2	2	3598	C	C5-C6-N1	5.98	123.99	121.00
2	2	3602	C	C6-N1-C2	-5.98	117.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1254	A	N1-C2-N3	-5.98	126.31	129.30
2	2	2537	A	N1-C2-N3	-5.98	126.31	129.30
8	8	153	C	C6-N1-C2	-5.98	117.91	120.30
2	2	2447	U	N1-C2-O2	5.98	126.98	122.80
2	2	2615	C	C2-N1-C1'	5.98	125.38	118.80
5	5	2	U	N3-C2-O2	-5.98	118.02	122.20
2	2	1913	C	C5-C6-N1	5.98	123.99	121.00
2	2	2892	C	C2-N1-C1'	5.98	125.37	118.80
2	2	155	C	N1-C2-O2	5.97	122.48	118.90
2	2	984	C	N1-C2-O2	5.97	122.48	118.90
2	2	4507	A	C2-N3-C4	5.97	113.59	110.60
2	2	1095	A	N1-C2-N3	-5.97	126.31	129.30
2	2	2667	C	C6-N1-C2	-5.97	117.91	120.30
2	2	3829	G	N3-C4-C5	-5.97	125.61	128.60
8	8	93	C	N1-C2-O2	5.97	122.48	118.90
2	2	4654	C	C5-C6-N1	5.97	123.99	121.00
2	2	1636	U	N3-C2-O2	-5.97	118.02	122.20
2	2	1957	U	N3-C2-O2	-5.97	118.02	122.20
2	2	3890	A	C5-C6-N1	5.97	120.68	117.70
2	2	1474	C	C5-C6-N1	5.96	123.98	121.00
2	2	986	C	C5-C6-N1	5.96	123.98	121.00
2	2	4955	A	C2-N3-C4	5.96	113.58	110.60
5	5	57	C	N1-C2-O2	5.96	122.48	118.90
2	2	1294	A	N1-C2-N3	-5.96	126.32	129.30
2	2	2412	A	C2-N3-C4	5.96	113.58	110.60
2	2	965	G	N3-C4-N9	5.96	129.57	126.00
2	2	1593	A	C4-C5-C6	-5.96	114.02	117.00
2	2	3854	C	C5-C6-N1	5.96	123.98	121.00
2	2	1275	G	O4'-C1'-N9	5.96	112.97	108.20
2	2	2589	C	C6-N1-C2	-5.96	117.92	120.30
2	2	4177	C	C5-C6-N1	5.96	123.98	121.00
2	2	4725	C	C6-N1-C2	-5.96	117.92	120.30
2	2	4860	G	N3-C4-N9	5.96	129.57	126.00
2	2	291	U	N3-C2-O2	-5.95	118.03	122.20
2	2	303	C	C5-C6-N1	5.95	123.98	121.00
5	5	33	U	N3-C2-O2	-5.95	118.03	122.20
2	2	917	A	C4-C5-C6	-5.95	114.02	117.00
2	2	1263	A	N1-C2-N3	-5.95	126.33	129.30
2	2	4860	G	C4-N9-C1'	5.95	134.24	126.50
2	2	4130	C	C5-C6-N1	5.95	123.97	121.00
2	2	2417	A	O4'-C1'-N9	5.95	112.96	108.20
2	2	3846	C	C5-C6-N1	5.95	123.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4332	C	C6-N1-C2	-5.95	117.92	120.30
9	9	15	LEU	CA-CB-CG	5.95	128.98	115.30
2	2	1447	C	N3-C2-O2	-5.95	117.74	121.90
2	2	1684	A	N1-C2-N3	-5.95	126.33	129.30
2	2	650	C	C6-N1-C2	-5.94	117.92	120.30
2	2	4144	C	C2-N1-C1'	5.94	125.34	118.80
2	2	4311	A	C4-C5-C6	-5.94	114.03	117.00
2	2	2375	A	C4-C5-C6	-5.94	114.03	117.00
2	2	2725	A	N1-C2-N3	-5.94	126.33	129.30
2	2	4561	C	N1-C2-O2	5.94	122.47	118.90
2	2	4639	G	C4-N9-C1'	5.94	134.22	126.50
2	2	1962	A	N1-C2-N3	-5.94	126.33	129.30
2	2	2692	U	N3-C2-O2	-5.94	118.04	122.20
2	2	4935	C	N3-C2-O2	-5.94	117.74	121.90
18	I	176	LEU	CA-CB-CG	5.94	128.95	115.30
2	2	1049	C	C6-N1-C1'	5.93	127.92	120.80
2	2	1344	C	C2-N1-C1'	5.93	125.33	118.80
2	2	2533	C	N1-C2-O2	5.93	122.46	118.90
2	2	2892	C	C6-N1-C2	-5.93	117.93	120.30
2	2	3711	A	N1-C2-N3	-5.93	126.33	129.30
5	5	102	U	C6-N1-C2	-5.93	117.44	121.00
2	2	1699	A	N1-C2-N3	-5.93	126.33	129.30
2	2	2059	C	C5-C6-N1	5.93	123.97	121.00
2	2	4723	A	N1-C2-N3	-5.93	126.33	129.30
2	2	4973	U	N3-C2-O2	-5.93	118.05	122.20
2	2	5038	A	N1-C2-N3	-5.93	126.33	129.30
8	8	28	C	N1-C2-O2	5.93	122.46	118.90
2	2	4074	C	C2-N1-C1'	5.93	125.32	118.80
2	2	4120	U	C2-N1-C1'	5.93	124.82	117.70
2	2	4983	C	C5-C6-N1	5.93	123.97	121.00
2	2	2371	U	C6-N1-C2	-5.92	117.45	121.00
2	2	1505	C	C6-N1-C2	-5.92	117.93	120.30
2	2	4569	U	N3-C2-O2	-5.92	118.06	122.20
2	2	4577	U	N3-C2-O2	-5.92	118.06	122.20
2	2	80	C	N1-C2-O2	5.92	122.45	118.90
2	2	1303	A	N1-C2-N3	-5.92	126.34	129.30
2	2	2445	C	N1-C2-O2	5.92	122.45	118.90
2	2	1505	C	C5-C6-N1	5.92	123.96	121.00
2	2	2329	U	N3-C2-O2	-5.92	118.06	122.20
2	2	3861	A	C2-N3-C4	5.92	113.56	110.60
5	5	30	C	C6-N1-C2	-5.92	117.93	120.30
2	2	4594	U	C6-N1-C2	-5.92	117.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1682	A	C2-N3-C4	5.91	113.56	110.60
11	B	304	SER	C-N-CA	5.91	136.48	121.70
2	2	2729	C	C2-N1-C1'	5.91	125.30	118.80
2	2	1254	A	N3-C4-N9	5.91	132.13	127.40
2	2	30	C	N3-C2-O2	-5.91	117.77	121.90
2	2	757	G	N3-C4-N9	5.91	129.54	126.00
2	2	4594	U	C2-N1-C1'	5.91	124.79	117.70
2	2	436	C	C5-C6-N1	5.91	123.95	121.00
2	2	2031	C	N3-C2-O2	-5.90	117.77	121.90
2	2	2721	G	C2-N3-C4	5.90	114.85	111.90
8	8	135	C	C6-N1-C2	-5.90	117.94	120.30
2	2	648	G	C8-N9-C1'	-5.90	119.33	127.00
2	2	1893	C	N3-C2-O2	-5.90	117.77	121.90
2	2	2704	C	N1-C2-O2	5.90	122.44	118.90
2	2	3632	C	C6-N1-C2	-5.90	117.94	120.30
2	2	1656	U	N1-C2-O2	5.90	126.93	122.80
2	2	294	G	C8-N9-C1'	-5.90	119.33	127.00
2	2	3830	A	N1-C2-N3	-5.90	126.35	129.30
2	2	4172	A	C2-N3-C4	5.90	113.55	110.60
8	8	118	C	N1-C2-O2	5.90	122.44	118.90
2	2	1859	C	C2-N3-C4	5.89	122.85	119.90
2	2	2292	C	C5-C6-N1	5.89	123.95	121.00
2	2	4969	C	C2-N3-C4	5.89	122.85	119.90
2	2	1726	U	C6-N1-C2	-5.89	117.47	121.00
2	2	4393	G	C8-N9-C4	-5.89	104.04	106.40
2	2	4905	C	C6-N1-C2	-5.89	117.94	120.30
2	2	2905	C	C6-N1-C2	-5.89	117.95	120.30
2	2	3781	C	C6-N1-C2	-5.89	117.95	120.30
2	2	1863	U	N1-C2-O2	5.88	126.92	122.80
2	2	2081	C	C5-C6-N1	5.88	123.94	121.00
2	2	2268	A	C4-C5-C6	-5.88	114.06	117.00
2	2	3848	U	N3-C2-O2	-5.88	118.08	122.20
2	2	4878	C	C5-C6-N1	5.88	123.94	121.00
2	2	1672	U	N1-C2-O2	5.88	126.92	122.80
2	2	2779	C	C6-N1-C2	-5.88	117.95	120.30
2	2	5037	U	N3-C2-O2	-5.88	118.08	122.20
2	2	209	U	C6-N1-C2	-5.88	117.47	121.00
4	4	417	TRP	CA-CB-CG	5.88	124.88	113.70
2	2	4639	G	N3-C4-C5	-5.88	125.66	128.60
2	2	2695	A	C4-C5-C6	-5.88	114.06	117.00
2	2	3604	A	C2-N3-C4	5.88	113.54	110.60
2	2	4746	C	N1-C2-O2	5.88	122.43	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1540	C	N3-C2-O2	-5.87	117.79	121.90
2	2	1499	C	C5-C6-N1	5.87	123.94	121.00
2	2	4668	U	N3-C2-O2	-5.87	118.09	122.20
5	5	69	U	N3-C2-O2	-5.87	118.09	122.20
2	2	1509	C	C5-C6-N1	5.87	123.94	121.00
2	2	1843	A	N1-C2-N3	-5.87	126.36	129.30
2	2	1203	G	N3-C4-N9	5.87	129.52	126.00
2	2	4674	C	N3-C2-O2	-5.87	117.79	121.90
2	2	2413	U	N3-C2-O2	-5.87	118.09	122.20
2	2	2611	A	C2-N3-C4	5.87	113.53	110.60
2	2	83	C	C6-N1-C2	-5.87	117.95	120.30
2	2	233	U	C4-C5-C6	5.87	123.22	119.70
2	2	256	G	C5-C6-O6	-5.87	125.08	128.60
2	2	4511	A	N1-C2-N3	-5.87	126.37	129.30
2	2	4561	C	C5-C6-N1	5.87	123.93	121.00
2	2	1906	U	C6-N1-C2	-5.86	117.48	121.00
2	2	2279	A	N1-C2-N3	-5.86	126.37	129.30
2	2	4886	C	N3-C2-O2	-5.86	117.80	121.90
2	2	1633	G	OP1-P-O3'	5.86	118.09	105.20
8	8	135	C	C5-C6-N1	5.86	123.93	121.00
2	2	304	C	C6-N1-C2	-5.86	117.96	120.30
2	2	734	G	C2-N3-C4	5.86	114.83	111.90
2	2	1274	A	N1-C2-N3	-5.86	126.37	129.30
2	2	2497	C	C2-N1-C1'	5.86	125.24	118.80
2	2	1190	C	N1-C2-O2	5.86	122.41	118.90
2	2	4749	C	C6-N1-C2	-5.86	117.96	120.30
2	2	4880	C	C2-N1-C1'	5.86	125.24	118.80
2	2	332	C	C6-N1-C2	-5.85	117.96	120.30
2	2	1404	G	C4-N9-C1'	5.85	134.11	126.50
2	2	152	U	C6-N1-C2	-5.85	117.49	121.00
2	2	1682	A	N1-C2-N3	-5.85	126.37	129.30
2	2	1850	A	C2-N3-C4	5.85	113.53	110.60
2	2	4770	U	N3-C2-O2	-5.85	118.10	122.20
2	2	2410	C	C2-N3-C4	5.85	122.82	119.90
8	8	59	A	C2-N3-C4	5.85	113.52	110.60
2	2	2537	A	C2-N3-C4	5.85	113.52	110.60
18	I	146	LEU	CA-CB-CG	5.85	128.75	115.30
2	2	1552	G	O4'-C1'-N9	5.85	112.88	108.20
2	2	4878	C	N1-C2-O2	5.84	122.41	118.90
2	2	376	A	C2-N3-C4	5.84	113.52	110.60
2	2	707	C	C5-C6-N1	5.84	123.92	121.00
2	2	663	G	C4-N9-C1'	5.84	134.09	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	105	A	C4-C5-C6	-5.84	114.08	117.00
2	2	905	C	C6-N1-C2	-5.84	117.97	120.30
2	2	3844	U	C6-N1-C2	-5.84	117.50	121.00
2	2	3847	C	C5-C6-N1	5.84	123.92	121.00
2	2	78	U	N1-C2-O2	5.84	126.89	122.80
2	2	421	C	C5-C6-N1	5.84	123.92	121.00
2	2	2372	U	N3-C2-O2	-5.84	118.11	122.20
2	2	4252	C	N1-C2-O2	5.84	122.40	118.90
2	2	1401	C	C5-C6-N1	5.83	123.92	121.00
2	2	1417	C	N3-C2-O2	-5.83	117.82	121.90
2	2	4722	G	N3-C4-C5	-5.83	125.68	128.60
8	8	83	C	C5-C6-N1	5.83	123.92	121.00
2	2	4158	C	C5-C6-N1	5.83	123.92	121.00
2	2	4145	C	C6-N1-C2	-5.83	117.97	120.30
2	2	4298	A	N1-C2-N3	-5.83	126.39	129.30
2	2	1837	A	C2-N3-C4	5.83	113.52	110.60
2	2	4348	A	C4-C5-C6	-5.83	114.08	117.00
2	2	4736	C	C6-N1-C2	-5.83	117.97	120.30
2	2	4350	C	C6-N1-C2	-5.83	117.97	120.30
2	2	152	U	N1-C2-O2	5.83	126.88	122.80
2	2	1921	C	C5-C6-N1	5.83	123.91	121.00
2	2	4303	C	O4'-C1'-N1	5.83	112.86	108.20
2	2	201	C	C6-N1-C2	-5.82	117.97	120.30
2	2	2601	A	N1-C2-N3	-5.82	126.39	129.30
2	2	4077	A	C2-N3-C4	5.82	113.51	110.60
2	2	2337	C	N3-C2-O2	-5.82	117.83	121.90
2	2	2690	C	C5-C6-N1	5.82	123.91	121.00
2	2	1345	A	C4-C5-C6	-5.82	114.09	117.00
2	2	1450	C	C2-N1-C1'	5.82	125.20	118.80
2	2	1901	C	C6-N1-C2	-5.82	117.97	120.30
2	2	2828	U	N3-C2-O2	-5.82	118.13	122.20
2	2	4274	A	N1-C2-N3	-5.82	126.39	129.30
2	2	436	C	C2-N1-C1'	5.82	125.20	118.80
2	2	1560	A	N1-C2-N3	-5.82	126.39	129.30
2	2	2762	G	C8-N9-C4	-5.82	104.07	106.40
2	2	4207	C	C5-C6-N1	5.82	123.91	121.00
2	2	4945	G	C5-N7-C8	-5.82	101.39	104.30
2	2	4896	G	C4-N9-C1'	5.81	134.06	126.50
2	2	2302	C	N1-C2-O2	5.81	122.39	118.90
2	2	2534	C	C5-C6-N1	5.81	123.91	121.00
2	2	3931	C	C5-C6-N1	5.81	123.91	121.00
2	2	3774	A	N1-C2-N3	-5.81	126.39	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2446	C	N1-C2-O2	5.81	122.39	118.90
2	2	2836	A	N1-C2-N3	-5.81	126.40	129.30
2	2	3824	A	C4-C5-C6	-5.80	114.10	117.00
2	2	86	U	N1-C2-O2	5.80	126.86	122.80
2	2	1201	U	N1-C2-O2	5.80	126.86	122.80
2	2	1960	A	C2-N3-C4	5.80	113.50	110.60
2	2	66	A	C4-C5-C6	-5.79	114.10	117.00
2	2	458	C	N1-C2-O2	5.79	122.38	118.90
2	2	4980	C	N1-C2-O2	5.79	122.38	118.90
2	2	1282	G	N3-C4-N9	5.79	129.48	126.00
2	2	2304	U	N1-C2-O2	5.79	126.86	122.80
2	2	2629	C	C5-C6-N1	5.79	123.90	121.00
8	8	26	C	N1-C2-O2	5.79	122.38	118.90
2	2	3734	U	N1-C2-O2	5.79	126.86	122.80
2	2	4158	C	C6-N1-C2	-5.79	117.98	120.30
2	2	204	U	C5-C6-N1	5.79	125.59	122.70
2	2	2561	C	N3-C2-O2	-5.79	117.85	121.90
2	2	2051	C	C5-C6-N1	5.79	123.89	121.00
8	8	96	C	C6-N1-C2	-5.79	117.98	120.30
38	e	90	ARG	C-N-CA	5.79	136.17	121.70
2	2	4687	A	N9-C4-C5	-5.79	103.48	105.80
2	2	4939	C	C6-N1-C2	-5.79	117.99	120.30
5	5	29	C	N3-C2-O2	-5.79	117.85	121.90
2	2	1877	G	N3-C4-C5	-5.78	125.71	128.60
2	2	2334	C	C6-N1-C2	-5.78	117.99	120.30
2	2	3680	U	C5-C6-N1	5.78	125.59	122.70
2	2	227	A	C4-C5-C6	-5.78	114.11	117.00
2	2	256	G	N7-C8-N9	5.78	115.99	113.10
2	2	1327	C	C5-C6-N1	5.78	123.89	121.00
2	2	2250	C	C5-C6-N1	5.78	123.89	121.00
2	2	2783	A	N7-C8-N9	5.78	116.69	113.80
2	2	4709	U	C5-C6-N1	5.78	125.59	122.70
2	2	4885	U	N1-C2-O2	5.78	126.84	122.80
2	2	1082	C	O4'-C1'-N1	5.77	112.82	108.20
2	2	1281	G	C4-N9-C1'	5.77	134.00	126.50
2	2	2853	C	N1-C2-O2	5.77	122.36	118.90
2	2	424	U	N3-C2-O2	-5.77	118.16	122.20
2	2	759	G	N3-C4-N9	5.77	129.46	126.00
2	2	754	U	N3-C2-O2	-5.77	118.16	122.20
2	2	966	A	N1-C2-N3	-5.77	126.42	129.30
2	2	1350	C	C6-N1-C2	-5.77	117.99	120.30
2	2	2066	C	N1-C2-O2	5.77	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3599	A	N1-C2-N3	-5.77	126.42	129.30
2	2	4336	A	C4-C5-C6	-5.77	114.11	117.00
2	2	4689	U	C5-C6-N1	5.77	125.58	122.70
4	4	261	CYS	CA-CB-SG	5.77	124.39	114.00
2	2	2772	C	N1-C2-O2	5.77	122.36	118.90
2	2	3844	U	N1-C2-O2	5.77	126.84	122.80
2	2	4363	A	N1-C2-N3	-5.77	126.42	129.30
2	2	4613	C	C5-C6-N1	5.77	123.88	121.00
2	2	4705	A	C2-N3-C4	5.77	113.48	110.60
2	2	5048	A	C2-N3-C4	5.77	113.48	110.60
8	8	71	A	N1-C2-N3	-5.77	126.42	129.30
2	2	455	C	N1-C2-O2	5.76	122.36	118.90
2	2	1944	A	N1-C2-N3	-5.76	126.42	129.30
2	2	4695	C	C2-N1-C1'	5.76	125.14	118.80
2	2	4608	G	C4-C5-N7	5.76	113.11	110.80
2	2	750	U	N1-C2-O2	5.76	126.83	122.80
2	2	919	C	N1-C2-O2	5.76	122.36	118.90
2	2	1255	A	N1-C2-N3	-5.76	126.42	129.30
2	2	4271	A	C4-C5-C6	-5.76	114.12	117.00
2	2	4707	A	C4-C5-C6	-5.76	114.12	117.00
2	2	196	C	C6-N1-C2	-5.76	118.00	120.30
2	2	4648	A	C2-N3-C4	5.76	113.48	110.60
2	2	5002	U	C2-N1-C1'	5.76	124.61	117.70
2	2	1812	C	C6-N1-C2	-5.76	118.00	120.30
2	2	3845	A	C2-N3-C4	5.76	113.48	110.60
2	2	5056	A	N1-C2-N3	-5.76	126.42	129.30
5	5	80	U	N3-C2-O2	-5.76	118.17	122.20
8	8	111	U	C6-N1-C1'	-5.75	113.14	121.20
2	2	74	G	C8-N9-C1'	-5.75	119.52	127.00
2	2	732	A	C2-N3-C4	5.75	113.47	110.60
2	2	1579	C	N1-C2-O2	5.75	122.35	118.90
2	2	1923	A	C2-N3-C4	5.75	113.48	110.60
2	2	204	U	C2-N1-C1'	5.75	124.60	117.70
2	2	1397	A	C4-C5-C6	-5.75	114.12	117.00
2	2	1832	C	C5-C6-N1	5.75	123.87	121.00
2	2	256	G	C4-C5-C6	5.75	122.25	118.80
2	2	1796	U	N1-C2-O2	5.75	126.82	122.80
2	2	4140	C	C2-N1-C1'	5.75	125.12	118.80
2	2	4224	A	C4-C5-C6	-5.75	114.13	117.00
2	2	4476	C	C6-N1-C1'	-5.75	113.91	120.80
2	2	4675	U	N3-C2-O2	-5.75	118.18	122.20
2	2	972	C	C2-N1-C1'	5.75	125.12	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1320	U	C2-N1-C1'	5.75	124.59	117.70
2	2	4985	U	N1-C2-O2	5.75	126.82	122.80
2	2	5061	A	C2-N3-C4	5.75	113.47	110.60
2	2	1293	G	C2-N3-C4	5.74	114.77	111.90
2	2	1357	C	C6-N1-C2	-5.74	118.00	120.30
2	2	2023	C	N1-C2-O2	5.74	122.35	118.90
2	2	338	A	C4-C5-C6	-5.74	114.13	117.00
2	2	757	G	N3-C4-C5	-5.74	125.73	128.60
2	2	2062	C	C5-C6-N1	5.74	123.87	121.00
2	2	3611	A	N1-C2-N3	-5.74	126.43	129.30
2	2	2484	A	N3-C4-N9	5.74	131.99	127.40
2	2	4251	A	N1-C2-N3	-5.74	126.43	129.30
2	2	126	C	C6-N1-C2	-5.74	118.00	120.30
2	2	1970	A	N1-C2-N3	-5.74	126.43	129.30
2	2	3831	U	N3-C2-O2	-5.74	118.18	122.20
5	5	46	C	C6-N1-C2	-5.74	118.00	120.30
2	2	1428	U	C5-C6-N1	5.74	125.57	122.70
2	2	5050	C	C5-C6-N1	5.74	123.87	121.00
2	2	1345	A	N1-C2-N3	-5.74	126.43	129.30
2	2	1801	A	C2-N3-C4	5.74	113.47	110.60
2	2	3882	C	C5-C6-N1	5.74	123.87	121.00
2	2	4396	A	C2-N3-C4	5.74	113.47	110.60
22	N	94	LEU	CA-CB-CG	5.74	128.49	115.30
2	2	2439	G	C8-N9-C1'	-5.73	119.55	127.00
2	2	4078	C	C5-C6-N1	5.73	123.87	121.00
2	2	4940	C	C6-N1-C2	-5.73	118.01	120.30
5	5	4	U	C2-N1-C1'	5.73	124.58	117.70
2	2	2701	U	N1-C2-O2	5.73	126.81	122.80
2	2	4388	A	N1-C2-N3	-5.73	126.43	129.30
2	2	1821	G	C4-N9-C1'	5.73	133.95	126.50
2	2	2505	C	N3-C2-O2	-5.73	117.89	121.90
2	2	2589	C	N1-C2-O2	5.73	122.34	118.90
2	2	4504	C	C5-C6-N1	5.73	123.86	121.00
8	8	92	U	C6-N1-C2	-5.73	117.56	121.00
2	2	319	A	C4-C5-C6	-5.72	114.14	117.00
2	2	4722	G	N3-C4-N9	5.72	129.43	126.00
2	2	4970	C	C5-C6-N1	5.72	123.86	121.00
4	4	72	LEU	CA-CB-CG	5.72	128.46	115.30
2	2	511	C	N1-C2-O2	5.72	122.33	118.90
2	2	1343	A	N1-C2-N3	-5.72	126.44	129.30
2	2	1418	C	C5-C6-N1	5.72	123.86	121.00
2	2	1401	C	C6-N1-C2	-5.72	118.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	333	U	N3-C2-O2	-5.71	118.20	122.20
2	2	2334	C	C5-C6-N1	5.71	123.86	121.00
2	2	3939	G	N3-C4-N9	5.71	129.43	126.00
8	8	153	C	C5-C6-N1	5.71	123.86	121.00
2	2	158	A	C4-C5-C6	-5.71	114.14	117.00
2	2	4728	U	N1-C2-O2	5.71	126.80	122.80
2	2	4424	A	C2-N3-C4	5.71	113.46	110.60
11	B	364	ASP	CB-CG-OD1	5.71	123.44	118.30
2	2	1926	C	C5-C6-N1	5.71	123.86	121.00
2	2	648	G	N3-C4-C5	-5.71	125.75	128.60
2	2	2384	U	N3-C2-O2	-5.71	118.20	122.20
2	2	4940	C	C5-C6-N1	5.71	123.85	121.00
2	2	5001	U	N3-C2-O2	-5.71	118.20	122.20
2	2	1214	C	N1-C2-O2	5.71	122.32	118.90
2	2	1966	C	C5-C6-N1	5.70	123.85	121.00
2	2	3890	A	C2-N3-C4	5.70	113.45	110.60
2	2	659	G	N3-C4-C5	-5.70	125.75	128.60
2	2	3870	C	C2-N3-C4	5.70	122.75	119.90
4	4	306	ILE	CG1-CB-CG2	-5.70	98.86	111.40
2	2	4071	U	N3-C2-O2	-5.70	118.21	122.20
2	2	4363	A	C2-N3-C4	5.70	113.45	110.60
8	8	26	C	C5-C6-N1	5.70	123.85	121.00
2	2	2110	C	N1-C2-O2	5.70	122.32	118.90
2	2	2295	C	C6-N1-C2	-5.70	118.02	120.30
2	2	1285	U	N3-C2-O2	-5.69	118.21	122.20
2	2	2351	C	N3-C2-O2	-5.69	117.91	121.90
2	2	4102	C	N3-C2-O2	-5.69	117.92	121.90
2	2	4343	U	N1-C2-O2	5.69	126.78	122.80
2	2	4515	G	C2-N3-C4	5.69	114.75	111.90
11	B	292	LEU	CA-CB-CG	5.69	128.39	115.30
2	2	256	G	N3-C4-C5	-5.69	125.75	128.60
2	2	3650	C	N1-C2-O2	5.69	122.31	118.90
2	2	4155	C	N3-C2-O2	-5.69	117.92	121.90
2	2	197	A	N1-C2-N3	-5.69	126.46	129.30
2	2	975	C	N1-C2-O2	5.69	122.31	118.90
2	2	2253	A	N1-C2-N3	-5.69	126.46	129.30
2	2	1197	C	C2-N1-C1'	5.68	125.05	118.80
2	2	1447	C	C2-N1-C1'	5.68	125.05	118.80
2	2	3846	C	C6-N1-C2	-5.68	118.03	120.30
2	2	493	G	N3-C4-C5	-5.68	125.76	128.60
2	2	2533	C	C5-C6-N1	5.68	123.84	121.00
2	2	221	C	C6-N1-C2	-5.68	118.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	358	C	C6-N1-C2	-5.68	118.03	120.30
2	2	2427	G	N1-C6-O6	-5.68	116.49	119.90
2	2	704	C	C2-N1-C1'	5.68	125.05	118.80
2	2	974	C	C5-C6-N1	5.68	123.84	121.00
2	2	5044	A	C2-N3-C4	5.68	113.44	110.60
6	6	131	ASP	CB-CG-OD1	5.68	123.41	118.30
2	2	4770	U	N1-C2-O2	5.67	126.77	122.80
2	2	2654	C	C5-C6-N1	5.67	123.84	121.00
8	8	88	A	C2-N3-C4	5.67	113.44	110.60
2	2	1198	G	C4-N9-C1'	5.67	133.87	126.50
8	8	130	C	C5-C6-N1	5.67	123.83	121.00
2	2	2083	C	C6-N1-C2	-5.67	118.03	120.30
2	2	2544	G	C8-N9-C1'	-5.67	119.63	127.00
5	5	115	A	C4-C5-C6	-5.67	114.17	117.00
2	2	1464	C	C6-N1-C2	-5.67	118.03	120.30
2	2	3748	A	C2-N3-C4	5.67	113.44	110.60
2	2	4738	C	N1-C2-O2	5.67	122.30	118.90
8	8	155	C	N1-C2-O2	5.67	122.30	118.90
2	2	326	C	C2-N1-C1'	5.67	125.03	118.80
2	2	2803	U	C6-N1-C2	-5.67	117.60	121.00
2	2	4186	A	C4-C5-C6	-5.67	114.17	117.00
2	2	4213	A	C2-N3-C4	5.67	113.43	110.60
2	2	406	C	C2'-C3'-O3'	5.66	122.76	113.70
2	2	4227	U	N3-C2-O2	-5.66	118.24	122.20
2	2	4513	A	N1-C2-N3	-5.66	126.47	129.30
2	2	706	C	C5-C6-N1	5.66	123.83	121.00
2	2	2031	C	C2-N1-C1'	5.66	125.03	118.80
2	2	2892	C	C5-C6-N1	5.66	123.83	121.00
2	2	70	A	C4-C5-C6	-5.66	114.17	117.00
2	2	2085	G	N3-C4-N9	5.66	129.39	126.00
2	2	1412	G	C4-C5-N7	5.65	113.06	110.80
2	2	4237	C	N1-C2-O2	5.65	122.29	118.90
2	2	365	U	C2-N1-C1'	5.65	124.48	117.70
2	2	458	C	C5-C6-N1	5.65	123.83	121.00
2	2	1343	A	C2-N3-C4	5.65	113.42	110.60
2	2	4414	A	C4-C5-C6	-5.65	114.17	117.00
2	2	5030	U	N3-C4-O4	5.65	123.36	119.40
5	5	29	C	C5-C6-N1	5.65	123.83	121.00
2	2	2458	C	N1-C2-O2	5.65	122.29	118.90
2	2	1387	A	C4-C5-C6	-5.65	114.18	117.00
2	2	1592	G	C8-N9-C1'	-5.65	119.66	127.00
2	2	2593	C	C2-N1-C1'	5.65	125.01	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2601	A	C4-C5-C6	-5.64	114.18	117.00
2	2	466	A	C2-N3-C4	5.64	113.42	110.60
2	2	3647	A	C4-C5-C6	-5.64	114.18	117.00
2	2	1072	C	C5-C6-N1	5.64	123.82	121.00
2	2	1929	A	N3-C4-N9	5.64	131.91	127.40
2	2	4469	U	N3-C2-O2	-5.64	118.25	122.20
2	2	991	C	N3-C2-O2	-5.64	117.95	121.90
2	2	1947	U	N1-C2-O2	5.64	126.75	122.80
2	2	4337	C	C6-N1-C2	-5.64	118.05	120.30
2	2	4350	C	C5-C6-N1	5.64	123.82	121.00
2	2	239	C	C6-N1-C2	-5.63	118.05	120.30
2	2	4950	U	C2-N1-C1'	5.63	124.46	117.70
2	2	3657	U	N1-C2-O2	5.63	126.74	122.80
2	2	2362	U	C6-N1-C2	-5.63	117.62	121.00
2	2	4963	G	C8-N9-C4	-5.63	104.15	106.40
8	8	45	C	C6-N1-C2	-5.63	118.05	120.30
2	2	117	C	C5-C6-N1	5.63	123.81	121.00
2	2	1807	C	C6-N1-C2	-5.63	118.05	120.30
2	2	2264	C	C5-C6-N1	5.63	123.81	121.00
2	2	2779	C	C5-C6-N1	5.63	123.81	121.00
2	2	1557	C	C5-C6-N1	5.62	123.81	121.00
2	2	717	U	N3-C2-O2	-5.62	118.26	122.20
2	2	2465	C	C2-N1-C1'	5.62	124.98	118.80
2	2	2551	A	C2-N3-C4	5.62	113.41	110.60
2	2	2869	U	N1-C2-O2	5.62	126.74	122.80
2	2	2439	G	N3-C4-C5	-5.62	125.79	128.60
2	2	2447	U	C6-N1-C2	-5.62	117.63	121.00
2	2	4262	C	C5-C6-N1	5.62	123.81	121.00
2	2	4337	C	C5-C6-N1	5.62	123.81	121.00
2	2	4773	C	C2-N1-C1'	5.62	124.98	118.80
2	2	4906	C	C2-N1-C1'	5.62	124.98	118.80
8	8	72	A	C2-N3-C4	5.62	113.41	110.60
2	2	2843	U	C6-N1-C2	-5.62	117.63	121.00
2	2	3902	A	N1-C2-N3	-5.62	126.49	129.30
2	2	4298	A	C5-C6-N1	5.62	120.51	117.70
2	2	47	A	C4-C5-C6	-5.62	114.19	117.00
2	2	1538	U	N3-C2-O2	-5.62	118.27	122.20
2	2	3779	A	N1-C2-N3	-5.62	126.49	129.30
2	2	3663	A	N1-C2-N3	-5.62	126.49	129.30
2	2	2347	A	C4-C5-C6	-5.61	114.19	117.00
2	2	3853	U	C2-N1-C1'	5.61	124.44	117.70
2	2	4609	G	C5-C6-O6	-5.61	125.23	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2036	C	C6-N1-C2	-5.61	118.06	120.30
2	2	4905	C	N1-C2-O2	5.61	122.27	118.90
2	2	27	C	C2-N1-C1'	5.61	124.97	118.80
2	2	2325	C	N1-C2-O2	5.61	122.27	118.90
2	2	2607	C	C5-C6-N1	5.61	123.81	121.00
2	2	2673	G	C2-N3-C4	5.61	114.70	111.90
8	8	57	C	N3-C2-O2	-5.61	117.97	121.90
2	2	111	C	C5-C6-N1	5.61	123.80	121.00
2	2	168	C	C6-N1-C2	-5.61	118.06	120.30
2	2	1634	A	C2-N3-C4	5.61	113.40	110.60
2	2	2806	A	C4-C5-N7	5.61	113.50	110.70
2	2	3733	A	N1-C2-N3	-5.61	126.50	129.30
2	2	4488	A	C4-C5-C6	-5.61	114.20	117.00
2	2	3905	A	OP2-P-O3'	5.61	117.53	105.20
2	2	4128	A	N1-C2-N3	-5.60	126.50	129.30
2	2	1094	G	N3-C4-N9	5.60	129.36	126.00
2	2	1572	U	N1-C2-O2	5.60	126.72	122.80
2	2	2021	G	C4-N9-C1'	5.60	133.78	126.50
2	2	3823	G	N3-C4-N9	5.60	129.36	126.00
2	2	4251	A	C4-C5-C6	-5.60	114.20	117.00
2	2	4319	C	C6-N1-C2	-5.60	118.06	120.30
2	2	4752	U	N3-C2-O2	-5.60	118.28	122.20
2	2	1967	A	C2-N3-C4	5.60	113.40	110.60
2	2	3690	U	N1-C2-O2	5.60	126.72	122.80
2	2	4559	A	C4-C5-C6	-5.60	114.20	117.00
2	2	4393	G	N9-C4-C5	5.60	107.64	105.40
2	2	4561	C	C2-N1-C1'	5.60	124.96	118.80
5	5	35	U	N1-C2-O2	5.60	126.72	122.80
2	2	1507	C	C5-C6-N1	5.60	123.80	121.00
2	2	2509	C	C6-N1-C2	-5.60	118.06	120.30
2	2	1294	A	O4'-C1'-N9	5.59	112.68	108.20
2	2	1365	C	N1-C2-O2	5.59	122.25	118.90
2	2	2249	C	C6-N1-C2	-5.59	118.06	120.30
2	2	2540	C	C5-C6-N1	5.59	123.79	121.00
8	8	52	A	C2-N3-C4	5.59	113.39	110.60
2	2	3915	U	C6-N1-C2	-5.59	117.65	121.00
2	2	4072	C	C6-N1-C2	-5.59	118.06	120.30
2	2	274	C	C2-N1-C1'	5.59	124.94	118.80
2	2	759	G	C2-N3-C4	5.59	114.69	111.90
2	2	1963	C	C5-C6-N1	5.59	123.79	121.00
2	2	4603	C	C6-N1-C2	-5.59	118.06	120.30
5	5	78	C	N1-C2-O2	5.59	122.25	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1896	A	C4-C5-C6	-5.58	114.21	117.00
2	2	723	A	C4-C5-C6	-5.58	114.21	117.00
2	2	1286	C	C5-C6-N1	5.58	123.79	121.00
5	5	44	C	C6-N1-C2	-5.58	118.07	120.30
23	O	13	LEU	CA-CB-CG	5.58	128.14	115.30
2	2	1731	C	N3-C2-O2	-5.58	117.99	121.90
2	2	4386	C	N1-C2-O2	5.58	122.25	118.90
2	2	4699	U	OP1-P-O3'	5.58	117.48	105.20
2	2	709	C	C5-C6-N1	5.58	123.79	121.00
2	2	300	A	C4-C5-C6	-5.58	114.21	117.00
2	2	2430	C	C6-N1-C2	-5.58	118.07	120.30
2	2	4945	G	C4-N9-C1'	5.58	133.75	126.50
2	2	299	C	C5-C6-N1	5.58	123.79	121.00
2	2	2538	U	N3-C2-O2	-5.58	118.30	122.20
2	2	89	C	C5-C6-N1	5.58	123.79	121.00
2	2	419	A	C4-C5-C6	-5.58	114.21	117.00
2	2	1907	A	C2-N3-C4	5.58	113.39	110.60
2	2	2627	C	N3-C2-O2	-5.58	118.00	121.90
2	2	2726	G	C4-N9-C1'	5.58	133.75	126.50
2	2	4907	G	N3-C4-N9	5.58	129.34	126.00
2	2	318	A	C2-N3-C4	5.57	113.39	110.60
2	2	703	G	C4-N9-C1'	5.57	133.75	126.50
2	2	1791	U	N1-C2-O2	5.57	126.70	122.80
2	2	4119	C	C6-N1-C1'	-5.57	114.11	120.80
2	2	4615	C	N1-C2-O2	5.57	122.24	118.90
8	8	148	A	C4-C5-C6	-5.57	114.21	117.00
2	2	88	A	C2-N3-C4	5.57	113.39	110.60
2	2	1818	G	O4'-C1'-N9	5.57	112.66	108.20
2	2	2304	U	C2-N1-C1'	5.57	124.39	117.70
2	2	4248	A	N1-C2-N3	-5.57	126.52	129.30
2	2	4314	C	N3-C2-O2	-5.57	118.00	121.90
2	2	2272	C	C5-C6-N1	5.57	123.78	121.00
2	2	2290	C	C6-N1-C2	-5.57	118.07	120.30
2	2	4119	C	C2-N3-C4	5.57	122.69	119.90
2	2	3668	C	N1-C2-O2	5.57	122.24	118.90
2	2	1085	C	C5-C6-N1	5.57	123.78	121.00
2	2	1577	G	N9-C4-C5	5.57	107.63	105.40
2	2	1839	U	N3-C2-O2	-5.57	118.30	122.20
2	2	2496	G	N3-C4-N9	5.57	129.34	126.00
2	2	4223	C	C5-C6-N1	5.57	123.78	121.00
2	2	4748	U	N3-C2-O2	-5.57	118.30	122.20
5	5	96	U	N3-C2-O2	-5.57	118.30	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	84	A	C4-C5-C6	-5.56	114.22	117.00
2	2	981	C	C6-N1-C2	-5.56	118.08	120.30
2	2	4393	G	C5-C6-N1	-5.56	108.72	111.50
2	2	62	A	C5-C6-N1	5.56	120.48	117.70
2	2	513	U	C5-C6-N1	5.56	125.48	122.70
5	5	74	A	C2-N3-C4	5.56	113.38	110.60
5	5	74	A	C4-C5-C6	-5.56	114.22	117.00
2	2	2017	A	C4-N9-C1'	5.56	136.30	126.30
2	2	2767	U	N3-C2-O2	-5.56	118.31	122.20
2	2	3709	U	C6-N1-C2	-5.56	117.67	121.00
2	2	3832	U	N3-C2-O2	-5.56	118.31	122.20
2	2	4461	C	C5-C6-N1	5.56	123.78	121.00
2	2	1947	U	N3-C2-O2	-5.56	118.31	122.20
2	2	3707	U	N3-C2-O2	-5.55	118.31	122.20
2	2	1439	C	N1-C2-O2	5.55	122.23	118.90
2	2	155	C	N3-C2-O2	-5.55	118.01	121.90
2	2	1737	A	C2-N3-C4	5.55	113.38	110.60
2	2	2426	U	N3-C2-O2	-5.55	118.31	122.20
2	2	489	C	C6-N1-C1'	-5.55	114.14	120.80
2	2	4532	U	C6-N1-C2	-5.55	117.67	121.00
2	2	4537	C	N1-C2-O2	5.55	122.23	118.90
2	2	4655	A	C4-C5-C6	-5.55	114.22	117.00
2	2	2511	A	C4-C5-C6	-5.55	114.23	117.00
2	2	4253	A	N1-C2-N3	-5.55	126.53	129.30
2	2	2671	C	C6-N1-C2	-5.55	118.08	120.30
2	2	4664	A	C2-N3-C4	5.55	113.37	110.60
2	2	5051	C	N1-C2-O2	5.55	122.23	118.90
13	D	229	LEU	CA-CB-CG	5.55	128.06	115.30
2	2	919	C	N3-C2-O2	-5.54	118.02	121.90
2	2	1443	A	N1-C2-N3	-5.54	126.53	129.30
2	2	2085	G	C8-N9-C1'	-5.54	119.79	127.00
2	2	2498	C	C6-N1-C2	-5.54	118.08	120.30
2	2	2563	C	N1-C2-O2	5.54	122.23	118.90
2	2	105	A	N1-C2-N3	-5.54	126.53	129.30
2	2	329	A	C2-N3-C4	5.54	113.37	110.60
2	2	1913	C	N3-C2-O2	-5.54	118.02	121.90
2	2	2595	C	N1-C2-O2	5.54	122.22	118.90
2	2	4268	A	C2-N3-C4	5.54	113.37	110.60
2	2	1870	C	N1-C2-O2	5.54	122.22	118.90
9	9	11	ARG	N-CA-C	5.54	125.96	111.00
2	2	1293	G	N3-C4-N9	5.54	129.32	126.00
8	8	1	C	C5-C6-N1	5.54	123.77	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1395	U	N1-C2-O2	5.54	126.68	122.80
2	2	2699	C	C5-C6-N1	5.54	123.77	121.00
2	2	2710	C	C5-C6-N1	5.54	123.77	121.00
2	2	4945	G	C5-C6-N1	5.54	114.27	111.50
8	8	89	U	N3-C2-O2	-5.54	118.33	122.20
2	2	5038	A	C4-C5-C6	-5.53	114.23	117.00
2	2	905	C	C5-C6-N1	5.53	123.77	121.00
2	2	975	C	C5-C6-N1	5.53	123.77	121.00
2	2	1650	A	C4-C5-C6	-5.53	114.23	117.00
2	2	2850	A	C4-N9-C1'	5.53	136.25	126.30
2	2	2894	A	C2-N3-C4	5.53	113.36	110.60
2	2	4243	C	N1-C2-O2	5.53	122.22	118.90
2	2	3612	C	C5-C6-N1	5.53	123.76	121.00
2	2	694	C	C5-C6-N1	5.53	123.76	121.00
2	2	3841	C	C5-C6-N1	5.53	123.76	121.00
2	2	1337	A	N1-C2-N3	-5.52	126.54	129.30
2	2	1378	C	C6-N1-C1'	-5.52	114.17	120.80
2	2	3824	A	C2-N3-C4	5.52	113.36	110.60
2	2	4107	G	C4-N9-C1'	5.52	133.68	126.50
2	2	4624	A	C2-N3-C4	5.52	113.36	110.60
2	2	1304	C	C6-N1-C2	-5.52	118.09	120.30
2	2	1428	U	C6-N1-C2	-5.52	117.69	121.00
2	2	3734	U	N3-C2-O2	-5.52	118.33	122.20
2	2	4508	C	C2-N3-C4	5.52	122.66	119.90
4	4	41	HIS	C-N-CA	5.52	135.50	121.70
2	2	2360	A	C4-C5-C6	-5.52	114.24	117.00
2	2	4281	A	C8-N9-C4	-5.52	103.59	105.80
2	2	383	A	C4-C5-C6	-5.52	114.24	117.00
2	2	2690	C	C6-N1-C2	-5.52	118.09	120.30
2	2	4913	G	OP2-P-O3'	5.52	117.33	105.20
2	2	1556	C	C5-C6-N1	5.51	123.76	121.00
2	2	1949	U	C6-N1-C2	-5.51	117.69	121.00
2	2	4295	U	N3-C2-O2	-5.51	118.34	122.20
2	2	4896	G	N3-C4-C5	-5.51	125.84	128.60
22	N	174	ILE	CG1-CB-CG2	-5.51	99.27	111.40
2	2	252	C	C6-N1-C2	-5.51	118.09	120.30
2	2	1663	C	C2-N1-C1'	5.51	124.86	118.80
2	2	2319	C	N1-C2-O2	5.51	122.21	118.90
5	5	34	C	C5-C6-N1	5.51	123.76	121.00
2	2	4188	U	N3-C2-O2	-5.51	118.34	122.20
2	2	4689	U	N3-C2-O2	-5.51	118.34	122.20
8	8	21	C	N1-C2-O2	5.51	122.21	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4928	C	C6-N1-C1'	-5.51	114.19	120.80
2	2	1901	C	C5-C6-N1	5.51	123.75	121.00
2	2	1178	G	N3-C4-N9	5.50	129.30	126.00
2	2	1812	C	N1-C2-O2	5.50	122.20	118.90
4	4	284	LEU	CB-CG-CD1	-5.50	101.64	111.00
5	5	34	C	C6-N1-C2	-5.50	118.10	120.30
48	p	220	MET	C-N-CA	5.50	135.46	121.70
2	2	1461	C	C6-N1-C2	-5.50	118.10	120.30
2	2	447	C	C6-N1-C2	-5.50	118.10	120.30
2	2	3597	G	O5'-P-OP1	-5.50	100.75	105.70
2	2	4608	G	O4'-C1'-N9	5.50	112.60	108.20
2	2	3823	G	N3-C4-C5	-5.50	125.85	128.60
2	2	488	G	N3-C4-C5	-5.50	125.85	128.60
2	2	1314	C	O5'-P-OP2	-5.50	100.75	105.70
2	2	2905	C	C5-C6-N1	5.50	123.75	121.00
2	2	4694	G	O4'-C1'-N9	5.50	112.60	108.20
2	2	141	C	C2-N1-C1'	5.50	124.85	118.80
2	2	2866	C	C5-C6-N1	5.50	123.75	121.00
2	2	4981	G	C8-N9-C1'	-5.50	119.86	127.00
16	G	131	LYS	C-N-CA	5.50	135.44	121.70
2	2	42	A	C4-C5-C6	-5.49	114.25	117.00
2	2	659	G	N3-C4-N9	5.49	129.30	126.00
2	2	1684	A	C4-C5-C6	-5.49	114.25	117.00
2	2	4319	C	C5-C6-N1	5.49	123.75	121.00
2	2	5025	C	C5-C6-N1	5.49	123.75	121.00
48	p	28	LEU	CA-CB-CG	5.49	127.94	115.30
2	2	450	G	N3-C4-N9	5.49	129.29	126.00
2	2	4559	A	C6-N1-C2	5.49	121.89	118.60
2	2	4977	A	C2-N3-C4	5.49	113.34	110.60
8	8	98	C	C6-N1-C2	-5.49	118.10	120.30
2	2	355	A	C2-N3-C4	5.49	113.34	110.60
2	2	1661	C	C6-N1-C2	-5.49	118.11	120.30
2	2	4308	C	C5-C6-N1	5.49	123.74	121.00
2	2	1873	A	N1-C2-N3	-5.49	126.56	129.30
2	2	4215	C	C2-N1-C1'	5.48	124.83	118.80
2	2	1655	C	C5-C6-N1	5.48	123.74	121.00
2	2	4230	C	C6-N1-C2	-5.48	118.11	120.30
2	2	504	G	C8-N9-C4	-5.48	104.21	106.40
2	2	3833	C	C6-N1-C2	-5.48	118.11	120.30
5	5	22	A	C4-N9-C1'	5.48	136.16	126.30
8	8	126	C	C2-N3-C4	5.48	122.64	119.90
2	2	51	A	C2-N3-C4	5.48	113.34	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1467	C	N1-C2-O2	5.48	122.19	118.90
2	2	1917	A	C4-C5-C6	-5.48	114.26	117.00
2	2	2041	A	N1-C2-N3	-5.48	126.56	129.30
2	2	4688	C	N1-C2-O2	5.48	122.19	118.90
2	2	195	C	C2-N1-C1'	5.48	124.82	118.80
2	2	1537	A	C5-C6-N1	5.48	120.44	117.70
2	2	4134	C	C6-N1-C2	-5.48	118.11	120.30
2	2	2302	C	N3-C2-O2	-5.47	118.07	121.90
2	2	2506	G	C8-N9-C1'	-5.47	119.88	127.00
2	2	4874	A	C4-C5-C6	-5.47	114.26	117.00
2	2	4927	G	C4-N9-C1'	5.47	133.62	126.50
2	2	2621	A	C4-C5-C6	-5.47	114.26	117.00
2	2	2860	C	C2-N1-C1'	5.47	124.82	118.80
2	2	3650	C	C2-N1-C1'	5.47	124.82	118.80
2	2	4177	C	N1-C2-O2	5.47	122.18	118.90
2	2	499	G	C6-C5-N7	-5.47	127.12	130.40
2	2	2593	C	N1-C2-O2	5.47	122.18	118.90
2	2	4939	C	C5-C6-N1	5.47	123.73	121.00
2	2	1694	C	C2-N1-C1'	5.47	124.81	118.80
2	2	2825	A	C4-C5-C6	-5.47	114.27	117.00
2	2	2908	U	C2-N1-C1'	5.47	124.26	117.70
2	2	4972	U	C6-N1-C2	-5.47	117.72	121.00
2	2	208	A	C4-C5-C6	-5.46	114.27	117.00
2	2	323	C	C6-N1-C2	-5.46	118.11	120.30
2	2	2672	C	C5-C6-N1	5.46	123.73	121.00
2	2	4426	C	C6-N1-C2	-5.46	118.11	120.30
2	2	5023	C	N1-C2-O2	5.46	122.18	118.90
2	2	1802	A	C4-C5-C6	-5.46	114.27	117.00
2	2	4552	U	N3-C2-O2	-5.46	118.38	122.20
2	2	1913	C	N1-C2-O2	5.46	122.18	118.90
2	2	4860	G	C8-N9-C1'	-5.46	119.90	127.00
2	2	5003	U	N3-C2-O2	-5.46	118.38	122.20
2	2	1947	U	C2-N1-C1'	5.46	124.25	117.70
5	5	30	C	N1-C2-O2	5.46	122.17	118.90
2	2	2598	A	C4-C5-C6	-5.46	114.27	117.00
2	2	2770	C	C5-C6-N1	5.46	123.73	121.00
2	2	4109	G	C2-N3-C4	5.46	114.63	111.90
2	2	1465	G	N3-C4-N9	5.46	129.27	126.00
2	2	1472	C	N3-C2-O2	-5.46	118.08	121.90
2	2	2772	C	N3-C2-O2	-5.46	118.08	121.90
2	2	4576	U	N1-C2-O2	5.46	126.62	122.80
2	2	1716	G	N3-C4-C5	-5.45	125.87	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2539	C	C5-C6-N1	5.45	123.73	121.00
2	2	4486	C	N3-C2-O2	-5.45	118.08	121.90
2	2	488	G	C4-C5-N7	5.45	112.98	110.80
2	2	4074	C	N3-C2-O2	-5.45	118.08	121.90
2	2	1812	C	C5-C6-N1	5.45	123.73	121.00
2	2	2708	U	N1-C2-O2	5.45	126.62	122.80
2	2	3643	A	C4-C5-C6	-5.45	114.28	117.00
2	2	4362	A	C2-N3-C4	5.45	113.33	110.60
2	2	4698	C	N1-C2-O2	5.45	122.17	118.90
2	2	56	A	C5-C6-N1	5.45	120.42	117.70
2	2	1598	C	N1-C2-O2	5.45	122.17	118.90
8	8	55	U	N1-C2-O2	5.45	126.61	122.80
2	2	4160	C	C6-N1-C2	-5.45	118.12	120.30
8	8	18	U	N3-C2-O2	-5.45	118.39	122.20
2	2	1175	A	C2-N3-C4	5.45	113.32	110.60
2	2	4775	C	C5-C6-N1	5.45	123.72	121.00
2	2	290	U	N1-C2-O2	5.44	126.61	122.80
2	2	1220	G	N3-C4-N9	5.44	129.27	126.00
2	2	2388	A	C4-C5-C6	-5.44	114.28	117.00
2	2	2478	C	C6-N1-C2	-5.44	118.12	120.30
2	2	4383	U	C6-N1-C2	-5.44	117.73	121.00
2	2	4429	C	C6-N1-C2	-5.44	118.12	120.30
2	2	2418	A	C2-N3-C4	5.44	113.32	110.60
2	2	2701	U	C6-N1-C2	-5.44	117.74	121.00
5	5	32	A	N1-C2-N3	-5.44	126.58	129.30
2	2	2105	A	N1-C2-N3	-5.44	126.58	129.30
2	2	4933	C	C6-N1-C2	-5.44	118.12	120.30
8	8	44	A	C4-C5-C6	-5.44	114.28	117.00
2	2	3932	U	N1-C2-O2	5.44	126.61	122.80
2	2	4713	G	N3-C4-C5	-5.44	125.88	128.60
2	2	2806	A	N9-C4-C5	-5.43	103.63	105.80
2	2	4153	C	C6-N1-C2	-5.43	118.13	120.30
2	2	4358	U	N3-C2-O2	-5.43	118.39	122.20
5	5	74	A	C5-C6-N1	5.43	120.42	117.70
2	2	1843	A	C4-C5-C6	-5.43	114.28	117.00
2	2	648	G	C6-C5-N7	-5.43	127.14	130.40
2	2	86	U	C2-N1-C1'	5.43	124.22	117.70
2	2	175	C	N3-C2-O2	-5.43	118.10	121.90
2	2	2395	A	C4-C5-C6	-5.43	114.28	117.00
2	2	1655	C	N1-C2-O2	5.43	122.16	118.90
5	5	94	C	N3-C2-O2	-5.43	118.10	121.90
5	5	95	C	N3-C2-O2	-5.43	118.10	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2257	C	C6-N1-C1'	-5.42	114.29	120.80
2	2	2849	A	C4-C5-C6	-5.42	114.29	117.00
2	2	4178	A	C4-C5-C6	-5.42	114.29	117.00
5	5	20	U	N3-C2-O2	-5.42	118.40	122.20
5	5	76	U	C2-N1-C1'	5.42	124.21	117.70
2	2	94	A	C4-C5-C6	-5.42	114.29	117.00
2	2	465	G	C4-N9-C1'	5.42	133.55	126.50
2	2	110	C	N1-C2-O2	5.42	122.15	118.90
2	2	4703	U	C6-N1-C2	-5.42	117.75	121.00
2	2	4990	C	OP1-P-O3'	5.42	117.12	105.20
2	2	1306	C	C5-C6-N1	5.42	123.71	121.00
2	2	389	A	C2-N3-C4	5.42	113.31	110.60
2	2	1643	A	N1-C2-N3	-5.42	126.59	129.30
2	2	2066	C	N3-C2-O2	-5.42	118.11	121.90
2	2	2382	A	C2-N3-C4	5.42	113.31	110.60
2	2	467	U	O4'-C1'-N1	5.42	112.53	108.20
2	2	2886	U	N1-C2-O2	5.42	126.59	122.80
2	2	985	C	N3-C2-O2	-5.41	118.11	121.90
2	2	4603	C	C5-C6-N1	5.41	123.71	121.00
2	2	1204	C	C6-N1-C2	-5.41	118.14	120.30
2	2	1901	C	N1-C2-O2	5.41	122.15	118.90
2	2	2017	A	N7-C8-N9	5.41	116.51	113.80
2	2	2553	A	C4-C5-C6	-5.41	114.29	117.00
2	2	3692	A	C2-N3-C4	5.41	113.31	110.60
34	a	38	ARG	C-N-CA	5.41	135.23	121.70
2	2	1702	C	C6-N1-C1'	-5.41	114.31	120.80
2	2	3638	G	C2-N3-C4	5.41	114.60	111.90
2	2	3594	C	N3-C2-O2	-5.41	118.11	121.90
2	2	3830	A	C4-C5-C6	-5.41	114.30	117.00
2	2	328	A	C4-C5-C6	-5.41	114.30	117.00
2	2	1429	C	N1-C2-O2	5.41	122.14	118.90
2	2	2396	A	C2-N3-C4	5.41	113.30	110.60
2	2	2423	A	N1-C2-N3	-5.41	126.60	129.30
2	2	4372	U	N1-C2-O2	5.41	126.58	122.80
2	2	4748	U	N1-C2-O2	5.41	126.58	122.80
7	7	7	TYR	C-N-CA	5.41	135.22	121.70
2	2	2026	A	N1-C2-N3	-5.40	126.60	129.30
2	2	3632	C	C5-C6-N1	5.40	123.70	121.00
2	2	1275	G	N9-C4-C5	5.40	107.56	105.40
2	2	4723	A	C2-N3-C4	5.40	113.30	110.60
2	2	4945	G	C8-N9-C1'	-5.40	119.98	127.00
2	2	220	C	C2-N3-C4	5.40	122.60	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	944	A	C4-C5-C6	-5.40	114.30	117.00
2	2	977	C	C5-C6-N1	5.40	123.70	121.00
2	2	1339	U	C6-N1-C2	-5.40	117.76	121.00
2	2	4717	A	C2-N3-C4	5.40	113.30	110.60
2	2	4493	U	C6-N1-C2	-5.40	117.76	121.00
5	5	30	C	C5-C6-N1	5.40	123.70	121.00
2	2	25	A	N1-C2-N3	-5.40	126.60	129.30
2	2	390	C	N1-C2-O2	5.40	122.14	118.90
2	2	4144	C	N1-C2-O2	5.40	122.14	118.90
2	2	4566	U	N3-C2-O2	-5.40	118.42	122.20
5	5	2	U	N1-C2-O2	5.40	126.58	122.80
8	8	27	U	N3-C2-O2	-5.40	118.42	122.20
2	2	77	U	C2-N1-C1'	5.40	124.18	117.70
2	2	3745	U	N1-C2-O2	5.40	126.58	122.80
2	2	205	C	N1-C2-O2	5.39	122.14	118.90
2	2	242	U	C2-N1-C1'	5.39	124.17	117.70
2	2	1473	U	N1-C2-O2	5.39	126.58	122.80
2	2	1936	C	C5-C6-N1	5.39	123.70	121.00
2	2	2419	C	N1-C2-O2	5.39	122.14	118.90
2	2	2731	C	C6-N1-C2	-5.39	118.14	120.30
2	2	3696	C	C5-C6-N1	5.39	123.70	121.00
2	2	3923	A	C2-N3-C4	5.39	113.30	110.60
2	2	4981	G	N3-C4-N9	5.39	129.24	126.00
2	2	5060	A	C2-N3-C4	5.39	113.30	110.60
2	2	1720	C	C2-N1-C1'	5.39	124.73	118.80
8	8	71	A	C4-C5-C6	-5.39	114.30	117.00
2	2	1610	C	N1-C2-O2	5.39	122.14	118.90
2	2	1907	A	C4-C5-C6	-5.39	114.30	117.00
2	2	4360	U	C6-N1-C2	-5.39	117.77	121.00
2	2	965	G	N3-C4-C5	-5.39	125.91	128.60
2	2	2497	C	C5-C6-N1	5.39	123.69	121.00
2	2	2630	U	N1-C2-O2	5.39	126.57	122.80
2	2	4722	G	C8-N9-C1'	-5.39	119.99	127.00
2	2	180	C	C4-C5-C6	-5.39	114.71	117.40
2	2	317	A	C4-C5-N7	5.39	113.39	110.70
2	2	4254	G	C8-N9-C1'	-5.39	120.00	127.00
2	2	205	C	N3-C2-O2	-5.39	118.13	121.90
2	2	975	C	N3-C2-O2	-5.39	118.13	121.90
2	2	1727	U	N1-C2-O2	5.39	126.57	122.80
2	2	2095	A	C2-N3-C4	5.39	113.29	110.60
2	2	2511	A	C2-N3-C4	5.39	113.29	110.60
2	2	4730	C	C6-N1-C1'	5.39	127.26	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4958	C	C2-N3-C4	5.39	122.59	119.90
2	2	5058	A	N1-C2-N3	-5.39	126.61	129.30
2	2	4226	G	C2-N3-C4	5.38	114.59	111.90
2	2	4626	A	O4'-C1'-N9	5.38	112.51	108.20
2	2	2264	C	N3-C2-O2	-5.38	118.13	121.90
2	2	429	A	C2-N3-C4	5.38	113.29	110.60
2	2	1954	U	N3-C2-O2	-5.38	118.43	122.20
2	2	4549	G	N3-C4-N9	5.38	129.23	126.00
2	2	4969	C	N3-C2-O2	-5.38	118.13	121.90
2	2	3853	U	N1-C2-O2	5.38	126.57	122.80
2	2	986	C	C6-N1-C2	-5.38	118.15	120.30
2	2	1879	C	N1-C2-O2	5.38	122.13	118.90
2	2	2659	A	N1-C2-N3	-5.38	126.61	129.30
2	2	3594	C	C6-N1-C2	-5.38	118.15	120.30
2	2	4375	C	OP1-P-O3'	5.38	117.03	105.20
11	B	67	VAL	CA-CB-CG1	5.38	118.97	110.90
2	2	1337	A	C4-C5-C6	-5.38	114.31	117.00
2	2	513	U	N3-C2-O2	-5.38	118.44	122.20
2	2	350	C	N3-C2-O2	-5.37	118.14	121.90
5	5	36	C	C5-C6-N1	5.37	123.69	121.00
8	8	64	U	C6-N1-C2	-5.37	117.78	121.00
2	2	2512	A	C4-C5-C6	-5.37	114.31	117.00
2	2	4329	G	C4-N9-C1'	5.37	133.48	126.50
2	2	4569	U	C6-N1-C2	-5.37	117.78	121.00
2	2	1810	G	N3-C4-N9	5.37	129.22	126.00
2	2	2447	U	C5-C6-N1	5.37	125.38	122.70
2	2	2651	C	C6-N1-C2	-5.37	118.15	120.30
2	2	3823	G	C4-N9-C1'	5.37	133.48	126.50
2	2	3930	U	N3-C2-O2	-5.37	118.44	122.20
2	2	4420	U	C2-N1-C1'	5.37	124.14	117.70
2	2	3854	C	N1-C2-O2	5.37	122.12	118.90
2	2	492	U	N1-C2-O2	5.37	126.56	122.80
2	2	1202	C	C6-N1-C2	-5.37	118.15	120.30
2	2	1637	A	C4-C5-C6	-5.37	114.32	117.00
2	2	2595	C	C5-C6-N1	5.37	123.68	121.00
2	2	4333	C	C5-C6-N1	5.37	123.68	121.00
2	2	4885	U	C6-N1-C2	-5.37	117.78	121.00
2	2	415	G	N3-C4-N9	5.36	129.22	126.00
2	2	1418	C	N1-C2-O2	5.36	122.12	118.90
2	2	4973	U	N1-C2-O2	5.36	126.55	122.80
2	2	736	C	C6-N1-C2	-5.36	118.16	120.30
2	2	4376	A	C4-C5-C6	-5.36	114.32	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1404	G	C2-N3-C4	5.36	114.58	111.90
2	2	1714	C	C5-C6-N1	5.36	123.68	121.00
2	2	2748	C	C5-C6-N1	5.36	123.68	121.00
2	2	4199	C	C5-C6-N1	5.36	123.68	121.00
2	2	2667	C	C5-C6-N1	5.36	123.68	121.00
2	2	2827	G	C4-N9-C1'	5.36	133.47	126.50
2	2	3682	A	C4-C5-C6	-5.36	114.32	117.00
2	2	4883	C	C5-C6-N1	5.36	123.68	121.00
2	2	907	C	C6-N1-C2	-5.36	118.16	120.30
2	2	2356	U	N1-C2-O2	5.36	126.55	122.80
2	2	2672	C	C6-N1-C2	-5.36	118.16	120.30
2	2	249	C	C6-N1-C2	-5.35	118.16	120.30
2	2	1264	C	C6-N1-C2	-5.35	118.16	120.30
2	2	181	C	N1-C2-O2	5.35	122.11	118.90
2	2	2041	A	C4-C5-C6	-5.35	114.32	117.00
2	2	2319	C	C6-N1-C2	-5.35	118.16	120.30
2	2	2583	C	N1-C2-O2	5.35	122.11	118.90
5	5	80	U	N1-C2-O2	5.35	126.55	122.80
2	2	4074	C	C5-C6-N1	5.35	123.67	121.00
2	2	4893	A	C2-N3-C4	5.35	113.28	110.60
2	2	304	C	N3-C2-O2	-5.35	118.16	121.90
2	2	353	A	C4-C5-C6	-5.35	114.33	117.00
2	2	3686	G	N1-C6-O6	-5.35	116.69	119.90
2	2	1298	C	N1-C2-O2	5.35	122.11	118.90
2	2	1497	A	C4-C5-C6	-5.35	114.33	117.00
2	2	1707	C	C5-C6-N1	5.35	123.67	121.00
2	2	2100	A	C2-N3-C4	5.35	113.27	110.60
2	2	4389	C	N1-C2-O2	5.35	122.11	118.90
5	5	17	C	C6-N1-C2	-5.35	118.16	120.30
2	2	74	G	N3-C4-N9	5.34	129.21	126.00
2	2	1262	G	N3-C4-N9	5.34	129.21	126.00
2	2	2409	U	C4-C5-C6	5.34	122.91	119.70
2	2	2859	G	C8-N9-C4	-5.34	104.26	106.40
2	2	3688	U	C6-N1-C2	-5.34	117.79	121.00
2	2	87	A	C4-C5-C6	-5.34	114.33	117.00
2	2	914	U	C5-C4-O4	-5.34	122.69	125.90
2	2	5016	A	C5-N7-C8	-5.34	101.23	103.90
5	5	104	C	C6-N1-C2	-5.34	118.16	120.30
2	2	454	U	C5-C6-N1	5.34	125.37	122.70
2	2	1537	A	C2-N3-C4	5.34	113.27	110.60
2	2	2061	U	N3-C2-O2	-5.34	118.46	122.20
2	2	4379	A	C4-C5-C6	-5.34	114.33	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4610	A	C4-N9-C1'	5.34	135.91	126.30
2	2	711	A	C2-N3-C4	5.34	113.27	110.60
2	2	4206	C	N3-C2-O2	-5.34	118.16	121.90
2	2	4596	C	N3-C2-O2	-5.34	118.16	121.90
2	2	76	A	C2-N3-C4	5.34	113.27	110.60
2	2	499	G	C8-N9-C4	-5.34	104.27	106.40
2	2	2713	C	N1-C2-O2	5.34	122.10	118.90
2	2	4611	A	C2-N3-C4	5.34	113.27	110.60
2	2	4717	A	C4-C5-C6	-5.34	114.33	117.00
2	2	4722	G	C2-N3-C4	5.34	114.57	111.90
2	2	692	A	C4-C5-C6	-5.33	114.33	117.00
2	2	1664	U	N3-C2-O2	-5.33	118.47	122.20
2	2	1796	U	C6-N1-C2	-5.33	117.80	121.00
2	2	2019	C	C6-N1-C1'	5.33	127.20	120.80
2	2	4865	C	C6-N1-C2	-5.33	118.17	120.30
2	2	1281	G	N3-C4-N9	5.33	129.20	126.00
2	2	2036	C	C5-C6-N1	5.33	123.67	121.00
2	2	3903	A	C4-C5-C6	-5.33	114.33	117.00
2	2	4521	U	N3-C2-O2	-5.33	118.47	122.20
2	2	4712	C	N3-C2-O2	-5.33	118.17	121.90
2	2	196	C	C5-C6-N1	5.33	123.66	121.00
2	2	344	A	C2-N3-C4	5.33	113.26	110.60
2	2	2563	C	C5-C6-N1	5.33	123.66	121.00
2	2	1477	C	C2-N1-C1'	5.33	124.66	118.80
2	2	1610	C	C5-C6-N1	5.33	123.66	121.00
8	8	32	C	C2-N1-C1'	5.33	124.66	118.80
2	2	1632	A	N7-C8-N9	5.32	116.46	113.80
2	2	1908	A	C4-C5-C6	-5.32	114.34	117.00
2	2	2325	C	N3-C2-O2	-5.32	118.17	121.90
2	2	3920	U	N1-C2-O2	5.32	126.53	122.80
2	2	4256	A	N1-C2-N3	-5.32	126.64	129.30
2	2	5050	C	N1-C2-O2	5.32	122.09	118.90
2	2	1254	A	C8-N9-C1'	-5.32	118.12	127.70
2	2	2107	C	C5-C6-N1	5.32	123.66	121.00
2	2	4517	A	C2-N3-C4	5.32	113.26	110.60
8	8	137	A	C2-N3-C4	5.32	113.26	110.60
2	2	3651	A	C4-C5-C6	-5.32	114.34	117.00
2	2	440	U	C2-N1-C1'	5.32	124.08	117.70
2	2	2607	C	C6-N1-C2	-5.32	118.17	120.30
2	2	4892	A	C2-N3-C4	5.32	113.26	110.60
2	2	3849	A	C4-C5-C6	-5.32	114.34	117.00
2	2	4295	U	C6-N1-C2	-5.32	117.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4299	U	C6-N1-C2	-5.32	117.81	121.00
10	A	81	ASP	CB-CG-OD1	5.32	123.08	118.30
2	2	343	C	C6-N1-C2	-5.31	118.17	120.30
2	2	4162	C	N3-C2-O2	-5.31	118.18	121.90
2	2	147	A	C2-N3-C4	5.31	113.26	110.60
2	2	1702	C	C5-C6-N1	5.31	123.66	121.00
5	5	94	C	C6-N1-C2	-5.31	118.17	120.30
2	2	4640	C	N3-C2-O2	-5.31	118.18	121.90
2	2	368	C	C5-C6-N1	5.31	123.66	121.00
2	2	400	A	C4-C5-C6	-5.31	114.35	117.00
2	2	477	C	C5-C6-N1	5.31	123.65	121.00
2	2	1520	C	C5-C6-N1	5.31	123.66	121.00
2	2	2844	A	C4-C5-C6	-5.31	114.35	117.00
19	K	73	ILE	CG1-CB-CG2	-5.31	99.72	111.40
2	2	450	G	N3-C4-C5	-5.31	125.95	128.60
2	2	2598	A	C5-C6-N1	5.31	120.35	117.70
2	2	3663	A	C4-C5-C6	-5.31	114.35	117.00
2	2	3831	U	N1-C2-O2	5.31	126.52	122.80
8	8	45	C	C5-C6-N1	5.31	123.65	121.00
2	2	4544	A	C4-C5-C6	-5.30	114.35	117.00
2	2	4926	C	C6-N1-C1'	-5.30	114.44	120.80
2	2	1838	A	C4-C5-C6	-5.30	114.35	117.00
2	2	2335	C	C5-C6-N1	5.30	123.65	121.00
2	2	3876	A	C4-C5-C6	-5.30	114.35	117.00
2	2	1600	A	C4-C5-C6	-5.30	114.35	117.00
2	2	1725	U	N3-C2-O2	-5.30	118.49	122.20
2	2	1726	U	C5-C6-N1	5.30	125.35	122.70
2	2	4568	A	C4-C5-C6	-5.30	114.35	117.00
2	2	1557	C	C6-N1-C2	-5.30	118.18	120.30
2	2	2835	A	C4-C5-C6	-5.30	114.35	117.00
2	2	4522	G	C4-N9-C1'	5.30	133.38	126.50
2	2	4565	C	C2-N3-C4	5.30	122.55	119.90
2	2	4588	U	N1-C2-O2	5.30	126.51	122.80
2	2	1638	A	C4-C5-C6	-5.29	114.35	117.00
2	2	1603	C	N1-C2-O2	5.29	122.08	118.90
2	2	3704	U	N3-C2-O2	-5.29	118.50	122.20
2	2	3826	C	N3-C2-O2	-5.29	118.19	121.90
2	2	3828	A	C4-C5-C6	-5.29	114.35	117.00
2	2	4639	G	C8-N9-C1'	-5.29	120.12	127.00
2	2	1302	U	C6-N1-C2	-5.29	117.83	121.00
2	2	1808	C	C5-C6-N1	5.29	123.65	121.00
2	2	2332	A	C5-C6-N1	5.29	120.35	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1858	A	C2-N3-C4	5.29	113.25	110.60
2	2	4713	G	C4-N9-C1'	5.29	133.38	126.50
2	2	465	G	N3-C4-N9	5.29	129.17	126.00
2	2	1197	C	N1-C2-O2	5.29	122.07	118.90
2	2	82	U	N3-C2-O2	-5.29	118.50	122.20
2	2	3587	C	C5-C6-N1	5.28	123.64	121.00
2	2	3747	A	C4-C5-C6	-5.28	114.36	117.00
2	2	1825	A	C4-C5-C6	-5.28	114.36	117.00
2	2	3666	C	C6-N1-C2	-5.28	118.19	120.30
2	2	3844	U	C5-C6-N1	5.28	125.34	122.70
2	2	4350	C	C2-N1-C1'	5.28	124.61	118.80
2	2	4539	U	N3-C2-O2	-5.28	118.50	122.20
2	2	204	U	C6-N1-C2	-5.28	117.83	121.00
2	2	1437	C	C5-C6-N1	5.28	123.64	121.00
2	2	3839	G	O4'-C1'-N9	-5.28	103.98	108.20
2	2	4280	A	C6-N1-C2	5.28	121.77	118.60
2	2	2814	C	C6-N1-C2	-5.27	118.19	120.30
2	2	4629	U	N3-C2-O2	-5.27	118.51	122.20
2	2	4975	G	O4'-C1'-N9	5.27	112.42	108.20
2	2	4922	C	C6-N1-C2	-5.27	118.19	120.30
2	2	239	C	C5-C6-N1	5.27	123.64	121.00
2	2	1630	A	C4-C5-C6	-5.27	114.37	117.00
2	2	1682	A	C4-C5-C6	-5.27	114.37	117.00
2	2	2669	C	C5-C6-N1	5.27	123.63	121.00
2	2	1609	U	N1-C2-O2	5.26	126.48	122.80
2	2	4770	U	C2-N1-C1'	5.26	124.02	117.70
2	2	1915	C	C6-N1-C2	-5.26	118.19	120.30
2	2	1929	A	N7-C8-N9	5.26	116.43	113.80
2	2	360	A	C2-N3-C4	5.26	113.23	110.60
2	2	2262	G	C2-N3-C4	5.26	114.53	111.90
5	5	79	U	N1-C2-O2	5.26	126.48	122.80
2	2	1297	U	C6-N1-C2	-5.26	117.84	121.00
2	2	3630	A	C4-C5-C6	-5.26	114.37	117.00
2	2	4646	U	N3-C2-O2	-5.26	118.52	122.20
2	2	4311	A	N1-C2-N3	-5.26	126.67	129.30
2	2	4968	A	N1-C2-N3	-5.26	126.67	129.30
2	2	171	U	C5-C6-N1	5.26	125.33	122.70
2	2	417	G	N1-C6-O6	-5.26	116.75	119.90
2	2	1533	A	C4-C5-C6	-5.26	114.37	117.00
2	2	2528	G	N7-C8-N9	5.26	115.73	113.10
2	2	1178	G	C8-N9-C1'	-5.25	120.17	127.00
2	2	2867	C	N3-C2-O2	-5.25	118.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	358	C	N3-C2-O2	-5.25	118.22	121.90
2	2	2257	C	C5-C6-N1	5.25	123.63	121.00
2	2	2633	U	N3-C2-O2	-5.25	118.52	122.20
2	2	4386	C	C6-N1-C2	-5.25	118.20	120.30
2	2	37	U	N3-C2-O2	-5.25	118.52	122.20
2	2	2507	A	C2-N3-C4	5.25	113.22	110.60
2	2	3779	A	N7-C8-N9	5.25	116.43	113.80
2	2	4178	A	C2-N3-C4	5.25	113.23	110.60
8	8	93	C	C5-C6-N1	5.25	123.63	121.00
2	2	446	C	N1-C2-O2	5.25	122.05	118.90
2	2	1644	C	N1-C2-O2	5.25	122.05	118.90
2	2	2899	C	C6-N1-C2	-5.25	118.20	120.30
2	2	4183	G	C4-N9-C1'	5.25	133.32	126.50
2	2	2021	G	C8-N9-C1'	-5.25	120.18	127.00
2	2	2634	C	N1-C2-O2	5.25	122.05	118.90
2	2	3631	U	N1-C2-O2	5.25	126.47	122.80
2	2	4120	U	N3-C2-O2	-5.25	118.53	122.20
8	8	103	A	C4-C5-C6	-5.25	114.38	117.00
2	2	3854	C	C6-N1-C2	-5.25	118.20	120.30
2	2	262	G	N3-C2-N2	5.24	123.57	119.90
2	2	415	G	N3-C4-C5	-5.24	125.98	128.60
2	2	713	C	C5-C6-N1	5.24	123.62	121.00
2	2	718	C	C6-N1-C2	-5.24	118.20	120.30
2	2	1591	U	N3-C2-O2	-5.24	118.53	122.20
2	2	5030	U	C2-N1-C1'	5.24	123.99	117.70
2	2	1478	C	N1-C2-O2	5.24	122.04	118.90
2	2	1671	U	N1-C2-O2	5.24	126.47	122.80
2	2	2460	A	C2-N3-C4	5.24	113.22	110.60
2	2	759	G	C4-N9-C1'	5.24	133.31	126.50
2	2	4610	A	N7-C8-N9	5.24	116.42	113.80
8	8	103	A	C5-C6-N1	5.24	120.32	117.70
2	2	2787	A	C2-N3-C4	5.24	113.22	110.60
2	2	4996	C	C2-N1-C1'	5.24	124.56	118.80
2	2	166	C	C5-C6-N1	5.24	123.62	121.00
2	2	455	C	C2-N1-C1'	5.24	124.56	118.80
2	2	1430	C	N1-C2-O2	5.24	122.04	118.90
2	2	1491	A	C4-C5-C6	-5.24	114.38	117.00
2	2	2026	A	C4-C5-C6	-5.24	114.38	117.00
2	2	2632	U	N3-C2-O2	-5.24	118.53	122.20
2	2	3919	C	N3-C2-O2	-5.24	118.23	121.90
2	2	5004	C	C4-C5-C6	-5.24	114.78	117.40
2	2	678	C	C6-N1-C2	-5.23	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1650	A	C4-C5-N7	5.23	113.32	110.70
2	2	3833	C	N1-C2-O2	5.23	122.04	118.90
4	4	269	LEU	CA-CB-CG	5.23	127.34	115.30
2	2	1498	G	N3-C4-C5	-5.23	125.98	128.60
2	2	2250	C	C6-N1-C2	-5.23	118.21	120.30
2	2	3617	G	C8-N9-C4	-5.23	104.31	106.40
2	2	4363	A	C4-C5-C6	-5.23	114.38	117.00
2	2	1520	C	C6-N1-C2	-5.23	118.21	120.30
2	2	2292	C	N1-C2-O2	5.23	122.04	118.90
2	2	4701	A	C4-C5-C6	-5.23	114.39	117.00
8	8	98	C	C5-C6-N1	5.23	123.61	121.00
2	2	244	G	C8-N9-C4	-5.23	104.31	106.40
2	2	1716	G	N3-C4-N9	5.23	129.14	126.00
2	2	248	C	C6-N1-C2	-5.23	118.21	120.30
2	2	709	C	N3-C2-O2	-5.23	118.24	121.90
2	2	1929	A	C5-C6-N1	5.23	120.31	117.70
2	2	2634	C	C5-C6-N1	5.23	123.61	121.00
2	2	3717	A	C4-C5-C6	-5.23	114.39	117.00
2	2	3605	C	C5-C6-N1	5.23	123.61	121.00
2	2	984	C	C2-N1-C1'	5.22	124.55	118.80
2	2	2087	C	C6-N1-C2	-5.22	118.21	120.30
2	2	1906	U	C5-C6-N1	5.22	125.31	122.70
2	2	3836	A	N7-C8-N9	5.22	116.41	113.80
2	2	2402	G	C2-N3-C4	5.22	114.51	111.90
2	2	2581	A	C4-C5-C6	-5.22	114.39	117.00
2	2	4619	U	N3-C2-O2	-5.22	118.55	122.20
8	8	84	A	C4-C5-C6	-5.22	114.39	117.00
2	2	343	C	C5-C6-N1	5.22	123.61	121.00
2	2	724	C	N1-C2-O2	5.22	122.03	118.90
2	2	1703	C	C6-N1-C1'	-5.22	114.54	120.80
2	2	2767	U	N1-C2-O2	5.22	126.45	122.80
2	2	3726	A	C4-C5-C6	-5.22	114.39	117.00
2	2	923	C	O4'-C1'-N1	5.21	112.37	108.20
2	2	1466	G	N1-C6-O6	-5.21	116.77	119.90
2	2	4188	U	C6-N1-C2	-5.21	117.87	121.00
2	2	4906	C	C5-C6-N1	5.21	123.61	121.00
5	5	76	U	C5-C6-N1	5.21	125.31	122.70
2	2	4584	A	C2-N3-C4	5.21	113.21	110.60
2	2	189	G	N7-C8-N9	5.21	115.71	113.10
2	2	2783	A	C4-C5-N7	5.21	113.31	110.70
2	2	4340	U	C5-C6-N1	5.21	125.31	122.70
2	2	2035	C	N1-C2-O2	5.21	122.03	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	2096	G	C2-N3-C4	5.21	114.50	111.90
2	2	3841	C	C6-N1-C2	-5.21	118.22	120.30
2	2	329	A	C4-C5-C6	-5.21	114.40	117.00
2	2	415	G	C2-N3-C4	5.21	114.50	111.90
2	2	4123	C	C5-C6-N1	5.21	123.60	121.00
2	2	4896	G	N3-C4-N9	5.20	129.12	126.00
5	5	20	U	N1-C2-O2	5.20	126.44	122.80
2	2	1536	U	C5-C6-N1	5.20	125.30	122.70
2	2	1877	G	C8-N9-C4	-5.20	104.32	106.40
2	2	2783	A	C4-C5-C6	-5.20	114.40	117.00
39	g	116	LEU	CA-CB-CG	5.20	127.26	115.30
2	2	1293	G	C8-N9-C1'	-5.20	120.24	127.00
2	2	1428	U	N1-C2-O2	5.20	126.44	122.80
2	2	2884	G	C2-N3-C4	5.20	114.50	111.90
5	5	83	A	C4-C5-C6	-5.20	114.40	117.00
2	2	2708	U	N3-C2-O2	-5.20	118.56	122.20
2	2	2849	A	N1-C2-N3	-5.20	126.70	129.30
2	2	3895	G	N1-C6-O6	-5.20	116.78	119.90
2	2	4591	U	N3-C2-O2	-5.20	118.56	122.20
2	2	4590	A	C4-C5-C6	-5.20	114.40	117.00
2	2	4462	C	C6-N1-C2	-5.20	118.22	120.30
5	5	66	G	C4-N9-C1'	5.20	133.25	126.50
2	2	2733	C	N1-C2-O2	5.19	122.02	118.90
2	2	1292	C	C6-N1-C2	-5.19	118.22	120.30
8	8	35	C	N1-C2-O2	5.19	122.02	118.90
2	2	201	C	C5-C6-N1	5.19	123.59	121.00
2	2	1650	A	N9-C4-C5	-5.19	103.72	105.80
2	2	2403	A	C2-N3-C4	5.19	113.20	110.60
2	2	3834	C	C5-C6-N1	5.19	123.60	121.00
2	2	2484	A	C8-N9-C1'	-5.19	118.36	127.70
2	2	23	C	N3-C2-O2	-5.19	118.27	121.90
2	2	372	A	C2-N3-C4	5.19	113.19	110.60
2	2	1437	C	C6-N1-C1'	5.19	127.03	120.80
2	2	1575	A	C4-C5-C6	-5.19	114.41	117.00
2	2	4340	U	C2-N1-C1'	5.19	123.92	117.70
2	2	4928	C	O4'-C1'-N1	5.19	112.35	108.20
2	2	738	C	C2-N3-C4	5.19	122.49	119.90
2	2	3858	C	N3-C2-O2	-5.19	118.27	121.90
2	2	1669	A	C5-C6-N1	5.18	120.29	117.70
2	2	3833	C	C5-C6-N1	5.18	123.59	121.00
2	2	3890	A	C4-C5-C6	-5.18	114.41	117.00
2	2	2042	A	C2-N3-C4	5.18	113.19	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4385	A	N9-C4-C5	-5.18	103.73	105.80
2	2	5023	C	C5-C6-N1	5.18	123.59	121.00
2	2	100	C	C5-C6-N1	5.18	123.59	121.00
2	2	175	C	C5-C6-N1	5.18	123.59	121.00
2	2	317	A	N7-C8-N9	5.18	116.39	113.80
2	2	2702	C	C6-N1-C2	-5.18	118.23	120.30
2	2	3693	U	C2-N1-C1'	5.18	123.91	117.70
2	2	256	G	C8-N9-C4	-5.18	104.33	106.40
2	2	1613	A	N1-C6-N6	-5.18	115.49	118.60
2	2	62	A	C4-C5-C6	-5.17	114.41	117.00
2	2	940	C	C6-N1-C2	-5.17	118.23	120.30
2	2	1414	C	N3-C2-O2	-5.17	118.28	121.90
2	2	4930	C	C5-C6-N1	5.17	123.59	121.00
8	8	27	U	C6-N1-C2	-5.17	117.89	121.00
2	2	940	C	C5-C6-N1	5.17	123.59	121.00
2	2	1216	C	O4'-C1'-N1	5.17	112.34	108.20
2	2	414	C	C5-C6-N1	5.17	123.59	121.00
2	2	757	G	C2-N3-C4	5.17	114.48	111.90
2	2	1077	C	N1-C2-O2	5.17	122.00	118.90
2	2	1623	A	C4-C5-C6	-5.17	114.41	117.00
2	2	2806	A	C4-C5-C6	-5.17	114.42	117.00
2	2	4673	U	C6-N1-C2	-5.17	117.90	121.00
2	2	4891	G	C4-N9-C1'	5.17	133.22	126.50
2	2	4967	A	C2-N3-C4	5.17	113.18	110.60
2	2	303	C	N1-C2-O2	5.17	122.00	118.90
2	2	2860	C	C2-N3-C4	5.17	122.48	119.90
2	2	3749	C	N1-C2-O2	5.17	122.00	118.90
2	2	3667	C	N1-C2-O2	5.17	122.00	118.90
2	2	1282	G	C2-N3-C4	5.16	114.48	111.90
2	2	2069	A	C4-C5-C6	-5.16	114.42	117.00
2	2	2780	C	N1-C2-O2	5.16	122.00	118.90
2	2	4346	U	N1-C2-O2	5.16	126.42	122.80
2	2	112	C	N3-C2-O2	-5.16	118.29	121.90
2	2	2067	C	N1-C2-O2	5.16	122.00	118.90
2	2	262	G	N1-C6-O6	-5.16	116.80	119.90
2	2	518	G	C8-N9-C1'	-5.16	120.30	127.00
2	2	4682	U	C6-N1-C2	-5.16	117.91	121.00
5	5	5	A	C2-N3-C4	5.16	113.18	110.60
2	2	954	C	C6-N1-C2	-5.16	118.24	120.30
2	2	2738	C	O4'-C1'-N1	5.16	112.33	108.20
2	2	4456	C	N1-C2-O2	5.16	121.99	118.90
2	2	362	A	C4-C5-C6	-5.16	114.42	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3667	C	N3-C2-O2	-5.16	118.29	121.90
2	2	3895	G	C2-N3-C4	5.16	114.48	111.90
2	2	4123	C	N1-C2-O2	5.16	121.99	118.90
2	2	5001	U	N1-C2-O2	5.16	126.41	122.80
2	2	1298	C	N3-C2-O2	-5.15	118.29	121.90
2	2	1632	A	N3-C4-N9	5.15	131.52	127.40
2	2	4138	C	N3-C2-O2	-5.15	118.29	121.90
2	2	4891	G	N3-C4-C5	-5.15	126.02	128.60
2	2	1810	G	C4-N9-C1'	5.15	133.20	126.50
2	2	1729	A	C5-C6-N1	5.15	120.28	117.70
2	2	2101	C	N1-C2-O2	5.15	121.99	118.90
5	5	58	A	C2-N3-C4	5.15	113.18	110.60
2	2	2460	A	C4-C5-C6	-5.15	114.43	117.00
2	2	2030	A	C2-N3-C4	5.15	113.17	110.60
2	2	1343	A	C4-C5-C6	-5.15	114.43	117.00
2	2	2341	A	C4-C5-C6	-5.15	114.43	117.00
2	2	2517	A	C4-C5-C6	-5.15	114.43	117.00
2	2	5025	C	N3-C2-O2	-5.15	118.30	121.90
2	2	18	C	N1-C2-O2	5.14	121.99	118.90
2	2	358	C	C5-C6-N1	5.14	123.57	121.00
2	2	385	A	C2-N3-C4	5.14	113.17	110.60
2	2	669	C	N1-C2-O2	5.14	121.99	118.90
2	2	1344	C	N3-C2-O2	-5.14	118.30	121.90
2	2	2774	C	N3-C2-O2	-5.14	118.30	121.90
2	2	2899	C	C5-C6-N1	5.14	123.57	121.00
2	2	3601	C	C6-N1-C2	-5.14	118.24	120.30
3	3	328	LYS	C-N-CA	5.14	134.56	121.70
2	2	4162	C	C6-N1-C1'	-5.14	114.63	120.80
2	2	5035	U	C6-N1-C2	-5.14	117.91	121.00
2	2	2255	C	C2-N3-C4	5.14	122.47	119.90
2	2	2258	C	C6-N1-C2	-5.14	118.24	120.30
2	2	906	C	C6-N1-C2	-5.14	118.25	120.30
2	2	1278	C	C6-N1-C2	-5.14	118.24	120.30
2	2	719	C	N1-C2-O2	5.14	121.98	118.90
2	2	215	C	C6-N1-C2	-5.14	118.25	120.30
2	2	2791	C	N3-C2-O2	-5.14	118.30	121.90
2	2	4073	A	C2-N3-C4	5.14	113.17	110.60
2	2	422	C	N1-C2-O2	5.13	121.98	118.90
2	2	485	C	C2-N3-C4	5.13	122.47	119.90
2	2	2262	G	N7-C8-N9	5.13	115.67	113.10
2	2	1809	C	N3-C2-O2	-5.13	118.31	121.90
2	2	2835	A	C2-N3-C4	5.13	113.17	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3931	C	N1-C2-O2	5.13	121.98	118.90
2	2	1527	A	C2-N3-C4	5.13	113.17	110.60
2	2	3781	C	N1-C2-O2	5.13	121.98	118.90
2	2	1254	A	N3-C4-C5	-5.13	123.21	126.80
2	2	1279	A	C4-C5-C6	-5.13	114.44	117.00
2	2	1318	C	C5-C6-N1	5.13	123.56	121.00
2	2	2429	A	C2-N3-C4	5.13	113.16	110.60
5	5	69	U	N1-C2-O2	5.13	126.39	122.80
8	8	96	C	C5-C6-N1	5.13	123.56	121.00
2	2	1178	G	N3-C4-C5	-5.12	126.04	128.60
2	2	1968	G	N3-C4-N9	5.12	129.07	126.00
2	2	2678	A	C2-N3-C4	5.12	113.16	110.60
2	2	2764	A	C2-N3-C4	5.12	113.16	110.60
2	2	4519	C	N1-C2-O2	5.12	121.97	118.90
2	2	1462	A	C2-N3-C4	5.12	113.16	110.60
2	2	1558	A	C4-C5-C6	-5.12	114.44	117.00
2	2	2573	A	C4-C5-C6	-5.12	114.44	117.00
5	5	52	C	C5-C6-N1	5.12	123.56	121.00
2	2	1535	C	N1-C2-O2	5.12	121.97	118.90
2	2	1705	G	N3-C4-C5	-5.12	126.04	128.60
2	2	2485	U	N3-C2-O2	-5.12	118.62	122.20
2	2	4414	A	N1-C2-N3	-5.12	126.74	129.30
2	2	4641	U	N1-C2-O2	5.12	126.38	122.80
2	2	4651	A	C2-N3-C4	5.12	113.16	110.60
2	2	120	A	C4-C5-C6	-5.12	114.44	117.00
2	2	2302	C	C2-N1-C1'	5.12	124.43	118.80
2	2	27	C	N1-C2-O2	5.11	121.97	118.90
2	2	440	U	C6-N1-C2	-5.11	117.93	121.00
2	2	1692	C	N1-C2-O2	5.11	121.97	118.90
2	2	4260	U	N3-C2-O2	-5.11	118.62	122.20
2	2	300	A	C2-N3-C4	5.11	113.16	110.60
2	2	935	A	C6-C5-N7	5.11	135.88	132.30
2	2	1367	C	C6-N1-C1'	-5.11	114.67	120.80
2	2	4304	A	C4-C5-C6	-5.11	114.44	117.00
2	2	304	C	C5-C6-N1	5.11	123.56	121.00
2	2	1498	G	C2-N3-C4	5.11	114.45	111.90
2	2	2472	A	C2-N3-C4	5.11	113.16	110.60
5	5	46	C	C5-C6-N1	5.11	123.56	121.00
2	2	4337	C	N1-C2-O2	5.11	121.97	118.90
8	8	37	A	C2-N3-C4	5.11	113.15	110.60
2	2	56	A	C2-N3-C4	5.11	113.15	110.60
2	2	663	G	N3-C2-N2	5.11	123.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1592	G	N3-C4-C5	-5.11	126.05	128.60
2	2	1848	C	N1-C2-O2	5.11	121.96	118.90
2	2	2263	A	C2-N3-C4	5.11	113.15	110.60
2	2	2430	C	N1-C2-O2	5.11	121.96	118.90
2	2	2431	A	C4-C5-C6	-5.11	114.45	117.00
2	2	3925	U	N3-C2-O2	-5.11	118.63	122.20
2	2	4764	A	N3-C4-C5	5.11	130.37	126.80
8	8	98	C	N1-C2-O2	5.11	121.96	118.90
2	2	757	G	C8-N9-C1'	-5.10	120.37	127.00
2	2	3911	C	N1-C2-O2	5.10	121.96	118.90
2	2	4426	C	C2-N1-C1'	5.10	124.41	118.80
8	8	79	G	N7-C8-N9	5.10	115.65	113.10
2	2	2021	G	N3-C4-N9	5.10	129.06	126.00
2	2	2419	C	N3-C2-O2	-5.10	118.33	121.90
5	5	4	U	C6-N1-C2	-5.10	117.94	121.00
2	2	257	C	N1-C2-O2	5.10	121.96	118.90
2	2	1715	C	C6-N1-C2	-5.10	118.26	120.30
2	2	1849	U	N1-C2-O2	5.10	126.37	122.80
2	2	2310	C	N1-C2-O2	5.10	121.96	118.90
5	5	11	A	C4-C5-C6	-5.10	114.45	117.00
8	8	82	A	N3-C4-N9	5.10	131.48	127.40
2	2	195	C	N1-C2-O2	5.10	121.96	118.90
2	2	3652	A	C2-N3-C4	5.10	113.15	110.60
2	2	3732	A	C2-N3-C4	5.10	113.15	110.60
2	2	4713	G	N3-C4-N9	5.10	129.06	126.00
2	2	2028	C	C6-N1-C2	-5.10	118.26	120.30
2	2	3658	C	C5-C6-N1	5.10	123.55	121.00
2	2	5046	U	C5-C6-N1	5.10	125.25	122.70
2	2	1463	C	C6-N1-C2	-5.09	118.26	120.30
2	2	2071	A	C5-C6-N1	5.09	120.25	117.70
2	2	5007	A	C2-N3-C4	5.09	113.15	110.60
2	2	906	C	C5-C6-N1	5.09	123.55	121.00
2	2	2277	C	N1-C2-O2	5.09	121.96	118.90
2	2	2532	C	N3-C2-O2	-5.09	118.33	121.90
2	2	4244	A	C4-C5-C6	-5.09	114.45	117.00
2	2	4696	C	C5-C6-N1	5.09	123.55	121.00
2	2	1791	U	C6-N1-C2	-5.09	117.95	121.00
2	2	2393	C	N1-C2-O2	5.09	121.95	118.90
2	2	4689	U	C6-N1-C2	-5.09	117.95	121.00
2	2	4758	U	O4'-C1'-N1	5.09	112.27	108.20
2	2	4970	C	N3-C2-O2	-5.09	118.34	121.90
2	2	518	G	C2-N3-C4	5.09	114.44	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1086	C	N1-C2-O2	5.09	121.95	118.90
2	2	1312	A	C4-C5-C6	-5.09	114.45	117.00
2	2	1597	G	O4'-C1'-N9	5.09	112.27	108.20
2	2	2362	U	C5-C6-N1	5.09	125.24	122.70
2	2	4520	G	N3-C4-N9	5.09	129.05	126.00
2	2	1094	G	C8-N9-C4	-5.09	104.37	106.40
2	2	2094	G	N7-C8-N9	5.09	115.64	113.10
2	2	3706	C	C6-N1-C2	-5.09	118.27	120.30
2	2	667	A	C2-N3-C4	5.08	113.14	110.60
2	2	3694	U	N1-C2-O2	5.08	126.36	122.80
2	2	4378	A	C4-C5-C6	-5.08	114.46	117.00
2	2	4602	A	C2-N3-C4	5.08	113.14	110.60
2	2	452	A	C4-C5-C6	-5.08	114.46	117.00
2	2	1049	C	C5-C6-N1	5.08	123.54	121.00
2	2	1282	G	C4-N9-C1'	5.08	133.11	126.50
2	2	2454	U	N3-C2-O2	-5.08	118.64	122.20
4	4	303	ASP	CB-CG-OD1	5.08	122.88	118.30
2	2	49	U	C2-N1-C1'	5.08	123.80	117.70
2	2	108	A	C2-N3-C4	5.08	113.14	110.60
2	2	1635	C	N1-C2-O2	5.08	121.95	118.90
2	2	2772	C	C5-C6-N1	5.08	123.54	121.00
2	2	4585	U	C5-C6-N1	5.08	125.24	122.70
5	5	76	U	C6-N1-C2	-5.08	117.95	121.00
2	2	1910	G	C4-N9-C1'	5.08	133.10	126.50
45	m	55	GLY	C-N-CA	5.08	134.40	121.70
2	2	426	A	C4-C5-C6	-5.08	114.46	117.00
2	2	3590	G	C2-N3-C4	5.08	114.44	111.90
2	2	32	G	C8-N9-C4	-5.08	104.37	106.40
2	2	4310	A	C2-N3-C4	5.08	113.14	110.60
8	8	62	A	C2-N3-C4	5.08	113.14	110.60
2	2	988	C	C2-N3-C4	5.08	122.44	119.90
2	2	1832	C	C2-N1-C1'	5.08	124.38	118.80
2	2	1970	A	C4-C5-C6	-5.08	114.46	117.00
2	2	2465	C	C4-C5-C6	-5.08	114.86	117.40
2	2	4902	C	C6-N1-C2	-5.08	118.27	120.30
2	2	1094	G	N7-C8-N9	5.07	115.64	113.10
2	2	1275	G	C8-N9-C1'	5.07	133.59	127.00
2	2	4467	A	C2-N3-C4	5.07	113.14	110.60
2	2	4614	G	N1-C6-O6	-5.07	116.86	119.90
2	2	1321	G	C8-N9-C4	-5.07	104.37	106.40
2	2	1343	A	C5-C6-N1	5.07	120.24	117.70
2	2	2258	C	C5-C6-N1	5.07	123.54	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4684	A	C2-N3-C4	5.07	113.14	110.60
27	S	127	VAL	CG1-CB-CG2	-5.07	102.78	110.90
2	2	920	C	C6-N1-C2	-5.07	118.27	120.30
2	2	1076	C	N1-C2-O2	5.07	121.94	118.90
2	2	1857	C	C5-C6-N1	5.07	123.53	121.00
2	2	4493	U	C5-C6-N1	5.07	125.24	122.70
2	2	366	A	C2-N3-C4	5.07	113.14	110.60
2	2	1478	C	C2-N1-C1'	5.07	124.38	118.80
2	2	2651	C	C5-C6-N1	5.07	123.53	121.00
2	2	467	U	C5-C6-N1	5.07	125.23	122.70
2	2	2285	A	C2-N3-C4	5.07	113.13	110.60
2	2	2371	U	C5-C6-N1	5.07	125.23	122.70
2	2	3930	U	C6-N1-C2	-5.07	117.96	121.00
2	2	4982	A	C2-N3-C4	5.07	113.13	110.60
2	2	2047	A	C4-C5-C6	-5.07	114.47	117.00
2	2	4739	C	C6-N1-C2	-5.07	118.27	120.30
2	2	278	G	O4'-C1'-N9	-5.06	104.15	108.20
2	2	422	C	C6-N1-C2	-5.06	118.28	120.30
2	2	1816	C	N1-C2-O2	5.06	121.94	118.90
2	2	4460	U	N3-C2-O2	-5.06	118.66	122.20
5	5	17	C	C5-C6-N1	5.06	123.53	121.00
2	2	495	C	N1-C2-O2	5.06	121.94	118.90
2	2	1637	A	C2-N3-C4	5.06	113.13	110.60
2	2	2279	A	C2-N3-C4	5.06	113.13	110.60
2	2	419	A	C2-N3-C4	5.06	113.13	110.60
2	2	2374	A	C2-N3-C4	5.06	113.13	110.60
2	2	3917	A	C4-C5-C6	-5.06	114.47	117.00
2	2	4267	G	N3-C4-C5	-5.06	126.07	128.60
2	2	4994	G	N3-C4-C5	-5.06	126.07	128.60
2	2	504	G	N7-C8-N9	5.06	115.63	113.10
2	2	1243	C	N3-C2-O2	-5.06	118.36	121.90
2	2	4616	A	C4-C5-C6	-5.06	114.47	117.00
2	2	941	C	N1-C2-O2	5.06	121.93	118.90
2	2	31	U	N1-C2-O2	5.05	126.34	122.80
2	2	1429	C	C2-N1-C1'	5.05	124.36	118.80
2	2	3623	C	N1-C2-O2	5.05	121.93	118.90
2	2	4911	A	C4-C5-C6	-5.05	114.47	117.00
2	2	1827	C	C5-C6-N1	5.05	123.53	121.00
2	2	3737	A	C4-C5-C6	-5.05	114.47	117.00
2	2	4319	C	N3-C2-O2	-5.05	118.36	121.90
2	2	4477	A	C2-N3-C4	5.05	113.13	110.60
2	2	4739	C	C5-C6-N1	5.05	123.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	5019	A	N1-C2-N3	-5.05	126.77	129.30
2	2	1807	C	N1-C2-O2	5.05	121.93	118.90
2	2	2853	C	C5-C6-N1	5.05	123.53	121.00
11	B	261	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	2	1087	A	C2-N3-C4	5.05	113.12	110.60
2	2	1567	U	N1-C2-O2	5.05	126.33	122.80
2	2	1628	C	N3-C2-O2	-5.05	118.37	121.90
2	2	3877	A	C2-N3-C4	5.05	113.12	110.60
2	2	4987	C	N3-C2-O2	-5.05	118.37	121.90
2	2	2628	U	N1-C2-O2	5.04	126.33	122.80
2	2	4476	C	C6-N1-C2	-5.04	118.28	120.30
2	2	2568	C	C6-N1-C2	-5.04	118.28	120.30
2	2	2647	A	C2-N3-C4	5.04	113.12	110.60
2	2	3930	U	C5-C6-N1	5.04	125.22	122.70
2	2	4383	U	N3-C2-O2	-5.04	118.67	122.20
2	2	4926	C	N3-C2-O2	-5.04	118.37	121.90
2	2	3851	U	C2-N1-C1'	5.04	123.75	117.70
2	2	4387	C	C2-N1-C1'	5.04	124.34	118.80
2	2	178	C	N3-C2-O2	-5.04	118.37	121.90
2	2	659	G	C4-N9-C1'	5.04	133.05	126.50
2	2	1078	A	O4'-C1'-N9	5.04	112.23	108.20
2	2	2083	C	C5-C6-N1	5.04	123.52	121.00
2	2	519	C	C6-N1-C2	-5.04	118.28	120.30
2	2	4193	C	C6-N1-C2	-5.04	118.28	120.30
2	2	4455	G	N3-C4-N9	5.04	129.02	126.00
2	2	4481	U	N3-C2-O2	-5.04	118.67	122.20
2	2	4507	A	C5-C6-N1	5.04	120.22	117.70
2	2	365	U	C6-N1-C2	-5.04	117.98	121.00
2	2	2334	C	N1-C2-O2	5.04	121.92	118.90
8	8	145	C	C6-N1-C2	-5.04	118.28	120.30
2	2	262	G	N3-C4-N9	5.04	129.02	126.00
2	2	3708	C	C5-C6-N1	5.04	123.52	121.00
2	2	110	C	N3-C2-O2	-5.03	118.38	121.90
2	2	414	C	C6-N1-C2	-5.03	118.29	120.30
2	2	1466	G	C2-N3-C4	5.03	114.42	111.90
2	2	1518	A	C2-N3-C4	5.03	113.12	110.60
2	2	2438	A	C4-C5-C6	-5.03	114.48	117.00
2	2	1405	C	N3-C2-O2	-5.03	118.38	121.90
2	2	3894	A	C2-N3-C4	5.03	113.11	110.60
2	2	1276	C	N1-C2-O2	5.03	121.92	118.90
2	2	1373	A	C2-N3-C4	5.03	113.11	110.60
2	2	1634	A	C4-C5-C6	-5.03	114.49	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1736	A	C2-N3-C4	5.03	113.11	110.60
2	2	2697	A	C4-C5-C6	-5.03	114.49	117.00
2	2	3692	A	C4-C5-C6	-5.03	114.49	117.00
2	2	4237	C	C2-N1-C1'	5.03	124.33	118.80
13	D	318	PRO	C-N-CA	5.03	134.27	121.70
2	2	222	C	C5-C6-N1	5.03	123.51	121.00
2	2	1810	G	N3-C4-C5	-5.03	126.09	128.60
2	2	1906	U	C2-N1-C1'	5.03	123.73	117.70
2	2	2078	C	N3-C2-O2	-5.03	118.38	121.90
2	2	2727	C	C5-C6-N1	5.03	123.51	121.00
5	5	14	C	C2-N1-C1'	5.02	124.33	118.80
2	2	125	C	C2-N1-C1'	5.02	124.32	118.80
2	2	440	U	N1-C2-O2	5.02	126.31	122.80
2	2	971	U	N1-C2-O2	5.02	126.31	122.80
2	2	1653	A	C4-C5-C6	-5.02	114.49	117.00
2	2	2755	A	C4-C5-C6	-5.02	114.49	117.00
5	5	66	G	N3-C4-C5	-5.02	126.09	128.60
2	2	2033	A	C2-N3-C4	5.02	113.11	110.60
2	2	3853	U	C6-N1-C2	-5.02	117.99	121.00
8	8	108	A	C2-N3-C4	5.02	113.11	110.60
2	2	59	A	C4-C5-C6	-5.02	114.49	117.00
2	2	1334	A	C4-C5-C6	-5.01	114.49	117.00
2	2	2077	C	N1-C2-O2	5.01	121.91	118.90
2	2	4958	C	N3-C2-O2	-5.01	118.39	121.90
2	2	2665	U	N3-C2-O2	-5.01	118.69	122.20
2	2	302	C	C6-N1-C2	-5.01	118.30	120.30
2	2	345	C	C2-N1-C1'	5.01	124.31	118.80
2	2	2534	C	N1-C2-O2	5.01	121.91	118.90
2	2	2670	C	C2-N1-C1'	5.01	124.31	118.80
2	2	3728	A	C4-C5-C6	-5.01	114.50	117.00
2	2	4506	C	C5-C6-N1	5.01	123.50	121.00
2	2	4895	C	C6-N1-C1'	-5.01	114.79	120.80
2	2	2397	G	O4'-C1'-N9	5.01	112.20	108.20
2	2	2548	C	C5-C6-N1	5.01	123.50	121.00
2	2	4766	C	N3-C2-O2	-5.00	118.40	121.90
2	2	1474	C	N1-C2-O2	5.00	121.90	118.90
2	2	1888	A	C2-N3-C4	5.00	113.10	110.60
2	2	4072	C	N1-C2-O2	5.00	121.90	118.90
2	2	4553	A	C2-N3-C4	5.00	113.10	110.60
2	2	1372	A	C2-N3-C4	5.00	113.10	110.60
2	2	1957	U	C6-N1-C2	-5.00	118.00	121.00
8	8	28	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	225	ARG	Peptide
3	3	328	LYS	Peptide
4	4	176	TYR	Peptide
4	4	198	TYR	Peptide
4	4	294	LYS	Peptide
4	4	299	LEU	Peptide
4	4	300	SER	Peptide
4	4	542	GLN	Peptide
6	6	7	PHE	Peptide
10	A	100	VAL	Peptide
10	A	159	MET	Peptide
10	A	160	LYS	Peptide
10	A	169	VAL	Mainchain
10	A	213	PRO	Peptide
10	A	46	ASP	Peptide
10	A	61	PRO	Peptide
11	B	16	PHE	Peptide
11	B	304	SER	Peptide
18	I	49	GLY	Peptide
22	N	94	LEU	Peptide
25	Q	154	VAL	Peptide
26	R	163	ALA	Peptide
27	S	31	ILE	Peptide
30	W	58	LYS	Peptide
41	i	124	THR	Peptide
45	m	54	ARG	Peptide
46	n	3	GLY	Peptide
47	o	176	THR	Peptide
47	o	203	ILE	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
1	1	17/731 (2%)	17 (100%)	0	0	100	100
3	3	237/503 (47%)	211 (89%)	25 (10%)	1 (0%)	34	67
4	4	601/634 (95%)	539 (90%)	59 (10%)	3 (0%)	29	63
6	6	242/245 (99%)	225 (93%)	17 (7%)	0	100	100
7	7	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
9	9	82/134 (61%)	71 (87%)	9 (11%)	2 (2%)	6	25
10	A	210/217 (97%)	176 (84%)	32 (15%)	2 (1%)	15	47
11	B	399/403 (99%)	373 (94%)	24 (6%)	2 (0%)	29	63
12	C	86/159 (54%)	82 (95%)	4 (5%)	0	100	100
13	D	355/427 (83%)	333 (94%)	22 (6%)	0	100	100
14	E	92/115 (80%)	88 (96%)	4 (4%)	0	100	100
15	F	107/117 (92%)	104 (97%)	3 (3%)	0	100	100
16	G	240/266 (90%)	224 (93%)	16 (7%)	0	100	100
17	H	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
18	I	188/192 (98%)	175 (93%)	13 (7%)	0	100	100
19	K	95/105 (90%)	90 (95%)	5 (5%)	0	100	100
20	L	145/148 (98%)	132 (91%)	13 (9%)	0	100	100
21	M	84/97 (87%)	76 (90%)	8 (10%)	0	100	100
22	N	163/178 (92%)	145 (89%)	18 (11%)	0	100	100
23	O	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
24	P	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
25	Q	208/211 (99%)	189 (91%)	18 (9%)	1 (0%)	29	63
26	R	148/203 (73%)	137 (93%)	9 (6%)	2 (1%)	11	39
27	S	133/215 (62%)	124 (93%)	9 (7%)	0	100	100
28	U	201/204 (98%)	190 (94%)	10 (5%)	1 (0%)	29	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	V	199/203 (98%)	192 (96%)	7 (4%)	0	100	100
30	W	101/106 (95%)	93 (92%)	8 (8%)	0	100	100
31	X	88/92 (96%)	84 (96%)	4 (4%)	0	100	100
32	Y	151/184 (82%)	143 (95%)	8 (5%)	0	100	100
33	Z	185/188 (98%)	176 (95%)	9 (5%)	0	100	100
34	a	146/196 (74%)	139 (95%)	7 (5%)	0	100	100
35	b	174/176 (99%)	165 (95%)	9 (5%)	0	100	100
36	c	153/160 (96%)	148 (97%)	5 (3%)	0	100	100
37	d	99/128 (77%)	92 (93%)	7 (7%)	0	100	100
38	e	129/140 (92%)	117 (91%)	12 (9%)	0	100	100
39	g	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
40	h	132/145 (91%)	126 (96%)	6 (4%)	0	100	100
41	i	133/136 (98%)	123 (92%)	10 (8%)	0	100	100
42	j	105/125 (84%)	93 (89%)	12 (11%)	0	100	100
43	k	126/135 (93%)	114 (90%)	12 (10%)	0	100	100
44	l	123/137 (90%)	112 (91%)	11 (9%)	0	100	100
45	m	246/257 (96%)	221 (90%)	24 (10%)	1 (0%)	34	67
46	n	107/110 (97%)	100 (94%)	7 (6%)	0	100	100
47	o	212/288 (74%)	189 (89%)	21 (10%)	2 (1%)	17	50
48	p	224/248 (90%)	211 (94%)	13 (6%)	0	100	100
49	r	291/297 (98%)	268 (92%)	23 (8%)	0	100	100
50	z	32/129 (25%)	30 (94%)	2 (6%)	0	100	100
All	All	7673/9647 (80%)	7100 (92%)	556 (7%)	17 (0%)	50	78

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	5	ARG
9	9	99	GLN
47	o	96	VAL
11	B	304	SER
11	B	305	THR
26	R	164	ASN
4	4	301	GLU

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Mol	Chain	Res	Type
10	A	160	LYS
10	A	169	VAL
4	4	396	LYS
26	R	18	HIS
47	o	101	ASN
3	3	192	HIS
45	m	55	GLY
4	4	34	ILE
25	Q	47	ALA
28	U	83	LYS

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	
1	1	17/654 (3%)	17 (100%)	0	100	100
3	3	223/457 (49%)	218 (98%)	5 (2%)	52	77
4	4	548/574 (96%)	541 (99%)	7 (1%)	69	86
6	6	212/213 (100%)	207 (98%)	5 (2%)	49	75
7	7	126/149 (85%)	126 (100%)	0	100	100
9	9	74/114 (65%)	73 (99%)	1 (1%)	67	85
10	A	191/196 (97%)	187 (98%)	4 (2%)	53	78
11	B	349/349 (100%)	347 (99%)	2 (1%)	86	94
12	C	76/126 (60%)	75 (99%)	1 (1%)	69	86
13	D	298/348 (86%)	294 (99%)	4 (1%)	69	86
14	E	79/97 (81%)	79 (100%)	0	100	100
15	F	94/100 (94%)	93 (99%)	1 (1%)	73	88
16	G	206/223 (92%)	206 (100%)	0	100	100
17	H	109/110 (99%)	107 (98%)	2 (2%)	59	81
18	I	169/171 (99%)	167 (99%)	2 (1%)	71	87
19	K	84/89 (94%)	83 (99%)	1 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	L	120/121 (99%)	120 (100%)	0	100	100
21	M	73/80 (91%)	73 (100%)	0	100	100
22	N	138/149 (93%)	137 (99%)	1 (1%)	84	93
23	O	64/65 (98%)	64 (100%)	0	100	100
24	P	47/48 (98%)	46 (98%)	1 (2%)	53	78
25	Q	176/177 (99%)	170 (97%)	6 (3%)	37	67
26	R	138/184 (75%)	136 (99%)	2 (1%)	67	85
27	S	115/161 (71%)	113 (98%)	2 (2%)	60	82
28	U	171/172 (99%)	168 (98%)	3 (2%)	59	81
29	V	173/174 (99%)	172 (99%)	1 (1%)	86	94
30	W	91/94 (97%)	90 (99%)	1 (1%)	73	88
31	X	73/75 (97%)	71 (97%)	2 (3%)	44	72
32	Y	134/163 (82%)	131 (98%)	3 (2%)	52	77
33	Z	164/165 (99%)	162 (99%)	2 (1%)	71	87
34	a	133/175 (76%)	132 (99%)	1 (1%)	81	92
35	b	157/157 (100%)	156 (99%)	1 (1%)	86	94
36	c	136/140 (97%)	132 (97%)	4 (3%)	42	70
37	d	91/115 (79%)	90 (99%)	1 (1%)	73	88
38	e	101/107 (94%)	100 (99%)	1 (1%)	76	89
39	g	106/133 (80%)	106 (100%)	0	100	100
40	h	124/135 (92%)	120 (97%)	4 (3%)	39	68
41	i	117/118 (99%)	115 (98%)	2 (2%)	60	82
42	j	98/110 (89%)	98 (100%)	0	100	100
43	k	114/121 (94%)	114 (100%)	0	100	100
44	l	109/121 (90%)	109 (100%)	0	100	100
45	m	190/199 (96%)	190 (100%)	0	100	100
46	n	88/89 (99%)	88 (100%)	0	100	100
47	o	192/252 (76%)	189 (98%)	3 (2%)	62	84
48	p	195/215 (91%)	195 (100%)	0	100	100
49	r	247/250 (99%)	246 (100%)	1 (0%)	91	96
50	z	30/115 (26%)	30 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6760/8350 (81%)	6683 (99%)	77 (1%)	74 88

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	290	GLN
3	3	298	THR
3	3	355	THR
3	3	375	VAL
3	3	404	ILE
4	4	125	ARG
4	4	195	VAL
4	4	207	VAL
4	4	346	THR
4	4	382	VAL
4	4	394	ARG
4	4	541	VAL
6	6	58	ILE
6	6	107	VAL
6	6	109	THR
6	6	153	VAL
6	6	161	VAL
9	9	55	LEU
10	A	25	ARG
10	A	54	ARG
10	A	154	THR
10	A	171	HIS
11	B	341[A]	LYS
11	B	341[B]	LYS
12	C	117	ARG
13	D	100	ARG
13	D	170	LEU
13	D	171	LEU
13	D	352	ASP
15	F	54	ARG
17	H	37	THR
17	H	82	ASP
18	I	64	ARG
18	I	84	VAL
19	K	29	ARG
22	N	57	VAL
24	P	21	ARG

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Mol	Chain	Res	Type
25	Q	63	THR
25	Q	67	HIS
25	Q	70	VAL
25	Q	97	SER
25	Q	197	LYS
25	Q	210	LYS
26	R	18	HIS
26	R	63	ASP
27	S	38	VAL
27	S	43	THR
28	U	80	THR
28	U	114	ARG
28	U	204	ARG
29	V	117	ARG
30	W	10	THR
31	X	45	THR
31	X	63	THR
32	Y	24	VAL
32	Y	30	ARG
32	Y	151	THR
33	Z	28	LEU
33	Z	42	THR
34	a	84	THR
35	b	169	THR
36	c	4	THR
36	c	68	THR
36	c	76	VAL
36	c	136	ARG
37	d	72	VAL
38	e	48	ARG
40	h	55	VAL
40	h	74	TYR
40	h	78	TYR
40	h	79	VAL
41	i	52	LYS
41	i	108	ARG
47	o	96	VAL
47	o	100	LYS
47	o	194	VAL
49	r	215	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	161	GLN
3	3	174	GLN
3	3	192	HIS
3	3	206	GLN
3	3	224	GLN
3	3	391	ASN
4	4	128	GLN
4	4	209	HIS
4	4	218	GLN
4	4	239	GLN
4	4	281	ASN
4	4	437	ASN
4	4	601	ASN
6	6	21	ASN
6	6	75	ASN
6	6	170	GLN
7	7	87	ASN
7	7	104	GLN
7	7	115	ASN
9	9	75	ASN
10	A	40	ASN
10	A	184	HIS
11	B	213	GLN
12	C	12	GLN
12	C	19	ASN
13	D	38	ASN
13	D	50	GLN
13	D	119	GLN
13	D	178	ASN
14	E	19	GLN
16	G	43	GLN
16	G	225	ASN
18	I	42	ASN
18	I	163	GLN
20	L	66	ASN
20	L	85	GLN
23	O	28	ASN
25	Q	111	GLN
25	Q	149	GLN
26	R	42	ASN
26	R	102	GLN
28	U	196	ASN
30	W	45	GLN

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Mol	Chain	Res	Type
31	X	56	HIS
32	Y	21	ASN
32	Y	80	GLN
36	c	127	GLN
37	d	38	ASN
37	d	116	GLN
38	e	27	ASN
39	g	93	ASN
39	g	111	GLN
40	h	14	ASN
40	h	20	ASN
42	j	69	ASN
43	k	117	GLN
44	l	100	ASN
45	m	132	ASN
46	n	80	ASN
48	p	39	GLN
48	p	63	GLN
49	r	195	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	3431/5070 (67%)	904 (26%)	25 (0%)
5	5	119/120 (99%)	24 (20%)	0
8	8	155/156 (99%)	39 (25%)	0
All	All	3705/5346 (69%)	967 (26%)	25 (0%)

All (967) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	17	A
2	2	20	U
2	2	25	A
2	2	36	U
2	2	39	A
2	2	42	A
2	2	48	G
2	2	56	A
2	2	59	A
2	2	64	A

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Mol	Chain	Res	Type
2	2	65	A
2	2	66	A
2	2	69	A
2	2	73	A
2	2	74	G
2	2	84	A
2	2	91	G
2	2	98	A
2	2	104	G
2	2	108	A
2	2	109	G
2	2	110	C
2	2	119	G
2	2	120	A
2	2	121	A
2	2	127	G
2	2	128	C
2	2	133	C
2	2	134	G
2	2	135	G
2	2	136	C
2	2	137	G
2	2	141	C
2	2	143	C
2	2	151	G
2	2	152	U
2	2	157	U
2	2	159	C
2	2	169	G
2	2	170	C
2	2	172	C
2	2	173	C
2	2	176	G
2	2	178	C
2	2	181	C
2	2	182	G
2	2	183	C
2	2	184	U
2	2	185	C
2	2	188	G
2	2	197	A
2	2	200	U

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Mol	Chain	Res	Type
2	2	207	G
2	2	209	U
2	2	216	C
2	2	218	A
2	2	220	C
2	2	225	G
2	2	234	G
2	2	254	G
2	2	255	C
2	2	256	G
2	2	259	C
2	2	260	C
2	2	262	G
2	2	264	C
2	2	265	C
2	2	266	C
2	2	267	G
2	2	279	A
2	2	280	G
2	2	297	U
2	2	306	A
2	2	315	G
2	2	316	U
2	2	326	C
2	2	340	C
2	2	345	C
2	2	347	A
2	2	349	A
2	2	353	A
2	2	370	U
2	2	379	G
2	2	387	G
2	2	395	A
2	2	406	C
2	2	407	A
2	2	408	A
2	2	409	G
2	2	410	A
2	2	411	G
2	2	412	G
2	2	413	G
2	2	433	A

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Mol	Chain	Res	Type
2	2	440	U
2	2	444	G
2	2	449	C
2	2	450	G
2	2	452	A
2	2	453	G
2	2	454	U
2	2	456	C
2	2	457	G
2	2	464	G
2	2	465	G
2	2	467	U
2	2	483	G
2	2	484	U
2	2	485	C
2	2	486	C
2	2	489	C
2	2	490	C
2	2	491	G
2	2	493	G
2	2	494	U
2	2	496	G
2	2	497	G
2	2	498	C
2	2	499	G
2	2	500	G
2	2	502	C
2	2	503	C
2	2	504	G
2	2	505	G
2	2	509	A
2	2	510	U
2	2	512	U
2	2	513	U
2	2	514	U
2	2	517	C
2	2	518	G
2	2	643	C
2	2	644	G
2	2	647	G
2	2	656	C
2	2	657	C

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Mol	Chain	Res	Type
2	2	658	C
2	2	667	A
2	2	668	C
2	2	670	G
2	2	673	C
2	2	685	C
2	2	686	A
2	2	687	U
2	2	692	A
2	2	696	C
2	2	697	G
2	2	699	C
2	2	700	G
2	2	704	C
2	2	705	G
2	2	708	G
2	2	730	G
2	2	731	G
2	2	738	C
2	2	739	G
2	2	740	G
2	2	742	G
2	2	904	C
2	2	905	C
2	2	906	C
2	2	910	G
2	2	913	U
2	2	914	U
2	2	915	A
2	2	916	C
2	2	917	A
2	2	918	G
2	2	924	C
2	2	925	C
2	2	926	G
2	2	932	A
2	2	933	G
2	2	934	C
2	2	935	A
2	2	936	C
2	2	941	C
2	2	943	A

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Mol	Chain	Res	Type
2	2	944	A
2	2	945	U
2	2	956	A
2	2	959	G
2	2	960	A
2	2	961	G
2	2	962	C
2	2	965	G
2	2	966	A
2	2	967	C
2	2	969	C
2	2	970	G
2	2	972	C
2	2	982	U
2	2	985	C
2	2	989	U
2	2	990	C
2	2	991	C
2	2	992	C
2	2	993	G
2	2	994	G
2	2	995	C
2	2	1048	G
2	2	1049	C
2	2	1051	G
2	2	1066	G
2	2	1067	G
2	2	1070	G
2	2	1071	C
2	2	1072	C
2	2	1074	G
2	2	1082	C
2	2	1083	U
2	2	1094	G
2	2	1095	A
2	2	1097	C
2	2	1098	G
2	2	1100	U
2	2	1173	G
2	2	1178	G
2	2	1179	U
2	2	1180	C

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Mol	Chain	Res	Type
2	2	1181	C
2	2	1183	C
2	2	1193	C
2	2	1194	G
2	2	1195	G
2	2	1197	C
2	2	1198	G
2	2	1199	G
2	2	1200	G
2	2	1202	C
2	2	1203	G
2	2	1211	G
2	2	1215	C
2	2	1216	C
2	2	1218	G
2	2	1220	G
2	2	1221	G
2	2	1222	A
2	2	1240	G
2	2	1241	C
2	2	1245	C
2	2	1251	C
2	2	1254	A
2	2	1255	A
2	2	1257	A
2	2	1259	G
2	2	1260	G
2	2	1262	G
2	2	1266	G
2	2	1271	G
2	2	1272	C
2	2	1273	G
2	2	1274	A
2	2	1275	G
2	2	1280	C
2	2	1283	G
2	2	1284	G
2	2	1287	G
2	2	1294	A
2	2	1296	G
2	2	1301	C
2	2	1303	A

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Mol	Chain	Res	Type
2	2	1314	C
2	2	1321	G
2	2	1324	A
2	2	1325	C
2	2	1326	A2M
2	2	1327	C
2	2	1337	A
2	2	1354	A
2	2	1358	G
2	2	1359	G
2	2	1365	C
2	2	1366	G
2	2	1367	C
2	2	1370	G
2	2	1377	G
2	2	1378	C
2	2	1379	C
2	2	1387	A
2	2	1394	G
2	2	1397	A
2	2	1398	A
2	2	1401	C
2	2	1402	C
2	2	1404	G
2	2	1405	C
2	2	1407	C
2	2	1409	C
2	2	1410	U
2	2	1412	G
2	2	1414	C
2	2	1417	C
2	2	1419	G
2	2	1439	C
2	2	1441	C
2	2	1443	A
2	2	1446	C
2	2	1447	C
2	2	1448	G
2	2	1476	C
2	2	1482	G
2	2	1483	C
2	2	1486	C

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Mol	Chain	Res	Type
2	2	1493	G
2	2	1497	A
2	2	1498	G
2	2	1501	C
2	2	1502	G
2	2	1503	A
2	2	1518	A
2	2	1525	A
2	2	1534	A2M
2	2	1543	G
2	2	1547	A
2	2	1566	C
2	2	1578	U
2	2	1582	PSU
2	2	1583	A
2	2	1592	G
2	2	1596	U
2	2	1612	G
2	2	1613	A
2	2	1614	C
2	2	1624	G
2	2	1625	OMG
2	2	1626	G
2	2	1631	A
2	2	1632	A
2	2	1633	G
2	2	1634	A
2	2	1637	A
2	2	1638	A
2	2	1640	C
2	2	1641	G
2	2	1642	A
2	2	1654	G
2	2	1661	C
2	2	1676	C
2	2	1677	PSU
2	2	1678	C
2	2	1691	G
2	2	1694	C
2	2	1697	G
2	2	1699	A
2	2	1700	G

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Mol	Chain	Res	Type
2	2	1701	A
2	2	1703	C
2	2	1704	C
2	2	1705	G
2	2	1708	G
2	2	1715	C
2	2	1717	C
2	2	1718	C
2	2	1719	A
2	2	1724	G
2	2	1726	U
2	2	1734	G
2	2	1803	G
2	2	1804	A
2	2	1810	G
2	2	1815	G
2	2	1821	G
2	2	1822	U
2	2	1834	U
2	2	1836	G
2	2	1837	A
2	2	1842	G
2	2	1854	G
2	2	1855	G
2	2	1856	C
2	2	1859	C
2	2	1861	U
2	2	1866	UR3
2	2	1867	A
2	2	1868	A
2	2	1871	A2M
2	2	1881	C
2	2	1882	U
2	2	1883	OMG
2	2	1897	A
2	2	1916	G
2	2	1917	A
2	2	1918	U
2	2	1919	G
2	2	1920	C
2	2	1921	C
2	2	1922	G

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Mol	Chain	Res	Type
2	2	1930	U
2	2	1931	C
2	2	1932	A
2	2	1935	C
2	2	1939	A
2	2	1940	G
2	2	1941	A
2	2	1947	U
2	2	1948	G
2	2	1951	G
2	2	1961	G
2	2	1962	A
2	2	1967	A
2	2	1968	G
2	2	2016	C
2	2	2018	C
2	2	2024	G
2	2	2025	A
2	2	2026	A
2	2	2033	A
2	2	2034	G
2	2	2040	A
2	2	2042	A
2	2	2043	A
2	2	2044	U
2	2	2046	G
2	2	2048	U
2	2	2055	G
2	2	2056	G
2	2	2062	C
2	2	2068	C
2	2	2069	A
2	2	2071	A
2	2	2084	C
2	2	2085	G
2	2	2090	U
2	2	2091	C
2	2	2092	G
2	2	2093	A
2	2	2095	A
2	2	2096	G
2	2	2097	U

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Mol	Chain	Res	Type
2	2	2098	G
2	2	2100	A
2	2	2102	G
2	2	2104	G
2	2	2105	A
2	2	2106	G
2	2	2108	G
2	2	2110	C
2	2	2111	G
2	2	2112	G
2	2	2113	C
2	2	2251	G
2	2	2252	G
2	2	2253	A
2	2	2256	C
2	2	2258	C
2	2	2259	G
2	2	2260	C
2	2	2262	G
2	2	2263	A
2	2	2266	C
2	2	2268	A
2	2	2280	G
2	2	2289	C
2	2	2300	A
2	2	2301	G
2	2	2306	G
2	2	2313	A
2	2	2314	G
2	2	2316	G
2	2	2331	G
2	2	2333	G
2	2	2348	G
2	2	2351	C
2	2	2360	A
2	2	2364	OMG
2	2	2369	U
2	2	2381	A
2	2	2389	A
2	2	2395	A
2	2	2402	G
2	2	2416	G

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Mol	Chain	Res	Type
2	2	2417	A
2	2	2422	OMC
2	2	2425	U
2	2	2436	U
2	2	2437	C
2	2	2441	C
2	2	2447	U
2	2	2450	G
2	2	2453	A
2	2	2461	G
2	2	2465	C
2	2	2471	G
2	2	2475	G
2	2	2483	G
2	2	2484	A
2	2	2485	U
2	2	2489	C
2	2	2490	U
2	2	2491	C
2	2	2492	C
2	2	2493	G
2	2	2494	U
2	2	2495	U
2	2	2497	C
2	2	2502	G
2	2	2503	G
2	2	2504	C
2	2	2505	C
2	2	2512	A
2	2	2513	A
2	2	2519	U
2	2	2520	C
2	2	2521	G
2	2	2529	A
2	2	2543	A
2	2	2544	G
2	2	2545	U
2	2	2546	G
2	2	2547	G
2	2	2553	A
2	2	2554	U
2	2	2560	C

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Mol	Chain	Res	Type
2	2	2561	C
2	2	2563	C
2	2	2564	G
2	2	2565	A
2	2	2566	G
2	2	2573	A
2	2	2583	C
2	2	2586	G
2	2	2587	A
2	2	2601	A
2	2	2611	A
2	2	2618	G
2	2	2627	C
2	2	2638	G
2	2	2639	U
2	2	2653	C
2	2	2659	A
2	2	2661	U
2	2	2662	G
2	2	2669	C
2	2	2670	C
2	2	2675	G
2	2	2687	U
2	2	2694	G
2	2	2695	A
2	2	2696	A
2	2	2703	G
2	2	2707	U
2	2	2708	U
2	2	2709	C
2	2	2710	C
2	2	2711	G
2	2	2723	U
2	2	2724	G
2	2	2726	G
2	2	2739	C
2	2	2742	G
2	2	2743	A
2	2	2756	G
2	2	2761	U
2	2	2763	U
2	2	2765	A

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Mol	Chain	Res	Type
2	2	2769	U
2	2	2770	C
2	2	2772	C
2	2	2788	U
2	2	2790	U
2	2	2795	A
2	2	2799	G
2	2	2814	C
2	2	2815	A
2	2	2826	U
2	2	2827	G
2	2	2829	U
2	2	2835	A
2	2	2842	G
2	2	2848	G
2	2	2855	G
2	2	2856	C
2	2	2867	C
2	2	2877	G
2	2	2882	A
2	2	2901	G
2	2	2902	G
2	2	2903	G
2	2	2904	U
2	2	2905	C
2	2	2906	G
2	2	2907	G
2	2	2908	U
2	2	2909	C
2	2	3585	G
2	2	3587	C
2	2	3590	G
2	2	3591	C
2	2	3592	G
2	2	3593	C
2	2	3594	C
2	2	3595	U
2	2	3596	A
2	2	3597	G
2	2	3599	A
2	2	3604	A
2	2	3605	C

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Mol	Chain	Res	Type
2	2	3606	U
2	2	3615	G
2	2	3616	U
2	2	3619	G
2	2	3620	G
2	2	3626	G
2	2	3635	A
2	2	3644	U
2	2	3646	A
2	2	3648	A
2	2	3649	A
2	2	3650	C
2	2	3662	A
2	2	3664	G
2	2	3672	G
2	2	3673	C
2	2	3674	G
2	2	3675	G
2	2	3678	G
2	2	3679	U
2	2	3680	U
2	2	3691	G
2	2	3709	U
2	2	3710	G
2	2	3711	A
2	2	3713	U
2	2	3714	G
2	2	3728	A
2	2	3729	PSU
2	2	3734	U
2	2	3735	G
2	2	3736	A
2	2	3747	A
2	2	3748	A
2	2	3750	G
2	2	3776	G
2	2	3777	G
2	2	3779	A
2	2	3823	G
2	2	3830	A
2	2	3832	U
2	2	3838	U

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Mol	Chain	Res	Type
2	2	3840	U
2	2	3843	C
2	2	3867	A2M
2	2	3868	G
2	2	3875	G
2	2	3877	A
2	2	3878	C
2	2	3879	G
2	2	3898	G
2	2	3902	A
2	2	3903	A
2	2	3904	G
2	2	3905	A
2	2	3906	A
2	2	3907	G
2	2	3915	U
2	2	3916	G
2	2	3922	G
2	2	3923	A
2	2	3938	G
2	2	3939	G
2	2	3943	A
2	2	4076	G
2	2	4084	G
2	2	4095	G
2	2	4097	G
2	2	4099	G
2	2	4100	C
2	2	4101	C
2	2	4102	C
2	2	4104	G
2	2	4110	C
2	2	4111	U
2	2	4112	C
2	2	4114	C
2	2	4115	G
2	2	4116	C
2	2	4117	U
2	2	4119	C
2	2	4122	G
2	2	4137	C
2	2	4139	G

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Mol	Chain	Res	Type
2	2	4140	C
2	2	4141	G
2	2	4143	G
2	2	4144	C
2	2	4145	C
2	2	4146	G
2	2	4162	C
2	2	4163	U
2	2	4170	A
2	2	4183	G
2	2	4184	G
2	2	4191	G
2	2	4195	G
2	2	4196	OMG
2	2	4203	A
2	2	4204	C
2	2	4205	A
2	2	4212	A
2	2	4225	G
2	2	4229	U
2	2	4233	A
2	2	4234	A
2	2	4243	C
2	2	4249	G
2	2	4252	C
2	2	4254	G
2	2	4265	U
2	2	4268	A
2	2	4271	A
2	2	4273	A
2	2	4281	A
2	2	4282	A
2	2	4283	G
2	2	4291	G
2	2	4293	PSU
2	2	4295	U
2	2	4297	G
2	2	4303	C
2	2	4304	A
2	2	4305	G
2	2	4312	U
2	2	4314	C

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Mol	Chain	Res	Type
2	2	4319	C
2	2	4326	G
2	2	4329	G
2	2	4330	G
2	2	4332	C
2	2	4338	G
2	2	4339	A
2	2	4349	C
2	2	4350	C
2	2	4354	U
2	2	4364	G
2	2	4372	U
2	2	4373	G
2	2	4376	A
2	2	4377	G
2	2	4378	A
2	2	4379	A
2	2	4380	A
2	2	4381	A
2	2	4387	C
2	2	4395	U
2	2	4396	A
2	2	4405	G
2	2	4414	A
2	2	4415	1MA
2	2	4418	G
2	2	4420	U
2	2	4422	A
2	2	4424	A
2	2	4428	A
2	2	4451	G
2	2	4452	U
2	2	4453	C
2	2	4464	A
2	2	4466	C
2	2	4475	G
2	2	4476	C
2	2	4480	A
2	2	4484	A
2	2	4488	A
2	2	4499	G
2	2	4500	U

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Mol	Chain	Res	Type
2	2	4502	C
2	2	4512	U
2	2	4513	A
2	2	4518	A
2	2	4519	C
2	2	4523	A2M
2	2	4524	G
2	2	4527	G
2	2	4530	UR3
2	2	4545	G
2	2	4548	A
2	2	4549	G
2	2	4554	G
2	2	4555	U
2	2	4556	U
2	2	4557	U
2	2	4558	U
2	2	4560	C
2	2	4567	G
2	2	4569	U
2	2	4570	G
2	2	4573	G
2	2	4575	G
2	2	4589	A
2	2	4590	A
2	2	4597	UR3
2	2	4600	G
2	2	4601	U
2	2	4606	G
2	2	4607	A
2	2	4608	G
2	2	4626	A
2	2	4632	U
2	2	4636	PSU
2	2	4637	OMG
2	2	4652	G
2	2	4656	A
2	2	4658	G
2	2	4664	A
2	2	4670	C
2	2	4678	G
2	2	4684	A

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Mol	Chain	Res	Type
2	2	4695	C
2	2	4699	U
2	2	4703	U
2	2	4708	A
2	2	4709	U
2	2	4719	G
2	2	4720	C
2	2	4721	G
2	2	4730	C
2	2	4732	G
2	2	4733	C
2	2	4734	A
2	2	4735	G
2	2	4740	G
2	2	4741	C
2	2	4742	G
2	2	4745	G
2	2	4750	G
2	2	4751	G
2	2	4754	G
2	2	4757	C
2	2	4759	C
2	2	4761	G
2	2	4765	G
2	2	4771	C
2	2	4775	C
2	2	4776	G
2	2	4859	C
2	2	4870	OMG
2	2	4871	C
2	2	4872	2MG
2	2	4874	A
2	2	4875	G
2	2	4876	U
2	2	4877	G
2	2	4880	C
2	2	4882	U
2	2	4883	C
2	2	4887	C
2	2	4888	U
2	2	4889	G
2	2	4894	A

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Mol	Chain	Res	Type
2	2	4895	C
2	2	4896	G
2	2	4899	G
2	2	4900	C
2	2	4901	G
2	2	4907	G
2	2	4910	G
2	2	4912	G
2	2	4914	C
2	2	4915	G
2	2	4923	C
2	2	4924	C
2	2	4925	U
2	2	4926	C
2	2	4927	G
2	2	4928	C
2	2	4935	C
2	2	4937	C
2	2	4938	A
2	2	4940	C
2	2	4941	G
2	2	4943	A
2	2	4947	U
2	2	4955	A
2	2	4966	A
2	2	4976	U
2	2	4985	U
2	2	4989	U
2	2	4990	C
2	2	4991	U
2	2	4995	U
2	2	5013	C
2	2	5014	A
2	2	5016	A
2	2	5017	G
2	2	5022	U
2	2	5024	C
2	2	5025	C
2	2	5026	U
2	2	5027	C
2	2	5028	G
2	2	5030	U

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Mol	Chain	Res	Type
2	2	5031	G
2	2	5034	A
2	2	5041	G
2	2	5047	C
2	2	5050	C
2	2	5053	U
2	2	5054	C
2	2	5055	G
2	2	5060	A
2	2	5061	A
2	2	5062	G
2	2	5069	U
5	5	5	A
5	5	11	A
5	5	22	A
5	5	24	C
5	5	29	C
5	5	33	U
5	5	37	G
5	5	38	U
5	5	41	G
5	5	50	A
5	5	52	C
5	5	53	U
5	5	54	A
5	5	63	C
5	5	64	G
5	5	70	G
5	5	71	G
5	5	74	A
5	5	88	A
5	5	97	G
5	5	100	A
5	5	108	G
5	5	110	G
5	5	118	C
8	8	24	G
8	8	25	G
8	8	34	U
8	8	35	C
8	8	38	U
8	8	39	G

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Mol	Chain	Res	Type
8	8	48	A
8	8	49	G
8	8	52	A
8	8	59	A
8	8	62	A
8	8	63	U
8	8	75	G
8	8	80	A
8	8	81	C
8	8	82	A
8	8	84	A
8	8	85	U
8	8	86	U
8	8	87	G
8	8	94	G
8	8	95	A
8	8	103	A
8	8	104	A
8	8	105	C
8	8	110	U
8	8	114	G
8	8	123	U
8	8	124	U
8	8	125	C
8	8	126	C
8	8	127	U
8	8	129	C
8	8	143	G
8	8	150	C
8	8	151	G
8	8	153	C
8	8	155	C
8	8	156	U

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	406	C
2	2	484	U
2	2	914	U
2	2	955	G
2	2	1302	U

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Mol	Chain	Res	Type
2	2	1322	1MA
2	2	1376	C
2	2	1613	A
2	2	1625	OMG
2	2	1633	G
2	2	1867	A
2	2	2033	A
2	2	2529	A
2	2	2760	G
2	2	3596	A
2	2	3673	C
2	2	3905	A
2	2	4136	G
2	2	4196	OMG
2	2	4378	A
2	2	4395	U
2	2	4498	U
2	2	4529	B8W
2	2	4555	U
2	2	4913	G

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

92 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BGH	2	3899	2	25,29,30	4.24	17 (68%)	31,43,46	2.46	11 (35%)
2	2MG	2	729	2	18,26,27	2.30	7 (38%)	16,38,41	1.43	4 (25%)
2	A2M	2	2363	51,2	18,25,26	4.14	7 (38%)	18,36,39	3.27	3 (16%)
2	B8W	2	4472	2	18,26,27	6.09	7 (38%)	21,38,41	2.62	7 (33%)
2	OMG	2	4494	2	18,26,27	2.39	8 (44%)	19,38,41	1.62	4 (21%)
2	PSU	2	4293	30,2	18,21,22	0.97	1 (5%)	22,30,33	1.78	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	1MA	2	1322	51,2	16,25,26	3.95	4 (25%)	18,37,40	1.63	3 (16%)
2	OMG	2	1883	2	18,26,27	2.34	6 (33%)	19,38,41	1.92	4 (21%)
2	M7A	2	4564	2	20,25,26	1.94	3 (15%)	28,37,40	3.99	6 (21%)
2	B8Q	2	1456	2	17,22,23	2.90	4 (23%)	22,32,35	2.63	6 (27%)
2	OMU	2	4306	2	19,22,23	2.68	7 (36%)	26,31,34	1.78	5 (19%)
2	UR3	2	4530	2	19,22,23	2.66	6 (31%)	26,32,35	1.37	3 (11%)
2	A2M	2	1871	2	18,25,26	4.31	7 (38%)	18,36,39	3.09	3 (16%)
2	OMC	2	2422	51,2,32	19,22,23	2.76	7 (36%)	26,31,34	1.39	3 (11%)
2	OMC	2	2861	2	19,22,23	2.85	8 (42%)	26,31,34	1.06	2 (7%)
2	2MG	2	978	2	18,26,27	2.41	7 (38%)	16,38,41	1.60	4 (25%)
2	OMG	2	4370	2	18,26,27	2.40	8 (44%)	19,38,41	1.56	4 (21%)
2	OMG	2	2424	2	18,26,27	2.33	7 (38%)	19,38,41	1.56	3 (15%)
2	I4U	2	1659	51,2	21,24,25	4.63	15 (71%)	27,34,37	1.65	4 (14%)
2	OMG	2	2364	2	18,26,27	2.27	7 (38%)	19,38,41	1.61	4 (21%)
2	B9H	2	2786	2	20,25,26	2.95	5 (25%)	22,35,38	3.29	7 (31%)
2	E7G	2	2297	2	24,27,28	3.74	11 (45%)	30,40,43	2.27	10 (33%)
2	MHG	2	4371	2	29,32,33	3.94	12 (41%)	34,46,49	2.61	10 (29%)
2	UR3	2	4597	2	19,22,23	2.69	7 (36%)	26,32,35	2.45	6 (23%)
2	7MG	2	4550	2	22,26,27	3.50	10 (45%)	29,39,42	2.08	10 (34%)
2	A2M	2	1534	51,2	18,25,26	4.17	7 (38%)	18,36,39	3.43	4 (22%)
2	P7G	2	3880	2	24,28,29	4.67	11 (45%)	27,41,44	1.58	3 (11%)
2	B8T	2	4483	2	19,22,23	3.49	8 (42%)	26,31,34	1.06	3 (11%)
2	A2M	2	1326	51,2	18,25,26	4.00	6 (33%)	18,36,39	3.29	4 (22%)
2	OMG	2	4623	2	18,26,27	2.28	8 (44%)	19,38,41	1.57	5 (26%)
2	OMG	2	373	2	18,26,27	2.27	7 (38%)	19,38,41	1.70	5 (26%)
2	5MU	2	4083	2	19,22,23	4.66	7 (36%)	28,32,35	3.87	10 (35%)
2	B8H	2	4296	2	19,22,23	6.87	6 (31%)	22,32,35	2.47	5 (22%)
2	PSU	2	3715	2	18,21,22	1.10	1 (5%)	22,30,33	1.68	4 (18%)
2	7MG	2	1605	2	22,26,27	3.19	10 (45%)	29,39,42	2.18	10 (34%)
2	A2M	2	4571	2	18,25,26	4.26	7 (38%)	18,36,39	3.17	3 (16%)
2	OMG	2	4637	2	18,26,27	2.38	6 (33%)	19,38,41	1.66	4 (21%)
2	PSU	2	4403	2	18,21,22	1.00	1 (5%)	22,30,33	1.70	5 (22%)
2	2MG	2	1517	2	18,26,27	2.33	7 (38%)	16,38,41	1.98	5 (31%)
2	A2M	2	3867	2	18,25,26	4.13	7 (38%)	18,36,39	3.16	4 (22%)
2	OMC	2	3869	2	19,22,23	2.80	7 (36%)	26,31,34	2.17	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OMG	2	1316	51,2	18,26,27	2.35	8 (44%)	19,38,41	1.77	5 (26%)
2	6MZ	2	4220	2	18,25,26	1.88	3 (16%)	16,36,39	3.77	4 (25%)
2	I4U	2	4194	2	21,24,25	4.72	15 (71%)	27,34,37	1.33	2 (7%)
2	UR3	2	1866	2	19,22,23	1.04	2 (10%)	26,32,35	1.62	2 (7%)
2	P4U	2	1348	2	21,24,25	3.51	7 (33%)	27,33,36	1.38	4 (14%)
2	PSU	2	4636	2	18,21,22	1.12	1 (5%)	22,30,33	1.79	3 (13%)
2	OMC	2	3909	2	19,22,23	2.98	8 (42%)	26,31,34	2.61	6 (23%)
2	OMG	2	1625	2	18,26,27	2.32	7 (38%)	19,38,41	1.58	4 (21%)
2	P7G	2	1909	2	24,28,29	4.57	11 (45%)	27,41,44	1.82	5 (18%)
2	OMG	2	2050	2	18,26,27	2.26	7 (38%)	19,38,41	1.61	4 (21%)
2	B9B	2	2754	2	21,28,29	5.50	8 (38%)	23,40,43	2.39	7 (30%)
2	B8T	2	4671	2	19,22,23	3.30	8 (42%)	26,31,34	1.04	1 (3%)
2	5MC	2	4335	2	18,22,23	3.34	7 (38%)	26,32,35	1.14	2 (7%)
2	2MG	2	4872	2	18,26,27	2.25	7 (38%)	16,38,41	1.58	4 (25%)
2	A2M	2	3718	2	18,25,26	4.20	7 (38%)	18,36,39	3.12	3 (16%)
2	OMU	2	4620	2	19,22,23	2.63	7 (36%)	26,31,34	1.75	5 (19%)
2	1MA	2	4415	2	16,25,26	3.95	4 (25%)	18,37,40	1.64	3 (16%)
2	B9B	2	237	2	21,28,29	5.70	9 (42%)	23,40,43	2.62	6 (26%)
2	OMG	2	4870	2	18,26,27	2.40	8 (44%)	19,38,41	1.58	4 (21%)
2	PSU	2	1582	2	18,21,22	1.07	1 (5%)	22,30,33	1.76	5 (22%)
2	B8W	2	4129	2	18,26,27	6.08	6 (33%)	21,38,41	2.83	8 (38%)
2	B8K	2	3897	2	24,28,29	4.33	16 (66%)	30,42,45	2.60	13 (43%)
2	A2M	2	3723	2	18,25,26	4.29	7 (38%)	18,36,39	3.06	3 (16%)
2	7MG	2	2522	2	22,26,27	3.44	10 (45%)	29,39,42	2.11	10 (34%)
2	OMC	2	3701	51,2	19,22,23	2.78	8 (42%)	26,31,34	0.93	0
2	B8W	2	4529	51,2	18,26,27	6.27	7 (38%)	21,38,41	2.85	10 (47%)
2	OMG	2	2773	2	18,26,27	2.37	8 (44%)	19,38,41	1.61	5 (26%)
2	OMG	2	1522	2	18,26,27	2.30	7 (38%)	19,38,41	1.51	4 (21%)
2	PSU	2	1677	2	18,21,22	1.31	3 (16%)	22,30,33	1.82	5 (22%)
8	OMU	8	14	8,2	19,22,23	2.58	6 (31%)	26,31,34	1.97	5 (19%)
2	PSU	2	3729	2	18,21,22	0.99	1 (5%)	22,30,33	1.68	4 (18%)
2	B9B	2	1574	2	21,28,29	5.64	8 (38%)	23,40,43	2.45	6 (26%)
2	E7G	2	1797	2	24,27,28	3.81	11 (45%)	30,40,43	2.26	10 (33%)
2	A2M	2	1524	2	18,25,26	4.07	7 (38%)	18,36,39	3.20	4 (22%)
2	OMC	2	3887	2	19,22,23	2.95	7 (36%)	26,31,34	1.31	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	B8W	2	4185	2	18,26,27	6.16	7 (38%)	21,38,41	2.63	6 (28%)
2	B8K	2	4690	2	24,28,29	4.45	16 (66%)	30,42,45	2.72	12 (40%)
2	A2M	2	3825	2	18,25,26	4.21	7 (38%)	18,36,39	3.34	3 (16%)
2	A2M	2	4523	2	18,25,26	4.24	7 (38%)	18,36,39	3.23	3 (16%)
2	PSU	2	2508	2	18,21,22	1.01	1 (5%)	22,30,33	1.66	4 (18%)
2	B8W	2	2380	2	18,26,27	6.12	7 (38%)	21,38,41	2.43	6 (28%)
2	E6G	2	4355	2	20,27,28	5.74	9 (45%)	22,39,42	3.05	8 (36%)
2	PSU	2	4628	2	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
2	PSU	2	1683	2	18,21,22	1.15	1 (5%)	22,30,33	1.90	5 (22%)
2	OMC	2	2804	2	19,22,23	2.63	7 (36%)	26,31,34	1.26	3 (11%)
2	A2M	2	398	2	18,25,26	4.23	6 (33%)	18,36,39	3.13	3 (16%)
2	B8H	2	1860	2	19,22,23	6.76	6 (31%)	22,32,35	2.21	5 (22%)
2	OMC	2	4536	2	19,22,23	2.78	7 (36%)	26,31,34	1.03	2 (7%)
2	OMG	2	4196	51,2,3	18,26,27	2.57	8 (44%)	19,38,41	1.93	6 (31%)
2	A2M	2	2401	2	18,25,26	4.12	6 (33%)	18,36,39	3.28	3 (16%)
2	OMC	2	2365	51,2	19,22,23	2.76	7 (36%)	26,31,34	0.97	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGH	2	3899	2	-	0/13/43/44	0/3/3/3
2	2MG	2	729	2	-	1/5/27/28	0/3/3/3
2	A2M	2	2363	51,2	-	1/5/27/28	0/3/3/3
2	B8W	2	4472	2	-	2/5/27/28	0/3/3/3
2	OMG	2	4494	2	-	0/5/27/28	0/3/3/3
2	PSU	2	4293	30,2	-	2/7/25/26	0/2/2/2
2	1MA	2	1322	51,2	-	0/3/25/26	0/3/3/3
2	OMG	2	1883	2	-	2/5/27/28	0/3/3/3
2	M7A	2	4564	2	-	0/7/37/38	0/3/3/3
2	B8Q	2	1456	2	-	0/7/42/43	0/2/2/2
2	OMU	2	4306	2	-	0/9/27/28	0/2/2/2
2	UR3	2	4530	2	-	0/7/25/26	0/2/2/2
2	A2M	2	1871	2	-	3/5/27/28	0/3/3/3
2	OMC	2	2422	51,2,32	-	1/9/27/28	0/2/2/2
2	OMC	2	2861	2	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2MG	2	978	2	-	0/5/27/28	0/3/3/3
2	OMG	2	4370	2	-	0/5/27/28	0/3/3/3
2	OMG	2	2424	2	-	2/5/27/28	0/3/3/3
2	I4U	2	1659	51,2	-	2/9/29/30	0/2/2/2
2	OMG	2	2364	2	-	2/5/27/28	0/3/3/3
2	B9H	2	2786	2	-	0/12/47/48	0/2/2/2
2	E7G	2	2297	2	-	1/9/39/40	0/3/3/3
2	MHG	2	4371	2	-	7/16/46/47	0/3/3/3
2	UR3	2	4597	2	-	2/7/25/26	0/2/2/2
2	7MG	2	4550	2	-	0/7/37/38	0/3/3/3
2	A2M	2	1534	51,2	-	2/5/27/28	0/3/3/3
2	P7G	2	3880	2	-	1/10/40/41	0/3/3/3
2	B8T	2	4483	2	-	0/7/27/28	0/2/2/2
2	A2M	2	1326	51,2	-	1/5/27/28	0/3/3/3
2	OMG	2	4623	2	-	0/5/27/28	0/3/3/3
2	OMG	2	373	2	-	1/5/27/28	0/3/3/3
2	5MU	2	4083	2	-	0/7/25/26	0/2/2/2
2	B8H	2	4296	2	-	2/7/25/26	0/2/2/2
2	PSU	2	3715	2	-	0/7/25/26	0/2/2/2
2	7MG	2	1605	2	-	1/7/37/38	0/3/3/3
2	A2M	2	4571	2	-	0/5/27/28	0/3/3/3
2	OMG	2	4637	2	-	2/5/27/28	0/3/3/3
2	PSU	2	4403	2	-	2/7/25/26	0/2/2/2
2	2MG	2	1517	2	-	0/5/27/28	0/3/3/3
2	A2M	2	3867	2	-	2/5/27/28	0/3/3/3
2	OMC	2	3869	2	-	3/9/27/28	0/2/2/2
2	OMG	2	1316	51,2	-	0/5/27/28	0/3/3/3
2	6MZ	2	4220	2	-	2/5/27/28	0/3/3/3
2	I4U	2	4194	2	-	4/9/29/30	0/2/2/2
2	UR3	2	1866	2	-	3/7/25/26	0/2/2/2
2	P4U	2	1348	2	-	1/10/29/30	0/2/2/2
2	PSU	2	4636	2	-	3/7/25/26	0/2/2/2
2	OMC	2	3909	2	-	0/9/27/28	0/2/2/2
2	OMG	2	1625	2	-	2/5/27/28	0/3/3/3
2	P7G	2	1909	2	-	1/10/40/41	0/3/3/3
2	OMG	2	2050	2	-	0/5/27/28	0/3/3/3
2	B9B	2	2754	2	-	2/7/29/30	0/3/3/3
2	B8T	2	4671	2	-	0/7/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	2	4335	2	-	0/7/25/26	0/2/2/2
2	2MG	2	4872	2	-	2/5/27/28	0/3/3/3
2	A2M	2	3718	2	-	1/5/27/28	0/3/3/3
2	OMU	2	4620	2	-	0/9/27/28	0/2/2/2
2	1MA	2	4415	2	-	2/3/25/26	0/3/3/3
2	B9B	2	237	2	-	6/7/29/30	0/3/3/3
2	OMG	2	4870	2	-	3/5/27/28	0/3/3/3
2	PSU	2	1582	2	-	2/7/25/26	0/2/2/2
2	B8W	2	4129	2	-	2/5/27/28	0/3/3/3
2	B8K	2	3897	2	-	3/11/41/42	0/3/3/3
2	A2M	2	3723	2	-	0/5/27/28	0/3/3/3
2	7MG	2	2522	2	-	0/7/37/38	0/3/3/3
2	OMC	2	3701	51,2	-	4/9/27/28	0/2/2/2
2	B8W	2	4529	51,2	-	4/5/27/28	0/3/3/3
2	OMG	2	2773	2	-	0/5/27/28	0/3/3/3
2	OMG	2	1522	2	-	0/5/27/28	0/3/3/3
2	PSU	2	1677	2	-	3/7/25/26	0/2/2/2
8	OMU	8	14	8,2	-	1/9/27/28	0/2/2/2
2	PSU	2	3729	2	-	2/7/25/26	0/2/2/2
2	B9B	2	1574	2	-	3/7/29/30	0/3/3/3
2	E7G	2	1797	2	-	2/9/39/40	0/3/3/3
2	A2M	2	1524	2	-	0/5/27/28	0/3/3/3
2	OMC	2	3887	2	-	1/9/27/28	0/2/2/2
2	B8W	2	4185	2	-	3/5/27/28	0/3/3/3
2	B8K	2	4690	2	-	0/11/41/42	0/3/3/3
2	A2M	2	3825	2	-	0/5/27/28	0/3/3/3
2	A2M	2	4523	2	-	4/5/27/28	0/3/3/3
2	PSU	2	2508	2	-	0/7/25/26	0/2/2/2
2	B8W	2	2380	2	-	4/5/27/28	0/3/3/3
2	E6G	2	4355	2	-	3/6/28/29	0/3/3/3
2	PSU	2	4628	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1683	2	-	0/7/25/26	0/2/2/2
2	OMC	2	2804	2	-	0/9/27/28	0/2/2/2
2	A2M	2	398	2	-	2/5/27/28	0/3/3/3
2	B8H	2	1860	2	-	0/7/25/26	0/2/2/2
2	OMC	2	4536	2	-	0/9/27/28	0/2/2/2
2	OMG	2	4196	51,2,3	-	3/5/27/28	0/3/3/3
2	A2M	2	2401	2	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	2	2365	51,2	-	0/9/27/28	0/2/2/2

All (644) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4529	B8W	O4'-C1'	18.29	1.66	1.41
2	2	4472	B8W	O4'-C1'	17.88	1.66	1.41
2	2	2380	B8W	O4'-C1'	17.65	1.65	1.41
2	2	4185	B8W	O4'-C1'	17.55	1.65	1.41
2	2	4129	B8W	O4'-C1'	17.42	1.65	1.41
2	2	4296	B8H	C6-C5	-17.22	1.10	1.34
2	2	237	B9B	C2'-C1'	-16.59	1.28	1.53
2	2	1860	B8H	C6-C5	-16.35	1.12	1.34
2	2	4296	B8H	C4-N3	-16.35	1.08	1.38
2	2	1574	B9B	C2'-C1'	-16.08	1.29	1.53
2	2	4355	E6G	C2'-C1'	-15.85	1.29	1.53
2	2	1860	B8H	C4-N3	-15.83	1.09	1.38
2	2	1871	A2M	O4'-C1'	15.61	1.62	1.41
2	2	2754	B9B	C2'-C1'	-15.60	1.30	1.53
2	2	4185	B8W	C2'-C1'	-15.42	1.30	1.53
2	2	3723	A2M	O4'-C1'	15.26	1.62	1.41
2	2	4523	A2M	O4'-C1'	15.21	1.62	1.41
2	2	4529	B8W	C2'-C1'	-15.20	1.30	1.53
2	2	2380	B8W	C2'-C1'	-15.18	1.30	1.53
2	2	398	A2M	O4'-C1'	15.14	1.62	1.41
2	2	4129	B8W	C2'-C1'	-15.02	1.31	1.53
2	2	4355	E6G	O4'-C1'	15.00	1.62	1.41
2	2	3825	A2M	O4'-C1'	14.94	1.61	1.41
2	2	4571	A2M	O4'-C1'	14.92	1.61	1.41
2	2	1574	B9B	O4'-C1'	14.86	1.61	1.41
2	2	237	B9B	O4'-C1'	14.79	1.61	1.41
2	2	3718	A2M	O4'-C1'	14.76	1.61	1.41
2	2	1534	A2M	O4'-C1'	14.76	1.61	1.41
2	2	2754	B9B	O4'-C1'	14.75	1.61	1.41
2	2	2401	A2M	O4'-C1'	14.73	1.61	1.41
2	2	3867	A2M	O4'-C1'	14.49	1.61	1.41
2	2	4472	B8W	C2'-C1'	-14.42	1.31	1.53
2	2	1322	1MA	C2-N3	14.36	1.46	1.29
2	2	2363	A2M	O4'-C1'	14.33	1.61	1.41
2	2	4415	1MA	C2-N3	14.32	1.46	1.29
2	2	3880	P7G	C8-N9	14.23	1.53	1.46
2	2	1524	A2M	O4'-C1'	14.16	1.60	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1326	A2M	O4'-C1'	14.05	1.60	1.41
2	2	1909	P7G	C8-N9	13.96	1.53	1.46
2	2	1860	B8H	C4-C5	13.19	1.81	1.44
2	2	4296	B8H	C4-C5	12.88	1.80	1.44
2	2	1860	B8H	C6-N1	12.10	1.66	1.36
2	2	4296	B8H	C6-N1	11.80	1.65	1.36
2	2	4083	5MU	C6-N1	11.00	1.56	1.38
2	2	4194	I4U	C3'-C2'	-10.56	1.24	1.53
2	2	1659	I4U	C3'-C2'	-10.55	1.24	1.53
2	2	3880	P7G	C5-N7	10.44	1.47	1.35
2	2	4690	B8K	C3'-C4'	-10.27	1.26	1.53
2	2	4083	5MU	C2-N1	10.21	1.54	1.38
2	2	3897	B8K	C3'-C4'	-9.98	1.27	1.53
2	2	1909	P7G	C5-N7	9.97	1.46	1.35
2	2	3899	BGH	C3'-C4'	-9.96	1.27	1.53
2	2	4690	B8K	O4'-C4'	9.90	1.67	1.45
2	2	1348	P4U	C4-N3	9.89	1.44	1.31
2	2	3897	B8K	O4'-C4'	9.81	1.66	1.45
2	2	4371	MHG	C8-N9	9.56	1.51	1.46
2	2	4371	MHG	C5-N7	9.48	1.46	1.35
2	2	3899	BGH	O4'-C4'	9.46	1.66	1.45
2	2	4194	I4U	C4-N3	9.31	1.43	1.31
2	2	1659	I4U	C4-N3	9.27	1.43	1.31
2	2	1797	E7G	C8-N9	9.22	1.51	1.46
2	2	2297	E7G	C8-N9	9.19	1.51	1.46
2	2	2297	E7G	C5-N7	9.17	1.45	1.35
2	2	1797	E7G	C5-N7	9.17	1.45	1.35
2	2	2786	B9H	C2-N3	8.94	1.48	1.37
2	2	4335	5MC	C6-C5	8.64	1.48	1.34
2	2	2522	7MG	C5-N7	8.47	1.45	1.35
2	2	4083	5MU	C4-C5	8.39	1.58	1.44
2	2	4550	7MG	C8-N9	8.35	1.50	1.46
2	2	1574	B9B	O4'-C4'	-8.31	1.26	1.45
2	2	4529	B8W	C2-N2	8.29	1.50	1.33
2	2	237	B9B	O4'-C4'	-8.25	1.26	1.45
2	2	4355	E6G	O4'-C4'	-8.13	1.26	1.45
2	2	4472	B8W	C2-N2	8.10	1.50	1.33
2	2	4129	B8W	C2-N2	8.09	1.50	1.33
2	2	4083	5MU	C4-N3	-8.02	1.23	1.38
2	2	2754	B9B	O4'-C4'	-7.97	1.27	1.45
2	2	1456	B8Q	C6-C5	7.95	1.51	1.33
2	2	4185	B8W	C2-N2	7.92	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4550	7MG	C5-N7	7.88	1.44	1.35
2	2	2380	B8W	C2-N2	7.84	1.49	1.33
2	2	1605	7MG	C5-N7	7.71	1.44	1.35
2	2	2522	7MG	C8-N9	7.47	1.50	1.46
2	2	1659	I4U	O4'-C4'	-7.47	1.28	1.45
2	2	4194	I4U	O4'-C4'	-7.46	1.28	1.45
2	2	4371	MHG	C2-N3	7.28	1.45	1.31
2	2	4483	B8T	C2-N3	7.13	1.50	1.36
2	2	3909	OMC	C6-C5	7.06	1.51	1.35
2	2	2363	A2M	O4'-C4'	-6.97	1.29	1.45
2	2	4371	MHG	C8-N7	6.94	1.52	1.45
2	2	1524	A2M	O4'-C4'	-6.89	1.29	1.45
2	2	1456	B8Q	C2-N3	6.86	1.47	1.35
2	2	4571	A2M	O4'-C4'	-6.85	1.29	1.45
2	2	1534	A2M	O4'-C4'	-6.82	1.29	1.45
2	2	3718	A2M	O4'-C4'	-6.70	1.30	1.45
2	2	4483	B8T	C4-N3	6.68	1.44	1.32
2	2	237	B9B	O6-C6	6.68	1.40	1.35
2	2	3867	A2M	O4'-C4'	-6.68	1.30	1.45
2	2	4671	B8T	C2-N3	6.65	1.49	1.36
2	2	1909	P7G	C4-N3	6.64	1.49	1.37
2	2	1605	7MG	C8-N9	6.58	1.49	1.46
2	2	3825	A2M	O4'-C4'	-6.58	1.30	1.45
2	2	3880	P7G	C4-N3	6.55	1.49	1.37
2	2	1348	P4U	C2-N3	6.53	1.49	1.36
2	2	4530	UR3	C6-C5	6.50	1.50	1.35
2	2	3723	A2M	O4'-C4'	-6.49	1.30	1.45
2	2	4483	B8T	C6-C5	6.49	1.50	1.35
2	2	1326	A2M	O4'-C4'	-6.46	1.30	1.45
2	2	4355	E6G	O6-C6	6.45	1.40	1.35
2	2	4671	B8T	C6-C5	6.42	1.50	1.35
2	2	4194	I4U	C6-C5	6.41	1.50	1.35
2	2	4220	6MZ	C6-N6	6.40	1.45	1.35
2	2	398	A2M	O4'-C4'	-6.39	1.30	1.45
2	2	1574	B9B	O6-C6	6.36	1.40	1.35
2	2	4483	B8T	C4-N4	6.35	1.48	1.35
2	2	4371	MHG	C2-N2	6.30	1.47	1.33
2	2	4597	UR3	C6-C5	6.25	1.49	1.35
2	2	2754	B9B	O6-C6	6.24	1.40	1.35
2	2	3887	OMC	C2-N3	6.22	1.49	1.36
2	2	2401	A2M	O4'-C4'	-6.20	1.31	1.45
2	2	4597	UR3	C2-N3	6.18	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4671	B8T	C4-N3	6.17	1.43	1.32
2	2	4523	A2M	O4'-C4'	-6.17	1.31	1.45
2	2	3897	B8K	O4'-C1'	-6.16	1.27	1.42
2	2	1348	P4U	C6-C5	6.08	1.49	1.35
2	2	4690	B8K	C8-N9	6.06	1.49	1.46
2	2	4335	5MC	C4-N3	6.06	1.44	1.34
2	2	3909	OMC	C4-N4	6.05	1.48	1.33
2	2	1871	A2M	O4'-C4'	-6.04	1.31	1.45
2	2	4690	B8K	C2-N3	6.01	1.47	1.33
2	2	2861	OMC	C2-N3	6.00	1.48	1.36
8	8	14	OMU	C2-N1	5.97	1.48	1.38
2	2	4536	OMC	C2-N3	5.96	1.48	1.36
2	2	3701	OMC	C6-C5	5.96	1.48	1.35
2	2	4620	OMU	C2-N3	5.92	1.48	1.38
2	2	4196	OMG	C2-N3	5.91	1.47	1.33
2	2	2786	B9H	C2-N1	5.89	1.47	1.38
2	2	1659	I4U	C6-C5	5.87	1.48	1.35
2	2	4306	OMU	C2-N1	5.86	1.47	1.38
2	2	3869	OMC	C2-N3	5.86	1.48	1.36
2	2	1909	P7G	C2-N2	5.84	1.48	1.34
2	2	4306	OMU	C2-N3	5.83	1.48	1.38
2	2	2786	B9H	C6-C5	5.83	1.46	1.33
2	2	1659	I4U	C2-N3	5.82	1.48	1.36
2	2	4671	B8T	C4-N4	5.82	1.47	1.35
2	2	4530	UR3	C2-N1	5.81	1.46	1.38
2	2	2861	OMC	C6-C5	5.81	1.48	1.35
2	2	3887	OMC	C6-C5	5.75	1.48	1.35
2	2	2365	OMC	C2-N3	5.72	1.47	1.36
2	2	3701	OMC	C2-N3	5.67	1.47	1.36
2	2	3880	P7G	C2-N2	5.66	1.47	1.34
2	2	4371	MHG	C2-N1	5.65	1.45	1.36
2	2	2422	OMC	C2-N3	5.62	1.47	1.36
2	2	4536	OMC	C6-C5	5.59	1.48	1.35
2	2	4597	UR3	C2-N1	5.59	1.46	1.38
2	2	4335	5MC	C2-N3	5.57	1.47	1.36
2	2	237	B9B	C2-N2	5.56	1.45	1.33
2	2	2422	OMC	C6-C5	5.56	1.48	1.35
2	2	2365	OMC	C6-C5	5.55	1.48	1.35
2	2	4194	I4U	C2-N3	5.54	1.47	1.36
8	8	14	OMU	C2-N3	5.53	1.47	1.38
2	2	4690	B8K	O4'-C1'	-5.51	1.28	1.42
2	2	4355	E6G	C2-N2	5.48	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2804	OMC	C6-C5	5.45	1.47	1.35
2	2	4530	UR3	C2-N3	5.43	1.49	1.39
2	2	3899	BGH	C8-N9	5.41	1.49	1.46
2	2	2297	E7G	C8-N7	5.40	1.50	1.45
2	2	4129	B8W	O4'-C4'	-5.39	1.33	1.45
2	2	4550	7MG	C2-N3	5.36	1.46	1.33
2	2	4185	B8W	O4'-C4'	-5.36	1.33	1.45
2	2	1574	B9B	C2-N2	5.36	1.44	1.33
2	2	1797	E7G	C4-N3	5.36	1.47	1.34
2	2	3869	OMC	C6-C5	5.36	1.47	1.35
2	2	4637	OMG	C2-N3	5.34	1.46	1.33
2	2	3897	B8K	C2-N3	5.34	1.46	1.33
2	2	2380	B8W	O4'-C4'	-5.34	1.33	1.45
2	2	4494	OMG	C2-N3	5.32	1.46	1.33
2	2	2804	OMC	C2-N3	5.32	1.47	1.36
2	2	4620	OMU	C2-N1	5.31	1.47	1.38
2	2	4550	7MG	C4-N3	5.28	1.46	1.34
2	2	3899	BGH	C4-N3	5.28	1.46	1.34
2	2	4371	MHG	C4-N3	5.27	1.46	1.34
2	2	1797	E7G	C4-N9	5.26	1.43	1.37
2	2	4529	B8W	O4'-C4'	-5.26	1.33	1.45
2	2	4306	OMU	C6-C5	5.25	1.47	1.35
2	2	3869	OMC	C2-N1	5.25	1.51	1.40
2	2	2754	B9B	C2-N2	5.22	1.44	1.33
2	2	1797	E7G	C2-N3	5.21	1.45	1.33
2	2	4472	B8W	O4'-C4'	-5.20	1.33	1.45
2	2	4620	OMU	C6-C5	5.19	1.47	1.35
2	2	2297	E7G	C4-N3	5.18	1.46	1.34
2	2	2522	7MG	C2-N3	5.18	1.45	1.33
2	2	4870	OMG	C2-N3	5.16	1.45	1.33
2	2	4083	5MU	C6-C5	5.16	1.43	1.34
2	2	3880	P7G	C2-N1	5.16	1.45	1.33
2	2	4370	OMG	C2-N3	5.15	1.45	1.33
2	2	2522	7MG	C4-N3	5.15	1.46	1.34
2	2	1909	P7G	C2-N1	5.14	1.45	1.33
2	2	3899	BGH	C2-N3	5.12	1.45	1.33
2	2	2424	OMG	C2-N3	5.11	1.45	1.33
2	2	978	2MG	C2-N2	5.10	1.44	1.33
2	2	1625	OMG	C2-N3	5.07	1.45	1.33
2	2	4371	MHG	C4-N9	5.06	1.43	1.37
2	2	4196	OMG	C4-N3	5.05	1.49	1.37
2	2	4690	B8K	O2'-C2'	-5.05	1.31	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1517	2MG	C2-N2	5.04	1.44	1.33
2	2	3897	B8K	C8-N9	5.03	1.48	1.46
2	2	4690	B8K	C4-N3	5.02	1.46	1.34
2	2	2297	E7G	C2-N3	5.02	1.45	1.33
2	2	4194	I4U	C3'-C4'	5.01	1.65	1.53
2	2	1797	E7G	C8-N7	5.00	1.50	1.45
2	2	729	2MG	C4-N3	4.98	1.49	1.37
2	2	4194	I4U	C1'-N1	-4.96	1.33	1.47
2	2	1605	7MG	C2-N3	4.93	1.45	1.33
2	2	4564	M7A	C6-N6	4.93	1.46	1.34
2	2	4185	B8W	O3'-C3'	-4.93	1.31	1.43
2	2	1797	E7G	C2-N2	4.92	1.45	1.34
2	2	3899	BGH	O4'-C1'	-4.90	1.30	1.42
2	2	3880	P7G	C4-N9	4.90	1.42	1.35
2	2	1517	2MG	C4-N3	4.89	1.49	1.37
2	2	3887	OMC	C2-N1	4.86	1.50	1.40
2	2	1316	OMG	C2-N3	4.86	1.45	1.33
2	2	2050	OMG	C2-N3	4.85	1.45	1.33
2	2	4564	M7A	C4-N9	4.85	1.47	1.38
2	2	3880	P7G	C8-N7	4.83	1.50	1.45
2	2	2297	E7G	C2-N2	4.82	1.45	1.34
2	2	2861	OMC	C4-N4	4.82	1.45	1.33
2	2	2364	OMG	C2-N3	4.81	1.44	1.33
2	2	4623	OMG	C2-N3	4.78	1.44	1.33
2	2	3887	OMC	C4-N4	4.78	1.45	1.33
2	2	4872	2MG	C2-N2	4.77	1.44	1.33
2	2	2773	OMG	C2-N3	4.77	1.44	1.33
2	2	1522	OMG	C2-N3	4.75	1.44	1.33
2	2	3897	B8K	C4-N3	4.75	1.45	1.34
2	2	4472	B8W	O3'-C3'	-4.74	1.31	1.43
2	2	4637	OMG	C4-N3	4.74	1.48	1.37
2	2	978	2MG	C4-N3	4.73	1.48	1.37
2	2	2422	OMC	C2-N1	4.73	1.50	1.40
2	2	1883	OMG	C4-N3	4.73	1.48	1.37
2	2	1605	7MG	C4-N3	4.72	1.45	1.34
2	2	2365	OMC	C4-N4	4.71	1.45	1.33
2	2	4536	OMC	C4-N4	4.70	1.45	1.33
2	2	3887	OMC	C4-N3	4.70	1.44	1.34
2	2	3897	B8K	C4-N9	4.70	1.43	1.37
2	2	729	2MG	C2-N2	4.70	1.43	1.33
2	2	1883	OMG	C2-N3	4.67	1.44	1.33
2	2	3869	OMC	C4-N4	4.63	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4370	OMG	C4-N3	4.61	1.48	1.37
2	2	2422	OMC	C4-N4	4.61	1.44	1.33
2	2	1348	P4U	C5-C4	4.60	1.49	1.43
2	2	4415	1MA	C2-N1	4.59	1.44	1.35
2	2	3701	OMC	C4-N4	4.59	1.44	1.33
2	2	4494	OMG	C4-N3	4.59	1.48	1.37
2	2	4550	7MG	C2-N2	4.59	1.45	1.34
2	2	373	OMG	C2-N3	4.57	1.44	1.33
8	8	14	OMU	C6-C5	4.56	1.45	1.35
2	2	3899	BGH	C2-N2	4.56	1.45	1.34
2	2	3897	B8K	O2'-C2'	-4.55	1.32	1.43
2	2	1605	7MG	C2-N2	4.55	1.45	1.34
2	2	2522	7MG	C2-N2	4.54	1.45	1.34
2	2	3909	OMC	C2-N1	4.53	1.49	1.40
2	2	4870	OMG	C4-N3	4.50	1.48	1.37
2	2	978	2MG	C2-N1	4.49	1.43	1.36
2	2	1659	I4U	C2-N1	4.49	1.49	1.40
2	2	1522	OMG	C4-N3	4.48	1.48	1.37
2	2	2804	OMC	C4-N4	4.47	1.44	1.33
2	2	1909	P7G	C4-N9	4.46	1.41	1.35
2	2	3899	BGH	C71-N7	4.44	1.49	1.39
2	2	4529	B8W	O3'-C3'	-4.44	1.32	1.43
2	2	1322	1MA	C2-N1	4.44	1.44	1.35
2	2	4129	B8W	O3'-C3'	-4.42	1.32	1.43
2	2	1625	OMG	C4-N3	4.41	1.48	1.37
2	2	373	OMG	C4-N3	4.40	1.48	1.37
2	2	1348	P4U	O4-C4	4.39	1.40	1.35
2	2	3701	OMC	C4-N3	4.38	1.43	1.34
2	2	2365	OMC	C4-N3	4.37	1.43	1.34
2	2	4690	B8K	C5-N7	4.35	1.47	1.39
2	2	4690	B8K	C4-N9	4.32	1.42	1.37
2	2	4483	B8T	C2-N1	4.31	1.49	1.40
2	2	4550	7MG	C4-N9	4.31	1.42	1.37
2	2	1909	P7G	C6-N1	4.30	1.45	1.38
2	2	2424	OMG	C4-N3	4.29	1.47	1.37
2	2	2861	OMC	C4-N3	4.29	1.43	1.34
2	2	3897	B8K	C5-N7	4.28	1.47	1.39
2	2	2050	OMG	C4-N3	4.28	1.47	1.37
2	2	2804	OMC	C2-N1	4.28	1.49	1.40
2	2	1316	OMG	C4-N3	4.28	1.47	1.37
2	2	2773	OMG	C4-N3	4.28	1.47	1.37
2	2	2861	OMC	C2-N1	4.26	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2522	7MG	C4-N9	4.26	1.42	1.37
2	2	3880	P7G	C6-N1	4.24	1.45	1.38
2	2	2364	OMG	C4-N3	4.24	1.47	1.37
2	2	1456	B8Q	C2-N1	4.23	1.44	1.38
2	2	1909	P7G	O6-C6	-4.22	1.17	1.23
2	2	2297	E7G	C4-N9	4.22	1.42	1.37
2	2	1860	B8H	C2-N3	4.21	1.45	1.38
2	2	4872	2MG	C4-N3	4.21	1.47	1.37
2	2	4536	OMC	C4-N3	4.19	1.43	1.34
2	2	4872	2MG	C2-N1	4.18	1.43	1.36
2	2	4194	I4U	C5-C4	4.17	1.48	1.43
2	2	3899	BGH	C4-N9	4.14	1.42	1.37
2	2	4671	B8T	C2-N1	4.13	1.48	1.40
2	2	4623	OMG	C4-N3	4.11	1.47	1.37
2	2	1659	I4U	O4'-C1'	4.11	1.51	1.42
2	2	3899	BGH	O2'-C2'	-4.10	1.32	1.42
2	2	1348	P4U	C6-N1	4.09	1.47	1.38
2	2	4335	5MC	C4-N4	4.09	1.44	1.34
2	2	4536	OMC	C2-N1	4.09	1.48	1.40
2	2	2422	OMC	C4-N3	4.09	1.42	1.34
2	2	3909	OMC	C2-N3	4.08	1.44	1.36
2	2	729	2MG	C2-N1	4.05	1.43	1.36
2	2	4690	B8K	O6-C6	-4.05	1.15	1.23
2	2	1659	I4U	C1'-N1	-4.04	1.35	1.47
2	2	2380	B8W	O3'-C3'	-4.02	1.33	1.43
2	2	1348	P4U	C2-N1	3.99	1.48	1.40
2	2	4196	OMG	C2-N2	3.93	1.43	1.34
2	2	2804	OMC	C4-N3	3.92	1.42	1.34
2	2	1605	7MG	C4-N9	3.91	1.42	1.37
2	2	4415	1MA	C4-N3	3.89	1.49	1.37
2	2	4564	M7A	C5-N7	3.88	1.48	1.39
2	2	3869	OMC	C4-N3	3.87	1.42	1.34
2	2	4371	MHG	C5-C6	3.87	1.53	1.43
2	2	2365	OMC	C2-N1	3.86	1.48	1.40
2	2	3899	BGH	C5-N7	3.84	1.46	1.39
2	2	1517	2MG	C2-N1	3.83	1.42	1.36
2	2	1659	I4U	C3'-C4'	3.83	1.62	1.53
2	2	3897	B8K	C5-C6	3.82	1.53	1.43
2	2	4494	OMG	C2-N2	3.82	1.43	1.34
2	2	4870	OMG	C2-N2	3.82	1.43	1.34
2	2	4196	OMG	C6-N1	3.81	1.43	1.37
2	2	3701	OMC	C2-N1	3.79	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4335	5MC	C6-N1	3.79	1.44	1.38
2	2	4690	B8K	C2-N2	3.78	1.43	1.34
2	2	1909	P7G	C2-N3	3.77	1.47	1.37
2	2	1316	OMG	C2-N2	3.76	1.43	1.34
2	2	3880	P7G	C5-C4	3.76	1.44	1.37
2	2	3909	OMC	C6-N1	3.76	1.47	1.38
2	2	1909	P7G	C5-C4	3.76	1.44	1.37
2	2	3880	P7G	O6-C6	-3.75	1.17	1.23
2	2	2773	OMG	C6-N1	3.75	1.43	1.37
2	2	1322	1MA	C4-N3	3.75	1.49	1.37
2	2	4083	5MU	O4-C4	-3.74	1.16	1.23
2	2	2424	OMG	C2-N2	3.72	1.43	1.34
2	2	4370	OMG	C2-N2	3.70	1.43	1.34
2	2	1797	E7G	C2-N1	3.70	1.46	1.37
2	2	3897	B8K	C2-N2	3.66	1.42	1.34
2	2	2773	OMG	C2-N2	3.65	1.42	1.34
2	2	3880	P7G	C2-N3	3.65	1.46	1.37
2	2	3909	OMC	C4-N3	3.65	1.41	1.34
2	2	4623	OMG	C2-N2	3.64	1.42	1.34
2	2	1677	PSU	C6-C5	3.63	1.39	1.35
2	2	4690	B8K	C5-C6	3.63	1.52	1.43
2	2	4671	B8T	C5-C4	3.61	1.48	1.40
2	2	4194	I4U	O4'-C1'	3.60	1.50	1.42
2	2	1625	OMG	C2-N2	3.59	1.42	1.34
2	2	1909	P7G	C8-N7	3.58	1.49	1.45
2	2	3715	PSU	C6-C5	3.58	1.39	1.35
2	2	4194	I4U	C2-N1	3.57	1.47	1.40
2	2	4296	B8H	C2-N3	3.57	1.44	1.38
2	2	2754	B9B	O2'-C2'	3.56	1.51	1.43
2	2	237	B9B	O3'-C3'	-3.56	1.34	1.43
2	2	3899	BGH	C5-C6	3.54	1.52	1.43
2	2	4620	OMU	O4-C4	-3.53	1.17	1.24
2	2	2364	OMG	C2-N2	3.53	1.42	1.34
2	2	978	2MG	C6-N1	3.51	1.43	1.37
2	2	1659	I4U	O2-C2	-3.51	1.17	1.23
2	2	1883	OMG	C2-N2	3.51	1.42	1.34
2	2	2050	OMG	C2-N2	3.49	1.42	1.34
2	2	4335	5MC	C2-N1	3.48	1.47	1.40
2	2	373	OMG	C5-C4	-3.47	1.34	1.43
2	2	373	OMG	C2-N2	3.46	1.42	1.34
2	2	3899	BGH	C2-N1	3.46	1.46	1.37
2	2	4194	I4U	O2-C2	-3.45	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4483	B8T	C6-N1	3.45	1.46	1.38
2	2	1797	E7G	C5-C6	3.44	1.52	1.43
2	2	4571	A2M	O3'-C3'	-3.44	1.34	1.43
2	2	4637	OMG	C2-N2	3.44	1.42	1.34
2	2	4370	OMG	C6-N1	3.39	1.42	1.37
2	2	1871	A2M	O3'-C3'	-3.38	1.35	1.43
2	2	1522	OMG	C5-C4	-3.38	1.34	1.43
2	2	1659	I4U	C5-C4	3.38	1.47	1.43
2	2	1582	PSU	C6-C5	3.36	1.39	1.35
2	2	1522	OMG	C2-N2	3.36	1.42	1.34
2	2	4870	OMG	C6-N1	3.36	1.42	1.37
2	2	1883	OMG	C5-C4	-3.35	1.34	1.43
2	2	2297	E7G	C2-N1	3.35	1.46	1.37
2	2	1574	B9B	O2'-C2'	3.34	1.50	1.43
2	2	1883	OMG	O6-C6	-3.33	1.16	1.23
2	2	1683	PSU	C6-C5	3.33	1.39	1.35
2	2	1574	B9B	O3'-C3'	-3.32	1.35	1.43
2	2	4550	7MG	C5-C6	3.32	1.52	1.43
8	8	14	OMU	O4-C4	-3.31	1.18	1.24
2	2	4483	B8T	C5-C4	3.31	1.47	1.40
2	2	4306	OMU	C4-N3	3.30	1.44	1.38
2	2	1524	A2M	O3'-C3'	-3.29	1.35	1.43
2	2	4335	5MC	O2-C2	-3.29	1.17	1.23
2	2	3723	A2M	O3'-C3'	-3.29	1.35	1.43
2	2	3899	BGH	C6-N1	3.29	1.44	1.38
2	2	1316	OMG	C5-C4	-3.28	1.34	1.43
2	2	4494	OMG	C6-N1	3.28	1.42	1.37
2	2	4671	B8T	O2-C2	-3.28	1.17	1.23
2	2	4637	OMG	C5-C4	-3.28	1.34	1.43
2	2	2522	7MG	C5-C6	3.27	1.52	1.43
2	2	2363	A2M	C5-C4	-3.27	1.32	1.40
2	2	1574	B9B	C5-C4	-3.26	1.32	1.40
2	2	1605	7MG	C5-C6	3.25	1.51	1.43
2	2	3869	OMC	O2-C2	-3.25	1.17	1.23
2	2	4355	E6G	O2'-C2'	3.25	1.50	1.43
2	2	4623	OMG	C5-C4	-3.24	1.34	1.43
2	2	2364	OMG	C5-C4	-3.24	1.34	1.43
2	2	4306	OMU	O4-C4	-3.24	1.18	1.24
2	2	3897	B8K	C2-N1	3.24	1.45	1.37
2	2	2050	OMG	C5-C4	-3.23	1.34	1.43
2	2	2365	OMC	O2-C2	-3.22	1.17	1.23
2	2	2297	E7G	C5-C6	3.22	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4370	OMG	C5-C4	-3.20	1.34	1.43
8	8	14	OMU	C4-N3	3.19	1.44	1.38
2	2	1326	A2M	C6-N6	3.19	1.45	1.34
2	2	398	A2M	O3'-C3'	-3.17	1.35	1.43
2	2	2522	7MG	C2-N1	3.17	1.45	1.37
2	2	1883	OMG	C6-N1	3.17	1.42	1.37
2	2	2424	OMG	C5-C4	-3.16	1.35	1.43
2	2	3899	BGH	O6-C6	-3.16	1.17	1.23
2	2	1625	OMG	C5-C4	-3.15	1.35	1.43
2	2	3825	A2M	O3'-C3'	-3.15	1.35	1.43
2	2	4623	OMG	C6-N1	3.15	1.42	1.37
2	2	4636	PSU	C6-C5	3.15	1.39	1.35
2	2	3723	A2M	O2'-C2'	3.14	1.50	1.42
2	2	3897	B8K	O6-C6	-3.14	1.17	1.23
2	2	1659	I4U	O4-C4	3.14	1.41	1.35
2	2	2363	A2M	O3'-C3'	-3.13	1.35	1.43
2	2	1625	OMG	C6-N1	3.13	1.42	1.37
2	2	2773	OMG	C5-C4	-3.13	1.35	1.43
2	2	4494	OMG	C5-C4	-3.12	1.35	1.43
2	2	4571	A2M	C5-C4	-3.12	1.32	1.40
2	2	3887	OMC	C6-N1	3.12	1.45	1.38
2	2	2424	OMG	C6-N1	3.11	1.42	1.37
2	2	373	OMG	C6-N1	3.11	1.42	1.37
2	2	2754	B9B	O3'-C3'	-3.10	1.35	1.43
2	2	4355	E6G	O3'-C3'	-3.10	1.35	1.43
2	2	1522	OMG	C6-N1	3.09	1.42	1.37
2	2	4620	OMU	C4-N3	3.09	1.44	1.38
2	2	1316	OMG	C6-N1	3.08	1.42	1.37
2	2	4371	MHG	C6-N1	3.06	1.44	1.38
2	2	4536	OMC	C6-N1	3.06	1.45	1.38
2	2	237	B9B	O2'-C2'	3.06	1.50	1.43
2	2	3701	OMC	C6-N1	3.05	1.45	1.38
2	2	4483	B8T	O2-C2	-3.04	1.18	1.23
2	2	4194	I4U	O2'-C2'	3.03	1.50	1.43
2	2	1605	7MG	C2-N1	3.02	1.45	1.37
2	2	2861	OMC	C6-N1	3.02	1.45	1.38
2	2	3718	A2M	O3'-C3'	-3.02	1.35	1.43
2	2	4550	7MG	C2-N1	3.02	1.45	1.37
2	2	4870	OMG	C5-C4	-3.02	1.35	1.43
2	2	4872	2MG	C6-N1	3.01	1.42	1.37
2	2	2401	A2M	C5-C4	-3.01	1.33	1.40
2	2	2364	OMG	O6-C6	-3.01	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4637	OMG	O6-C6	-3.00	1.17	1.23
2	2	4196	OMG	C5-C6	3.00	1.53	1.47
2	2	4220	6MZ	C5-C4	-3.00	1.33	1.40
2	2	1517	2MG	C5-C4	-3.00	1.35	1.43
2	2	4523	A2M	C6-N6	2.99	1.45	1.34
2	2	3867	A2M	C6-N6	2.99	1.44	1.34
2	2	3897	B8K	C6-N1	2.98	1.44	1.38
2	2	1524	A2M	C6-N6	2.98	1.44	1.34
2	2	4690	B8K	C2-N1	2.98	1.45	1.37
2	2	2365	OMC	C6-N1	2.98	1.45	1.38
2	2	4571	A2M	C6-N6	2.98	1.44	1.34
2	2	3867	A2M	O3'-C3'	-2.98	1.36	1.43
2	2	4523	A2M	O3'-C3'	-2.97	1.36	1.43
2	2	1871	A2M	C6-N6	2.96	1.44	1.34
2	2	2522	7MG	O6-C6	-2.96	1.17	1.23
2	2	2786	B9H	C6-N1	2.96	1.45	1.38
2	2	1534	A2M	C5-C4	-2.95	1.33	1.40
2	2	4194	I4U	O4-C4	2.95	1.41	1.35
2	2	1316	OMG	O6-C6	-2.94	1.17	1.23
2	2	4523	A2M	C5-C4	-2.93	1.33	1.40
2	2	4637	OMG	C6-N1	2.93	1.42	1.37
2	2	4083	5MU	O2-C2	-2.93	1.17	1.23
2	2	2424	OMG	O6-C6	-2.92	1.17	1.23
2	2	3718	A2M	C6-N6	2.92	1.44	1.34
2	2	2050	OMG	C6-N1	2.92	1.42	1.37
2	2	398	A2M	C6-N6	2.92	1.44	1.34
2	2	1517	2MG	C6-N1	2.91	1.42	1.37
2	2	2401	A2M	C6-N6	2.91	1.44	1.34
2	2	3825	A2M	C5-C4	-2.91	1.33	1.40
2	2	1522	OMG	O6-C6	-2.91	1.17	1.23
2	2	4620	OMU	O2-C2	-2.90	1.17	1.23
2	2	3701	OMC	O2-C2	-2.90	1.18	1.23
2	2	398	A2M	C5-C4	-2.90	1.33	1.40
2	2	3718	A2M	C5-C4	-2.90	1.33	1.40
2	2	3825	A2M	C6-N6	2.89	1.44	1.34
2	2	4628	PSU	C6-C5	2.89	1.38	1.35
2	2	3723	A2M	C6-N6	2.89	1.44	1.34
2	2	3867	A2M	C5-C4	-2.89	1.33	1.40
2	2	978	2MG	C5-C4	-2.89	1.35	1.43
2	2	4355	E6G	C5-C4	-2.88	1.33	1.40
2	2	1517	2MG	O6-C6	-2.88	1.17	1.23
2	2	2363	A2M	C6-N6	2.87	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2401	A2M	O3'-C3'	-2.87	1.36	1.43
2	2	2422	OMC	O2-C2	-2.87	1.18	1.23
2	2	1524	A2M	C5-C4	-2.86	1.33	1.40
2	2	237	B9B	C5-C4	-2.86	1.33	1.40
2	2	4536	OMC	O2-C2	-2.86	1.18	1.23
2	2	4623	OMG	O6-C6	-2.85	1.17	1.23
2	2	1326	A2M	C5-C4	-2.85	1.33	1.40
2	2	3729	PSU	C6-C5	2.85	1.38	1.35
2	2	3897	B8K	O3'-C3'	2.85	1.49	1.43
2	2	2297	E7G	C6-N1	2.84	1.44	1.38
2	2	3718	A2M	O2'-C2'	2.84	1.49	1.42
2	2	2754	B9B	C5-C4	-2.84	1.33	1.40
2	2	4306	OMU	O2-C2	-2.84	1.17	1.23
2	2	4550	7MG	C6-N1	2.84	1.44	1.38
2	2	2861	OMC	O2-C2	-2.83	1.18	1.23
2	2	4530	UR3	C6-N1	2.83	1.44	1.38
2	2	1659	I4U	C6-N1	2.82	1.44	1.38
2	2	2773	OMG	C5-C6	2.82	1.53	1.47
2	2	2422	OMC	C6-N1	2.82	1.44	1.38
2	2	1534	A2M	C6-N6	2.82	1.44	1.34
2	2	3909	OMC	O2-C2	-2.81	1.18	1.23
2	2	729	2MG	C6-N1	2.81	1.42	1.37
2	2	1605	7MG	O6-C6	-2.80	1.18	1.23
2	2	2804	OMC	C6-N1	2.80	1.44	1.38
2	2	373	OMG	O6-C6	-2.80	1.17	1.23
8	8	14	OMU	O2-C2	-2.79	1.18	1.23
2	2	4550	7MG	O6-C6	-2.77	1.18	1.23
2	2	2297	E7G	O6-C6	-2.77	1.18	1.23
2	2	4872	2MG	C5-C6	2.77	1.53	1.47
2	2	4370	OMG	O6-C6	-2.75	1.17	1.23
2	2	4529	B8W	O2'-C2'	2.75	1.49	1.43
2	2	2804	OMC	O2-C2	-2.74	1.18	1.23
2	2	1797	E7G	C6-N1	2.74	1.43	1.38
2	2	4870	OMG	C5-C6	2.73	1.53	1.47
2	2	1797	E7G	O6-C6	-2.73	1.18	1.23
2	2	729	2MG	C5-C6	2.72	1.52	1.47
2	2	2786	B9H	O2-C2	-2.72	1.17	1.22
2	2	3723	A2M	C5-C4	-2.72	1.33	1.40
2	2	4872	2MG	C5-C4	-2.70	1.36	1.43
2	2	1871	A2M	C5-C4	-2.70	1.33	1.40
2	2	1871	A2M	O2'-C2'	2.69	1.49	1.42
2	2	2364	OMG	C6-N1	2.68	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1456	B8Q	C6-N1	2.67	1.44	1.38
2	2	4371	MHG	C72-C71	2.67	1.58	1.52
2	2	4494	OMG	O6-C6	-2.66	1.17	1.23
2	2	1326	A2M	O2'-C2'	2.66	1.49	1.42
2	2	2050	OMG	O6-C6	-2.65	1.17	1.23
2	2	4690	B8K	C71-N7	2.65	1.45	1.39
2	2	4129	B8W	O2'-C2'	2.63	1.49	1.43
2	2	4472	B8W	O2'-C2'	2.63	1.49	1.43
2	2	4870	OMG	O6-C6	-2.62	1.18	1.23
2	2	4403	PSU	C6-C5	2.62	1.38	1.35
2	2	1625	OMG	O6-C6	-2.60	1.18	1.23
2	2	398	A2M	O2'-C2'	2.60	1.49	1.42
2	2	3825	A2M	O2'-C2'	2.60	1.49	1.42
2	2	2508	PSU	C6-C5	2.60	1.38	1.35
2	2	4690	B8K	O3'-C3'	2.60	1.49	1.43
2	2	4671	B8T	C6-N1	2.60	1.44	1.38
2	2	729	2MG	C5-C4	-2.59	1.36	1.43
2	2	2522	7MG	C6-N1	2.59	1.43	1.38
2	2	1322	1MA	C5-C4	-2.58	1.36	1.43
2	2	1534	A2M	O3'-C3'	-2.58	1.36	1.43
2	2	3887	OMC	O2-C2	-2.58	1.18	1.23
2	2	4196	OMG	C2-N1	2.57	1.44	1.37
2	2	3867	A2M	O2'-C2'	2.57	1.49	1.42
2	2	4293	PSU	C6-C5	2.57	1.38	1.35
2	2	4690	B8K	C6-N1	2.56	1.43	1.38
2	2	4571	A2M	O2'-C2'	2.56	1.49	1.42
2	2	1659	I4U	O2'-C2'	2.55	1.49	1.43
2	2	3897	B8K	C71-N7	2.53	1.45	1.39
2	2	2773	OMG	O6-C6	-2.52	1.18	1.23
2	2	2380	B8W	O2'-C2'	2.52	1.48	1.43
2	2	3909	OMC	C5-C4	2.51	1.48	1.42
2	2	4597	UR3	C6-N1	2.50	1.44	1.38
2	2	2401	A2M	O2'-C2'	2.50	1.49	1.42
2	2	2380	B8W	C5-C4	-2.50	1.34	1.40
2	2	4185	B8W	C5-C4	-2.50	1.34	1.40
2	2	978	2MG	C5-C6	2.48	1.52	1.47
2	2	2050	OMG	C5-C6	2.48	1.52	1.47
2	2	4523	A2M	C2-N3	2.46	1.36	1.32
2	2	2363	A2M	O2'-C2'	2.46	1.48	1.42
2	2	4597	UR3	O2-C2	-2.46	1.18	1.22
2	2	4523	A2M	O2'-C2'	2.44	1.48	1.42
2	2	2364	OMG	C5-C6	2.44	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1316	OMG	C5-C6	2.44	1.52	1.47
2	2	978	2MG	O6-C6	-2.44	1.18	1.23
2	2	1625	OMG	C5-C6	2.44	1.52	1.47
2	2	4196	OMG	O6-C6	-2.43	1.18	1.23
2	2	4415	1MA	C5-C4	-2.43	1.36	1.43
2	2	4371	MHG	O6-C6	-2.42	1.19	1.23
2	2	4571	A2M	C2-N3	2.42	1.36	1.32
2	2	1605	7MG	C6-N1	2.41	1.43	1.38
2	2	4296	B8H	O4-C4	-2.40	1.19	1.23
2	2	4194	I4U	C6-N1	2.40	1.43	1.38
2	2	3723	A2M	C2-N3	2.39	1.35	1.32
2	2	4355	E6G	O5'-C5'	-2.37	1.39	1.44
2	2	1677	PSU	O4'-C1'	-2.37	1.40	1.43
2	2	3869	OMC	C6-N1	2.36	1.43	1.38
2	2	729	2MG	O6-C6	-2.34	1.18	1.23
2	2	4870	OMG	C2-N1	2.33	1.43	1.37
2	2	1326	A2M	O3'-C3'	-2.33	1.37	1.43
2	2	2773	OMG	C2-N1	2.32	1.43	1.37
2	2	4370	OMG	C5-C6	2.32	1.52	1.47
2	2	4872	2MG	O6-C6	-2.32	1.18	1.23
2	2	1534	A2M	O5'-C5'	-2.31	1.39	1.44
2	2	3867	A2M	C2-N3	2.31	1.35	1.32
2	2	4530	UR3	C4-N3	2.31	1.45	1.40
2	2	373	OMG	C5-C6	2.30	1.52	1.47
2	2	4530	UR3	O2-C2	-2.30	1.18	1.22
2	2	237	B9B	O5'-C5'	-2.30	1.39	1.44
2	2	4620	OMU	C6-N1	2.30	1.43	1.38
2	2	1677	PSU	C4-C5	-2.30	1.37	1.44
2	2	3701	OMC	C5-C4	2.30	1.48	1.42
2	2	4472	B8W	C5-C4	-2.29	1.34	1.40
2	2	4529	B8W	C5-C4	-2.29	1.34	1.40
2	2	4196	OMG	C5-C4	-2.25	1.37	1.43
2	2	4220	6MZ	C2-N3	2.24	1.35	1.32
2	2	3825	A2M	O5'-C5'	-2.24	1.39	1.44
2	2	1659	I4U	O5'-C5'	-2.24	1.39	1.44
2	2	4370	OMG	C2-N1	2.23	1.43	1.37
2	2	4185	B8W	O2'-C2'	2.20	1.48	1.43
2	2	2363	A2M	O5'-C5'	-2.19	1.39	1.44
2	2	4306	OMU	C6-N1	2.18	1.43	1.38
2	2	4597	UR3	C4-N3	2.18	1.45	1.40
2	2	3899	BGH	C3'-C2'	2.18	1.57	1.52
2	2	4494	OMG	C5-C6	2.16	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4623	OMG	C2-N1	2.16	1.43	1.37
2	2	1524	A2M	O5'-C5'	-2.16	1.39	1.44
2	2	1517	2MG	C5-C6	2.15	1.51	1.47
2	2	2424	OMG	C2-N1	2.14	1.43	1.37
2	2	1871	A2M	C2-N3	2.13	1.35	1.32
2	2	3899	BGH	O5'-C5'	-2.12	1.39	1.44
2	2	2861	OMC	C5-C4	2.10	1.47	1.42
2	2	1534	A2M	C2-N3	2.10	1.35	1.32
2	2	1860	B8H	O4-C4	-2.06	1.19	1.23
2	2	1316	OMG	C2-N1	2.06	1.42	1.37
2	2	1866	UR3	C6-C5	2.05	1.39	1.35
2	2	3718	A2M	O5'-C5'	-2.04	1.39	1.44
2	2	1524	A2M	O2'-C2'	2.03	1.47	1.42
2	2	1522	OMG	C5-C6	2.03	1.51	1.47
2	2	1866	UR3	C2-N1	2.03	1.41	1.38
2	2	4623	OMG	C5-C6	2.02	1.51	1.47
2	2	4597	UR3	C5-C4	2.02	1.49	1.43
2	2	4194	I4U	O5'-C5'	-2.02	1.39	1.44
2	2	4494	OMG	C2-N1	2.01	1.42	1.37

All (455) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4564	M7A	C5-C6-N6	13.77	147.26	123.74
2	2	4083	5MU	C5-C4-N3	13.36	126.71	115.31
2	2	4220	6MZ	C1'-N9-C4	-12.25	105.12	126.64
2	2	4564	M7A	N6-C6-N1	-11.95	92.17	118.35
2	2	2786	B9H	C6-N1-C2	-10.19	112.66	121.79
2	2	4597	UR3	C4-N3-C2	-9.93	115.21	124.56
2	2	1534	A2M	C5-C6-N6	9.77	135.21	120.35
2	2	3825	A2M	C5-C6-N6	9.52	134.82	120.35
2	2	1326	A2M	C5-C6-N6	9.47	134.74	120.35
2	2	2401	A2M	C5-C6-N6	9.17	134.29	120.35
2	2	4083	5MU	C5-C6-N1	-9.13	113.95	123.34
2	2	2363	A2M	C5-C6-N6	9.08	134.15	120.35
2	2	3718	A2M	C5-C6-N6	9.02	134.05	120.35
2	2	4571	A2M	C5-C6-N6	8.83	133.78	120.35
2	2	4523	A2M	C5-C6-N6	8.79	133.71	120.35
2	2	3867	A2M	C5-C6-N6	8.71	133.59	120.35
2	2	1524	A2M	C5-C6-N6	8.69	133.56	120.35
2	2	3723	A2M	C5-C6-N6	8.60	133.42	120.35
2	2	1871	A2M	C5-C6-N6	8.46	133.21	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	398	A2M	C5-C6-N6	8.46	133.21	120.35
2	2	4371	MHG	C72-C71-N7	7.73	120.02	112.41
2	2	2786	B9H	C31-N3-C2	7.41	126.47	117.21
2	2	2401	A2M	N3-C2-N1	-7.40	117.12	128.68
2	2	1534	A2M	N6-C6-N1	-7.34	103.34	118.57
2	2	2363	A2M	N3-C2-N1	-7.33	117.22	128.68
2	2	398	A2M	N3-C2-N1	-7.26	117.34	128.68
2	2	4523	A2M	N3-C2-N1	-7.24	117.37	128.68
2	2	4296	B8H	C4-N3-C2	-7.19	118.05	127.35
2	2	4220	6MZ	N3-C2-N1	-7.13	117.54	128.68
2	2	3825	A2M	N6-C6-N1	-7.11	103.82	118.57
2	2	1326	A2M	N3-C2-N1	-7.06	117.64	128.68
2	2	4690	B8K	C72-C71-N7	7.05	129.47	118.86
2	2	1534	A2M	N3-C2-N1	-7.00	117.74	128.68
2	2	1871	A2M	N3-C2-N1	-6.99	117.75	128.68
2	2	4083	5MU	O4-C4-C5	-6.98	116.82	124.90
2	2	1524	A2M	N3-C2-N1	-6.96	117.81	128.68
2	2	2363	A2M	N6-C6-N1	-6.95	104.16	118.57
2	2	4571	A2M	N3-C2-N1	-6.94	117.83	128.68
2	2	237	B9B	O6-C6-N1	-6.93	114.14	120.12
2	2	3825	A2M	N3-C2-N1	-6.91	117.88	128.68
2	2	4371	MHG	C2-N3-C4	6.88	120.57	112.04
2	2	4564	M7A	N3-C2-N1	-6.86	117.87	128.60
2	2	3867	A2M	N3-C2-N1	-6.85	117.97	128.68
2	2	3723	A2M	N3-C2-N1	-6.77	118.10	128.68
2	2	3718	A2M	N3-C2-N1	-6.74	118.15	128.68
2	2	2401	A2M	N6-C6-N1	-6.70	104.67	118.57
2	2	4571	A2M	N6-C6-N1	-6.69	104.68	118.57
2	2	4523	A2M	N6-C6-N1	-6.69	104.69	118.57
2	2	3867	A2M	N6-C6-N1	-6.60	104.87	118.57
2	2	3909	OMC	O2-C2-N3	-6.54	111.69	122.33
2	2	3897	B8K	C72-C71-N7	6.52	128.67	118.86
2	2	1524	A2M	N6-C6-N1	-6.52	105.03	118.57
2	2	1326	A2M	N6-C6-N1	-6.52	105.04	118.57
2	2	3723	A2M	N6-C6-N1	-6.42	105.25	118.57
2	2	4690	B8K	C5-C6-N1	6.41	122.28	110.99
2	2	4129	B8W	N3-C2-N1	-6.38	118.71	127.22
2	2	4355	E6G	N2-C2-N3	6.33	128.10	117.79
2	2	1860	B8H	C4-N3-C2	-6.29	119.21	127.35
2	2	1909	P7G	C4-C5-N7	6.27	109.98	106.67
2	2	1871	A2M	N6-C6-N1	-6.24	105.63	118.57
2	2	3718	A2M	N6-C6-N1	-6.23	105.63	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3909	OMC	C5-C4-N4	6.22	130.36	120.57
2	2	4355	E6G	O6-C6-N1	6.21	125.49	120.12
2	2	398	A2M	N6-C6-N1	-6.21	105.68	118.57
2	2	237	B9B	N3-C2-N1	-6.20	118.95	127.22
2	2	4355	E6G	N3-C2-N1	-6.17	118.99	127.22
8	8	14	OMU	C4-N3-C2	-6.14	118.48	126.58
2	2	4185	B8W	N3-C2-N1	-6.12	119.05	127.22
2	2	2754	B9B	O6-C6-N1	-6.12	114.84	120.12
2	2	1456	B8Q	O2-C2-N3	-6.12	113.97	122.95
2	2	1574	B9B	N3-C2-N1	-6.07	119.12	127.22
2	2	1574	B9B	O6-C6-N1	-6.05	114.90	120.12
2	2	1866	UR3	C4-N3-C2	-6.05	118.87	124.56
2	2	4472	B8W	N3-C2-N1	-5.93	119.31	127.22
2	2	3899	BGH	C72-C71-N7	5.90	127.74	118.86
2	2	4529	B8W	O6-C6-N1	5.90	127.21	119.03
2	2	1456	B8Q	C31-N3-C4	5.86	123.08	114.25
2	2	3880	P7G	C4-C5-N7	5.83	109.75	106.67
2	2	3869	OMC	O2-C2-N3	-5.77	112.95	122.33
2	2	2754	B9B	N3-C2-N1	-5.74	119.57	127.22
2	2	4296	B8H	N3-C2-N1	5.71	121.31	115.14
2	2	4185	B8W	C2-N3-C4	5.69	121.85	115.36
2	2	237	B9B	C2-N3-C4	5.64	121.80	115.36
2	2	3897	B8K	C5-C6-N1	5.56	120.78	110.99
2	2	2297	E7G	C5-C6-N1	5.53	120.73	110.99
2	2	4529	B8W	N3-C2-N1	-5.52	119.86	127.22
2	2	3869	OMC	C1'-N1-C2	5.50	130.68	118.42
2	2	4306	OMU	C4-N3-C2	-5.49	119.33	126.58
2	2	1605	7MG	C5-C6-N1	5.41	120.52	110.99
2	2	2380	B8W	N3-C2-N1	-5.41	120.01	127.22
2	2	4083	5MU	C4-N3-C2	-5.38	120.39	127.35
2	2	2522	7MG	C5-C6-N1	5.36	120.44	110.99
2	2	3899	BGH	C5-C6-N1	5.31	120.36	110.99
2	2	3909	OMC	C4-N3-C2	5.31	128.83	120.25
2	2	4472	B8W	C2-N3-C4	5.30	121.41	115.36
2	2	4564	M7A	N3-C4-N9	5.29	133.55	126.87
2	2	3909	OMC	O2-C2-N1	5.23	129.68	118.89
2	2	1797	E7G	C5-C6-N1	5.22	120.19	110.99
2	2	2297	E7G	C4-C5-N7	5.21	109.55	104.91
2	2	1456	B8Q	N3-C2-N1	5.21	123.25	117.13
2	2	1860	B8H	N3-C2-N1	5.19	120.75	115.14
2	2	4355	E6G	C2-N3-C4	5.16	121.25	115.36
2	2	4550	7MG	C5-C6-N1	5.12	120.01	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4371	MHG	C5-C6-N1	5.10	119.98	110.99
2	2	4129	B8W	O6-C6-C5	5.10	123.30	116.01
2	2	4636	PSU	C4-N3-C2	-5.06	119.05	126.34
2	2	1797	E7G	C2-N3-C4	5.05	121.30	112.30
2	2	2297	E7G	C2-N3-C4	5.01	121.23	112.30
2	2	2786	B9H	C32-C31-N3	4.97	122.85	112.47
2	2	4690	B8K	C4-C5-N7	4.97	109.33	104.91
2	2	4530	UR3	C4-N3-C2	-4.95	119.91	124.56
2	2	4529	B8W	C2-N3-C4	4.91	120.96	115.36
2	2	4083	5MU	N3-C2-N1	4.90	121.39	114.89
2	2	1605	7MG	C2-N3-C4	4.86	120.96	112.30
2	2	4415	1MA	N1-C2-N3	-4.84	120.38	126.02
2	2	4129	B8W	C2-N3-C4	4.83	120.88	115.36
2	2	2754	B9B	C2-N3-C4	4.81	120.85	115.36
2	2	4472	B8W	O6-C6-N1	4.80	125.69	119.03
2	2	1683	PSU	N1-C2-N3	4.80	120.57	115.13
2	2	1517	2MG	C5-C6-N1	4.80	122.42	113.95
2	2	4620	OMU	C4-N3-C2	-4.78	120.27	126.58
2	2	4529	B8W	N2-C2-N3	4.75	125.53	117.79
2	2	2380	B8W	O6-C6-N1	4.73	125.59	119.03
2	2	1797	E7G	C4-C5-N7	4.68	109.08	104.91
2	2	3899	BGH	C2-N3-C4	4.68	120.64	112.30
2	2	4185	B8W	N2-C2-N3	4.67	125.40	117.79
2	2	4196	OMG	CM2-O2'-C2'	4.67	126.77	114.52
2	2	1677	PSU	N1-C2-N3	4.66	120.41	115.13
2	2	4628	PSU	N1-C2-N3	4.63	120.38	115.13
2	2	1456	B8Q	C6-N1-C2	-4.62	117.65	121.79
2	2	3899	BGH	C4-C5-N7	4.60	109.00	104.91
2	2	3897	B8K	C2-N3-C4	4.53	120.37	112.30
2	2	4550	7MG	C2-N3-C4	4.52	120.36	112.30
2	2	4220	6MZ	C2-N1-C6	4.51	120.46	116.59
2	2	4371	MHG	C4-C5-N7	4.49	108.90	104.91
2	2	2380	B8W	C2-N3-C4	4.48	120.47	115.36
2	2	2522	7MG	C2-N3-C4	4.47	120.27	112.30
2	2	1883	OMG	C5-C6-N1	4.47	121.84	113.95
8	8	14	OMU	C5-C4-N3	4.46	121.50	114.84
2	2	2508	PSU	N1-C2-N3	4.44	120.16	115.13
2	2	1883	OMG	O6-C6-C5	-4.40	115.78	124.37
2	2	4636	PSU	N1-C2-N3	4.39	120.10	115.13
2	2	2786	B9H	O3'-C3'-C2'	4.37	123.59	111.17
2	2	1574	B9B	C2-N3-C4	4.37	120.34	115.36
2	2	4129	B8W	N2-C2-N3	4.33	124.85	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3715	PSU	N1-C2-N3	4.33	120.04	115.13
2	2	4472	B8W	N2-C2-N3	4.32	124.83	117.79
2	2	4129	B8W	C2-N1-C6	4.31	123.00	116.08
2	2	3899	BGH	N9-C8-N7	4.31	109.12	103.33
2	2	4403	PSU	N1-C2-N3	4.31	120.01	115.13
2	2	4690	B8K	C2-N3-C4	4.30	119.95	112.30
2	2	1797	E7G	C5-C4-N3	-4.29	119.95	128.13
2	2	1677	PSU	C4-N3-C2	-4.28	120.17	126.34
2	2	1683	PSU	C4-N3-C2	-4.25	120.22	126.34
2	2	1322	1MA	N1-C2-N3	-4.20	121.12	126.02
2	2	4306	OMU	N3-C2-N1	4.20	120.47	114.89
2	2	1456	B8Q	C1'-N1-C2	4.19	124.07	116.99
2	2	1659	I4U	C5-C4-N3	-4.17	118.56	124.91
2	2	2422	OMC	O2-C2-N3	-4.16	115.56	122.33
2	2	4293	PSU	N1-C2-N3	4.16	119.85	115.13
2	2	1322	1MA	C5-C6-N1	4.15	120.09	113.90
2	2	4403	PSU	C4-N3-C2	-4.14	120.38	126.34
2	2	4194	I4U	C5-C4-N3	-4.14	118.62	124.91
2	2	3909	OMC	C5-C4-N3	-4.10	114.34	121.33
2	2	2380	B8W	N2-C2-N3	4.08	124.44	117.79
2	2	4415	1MA	C5-C6-N1	4.07	119.97	113.90
2	2	2508	PSU	C4-N3-C2	-4.05	120.50	126.34
2	2	3897	B8K	C5-C4-N9	4.04	111.60	106.35
2	2	1574	B9B	C1'-N9-C4	-4.04	119.55	126.64
2	2	3729	PSU	N1-C2-N3	4.03	119.70	115.13
2	2	4185	B8W	O6-C6-N1	4.01	124.59	119.03
2	2	1605	7MG	C5-C4-N9	4.01	111.56	106.35
2	2	1348	P4U	C5-C4-N3	-4.00	118.82	124.91
2	2	4550	7MG	C5-C4-N9	3.99	111.53	106.35
2	2	4371	MHG	C5-C4-N9	3.97	111.51	106.35
2	2	3897	B8K	C4-C5-N7	3.93	108.41	104.91
2	2	4529	B8W	O4'-C4'-C3'	-3.92	97.35	105.11
2	2	1517	2MG	O6-C6-C5	-3.91	116.74	124.37
2	2	4296	B8H	C5-C4-N3	3.88	125.36	116.58
2	2	4637	OMG	C5-C6-N1	3.87	120.79	113.95
2	2	4628	PSU	C4-N3-C2	-3.86	120.78	126.34
2	2	4494	OMG	C5-C6-N1	3.85	120.75	113.95
2	2	4620	OMU	N3-C2-N1	3.84	119.99	114.89
2	2	1582	PSU	N1-C2-N3	3.84	119.48	115.13
2	2	3869	OMC	C1'-N1-C6	-3.81	112.53	120.84
2	2	1316	OMG	C5-C6-N1	3.79	120.65	113.95
2	2	4872	2MG	CM2-N2-C2	-3.79	115.48	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4564	M7A	C2-N3-C4	3.78	120.68	111.75
2	2	1605	7MG	C5-C4-N3	-3.78	120.94	128.13
2	2	2297	E7G	C5-C4-N3	-3.77	120.95	128.13
2	2	978	2MG	C5-C6-N1	3.77	120.60	113.95
2	2	2380	B8W	C3'-C2'-C1'	3.76	106.64	100.98
2	2	3729	PSU	C4-N3-C2	-3.75	120.94	126.34
2	2	2804	OMC	O2-C2-N3	-3.74	116.24	122.33
2	2	373	OMG	C5-C6-N1	3.74	120.56	113.95
2	2	1625	OMG	C5-C6-N1	3.70	120.48	113.95
2	2	3715	PSU	C4-N3-C2	-3.69	121.03	126.34
2	2	2364	OMG	C5-C6-N1	3.69	120.46	113.95
2	2	1909	P7G	N9-C8-N7	3.67	108.63	103.38
2	2	2424	OMG	C5-C6-N1	3.66	120.42	113.95
2	2	1797	E7G	C5-C4-N9	3.65	111.08	106.35
2	2	237	B9B	C3'-C2'-C1'	3.63	106.45	100.98
2	2	1582	PSU	O4-C4-N3	-3.63	113.15	120.12
2	2	2050	OMG	C5-C6-N1	3.62	120.34	113.95
2	2	4083	5MU	C5M-C5-C4	3.61	122.74	118.77
8	8	14	OMU	O4-C4-C5	-3.58	118.86	125.16
2	2	2522	7MG	C5-C4-N9	3.57	110.98	106.35
2	2	4690	B8K	C5-C4-N9	3.56	110.97	106.35
2	2	1909	P7G	C71-N7-C5	3.55	132.94	124.52
2	2	1522	OMG	C5-C6-N1	3.55	120.22	113.95
2	2	3897	B8K	N9-C8-N7	3.54	108.09	103.33
2	2	4690	B8K	C6-C5-C4	-3.54	115.32	122.62
2	2	1582	PSU	C4-N3-C2	-3.54	121.24	126.34
2	2	1860	B8H	C5-C4-N3	3.54	124.58	116.58
2	2	2050	OMG	C2-N1-C6	-3.50	118.66	125.10
2	2	1883	OMG	C2-N1-C6	-3.49	118.68	125.10
2	2	4355	E6G	O4'-C1'-C2'	-3.48	101.84	106.93
2	2	4690	B8K	N9-C8-N7	3.48	108.00	103.33
2	2	729	2MG	C5-C6-N1	3.46	120.06	113.95
2	2	4870	OMG	C5-C6-N1	3.46	120.06	113.95
2	2	4620	OMU	C5-C4-N3	3.45	120.00	114.84
2	2	2754	B9B	C3'-C2'-C1'	3.44	106.15	100.98
2	2	4550	7MG	C5-C4-N3	-3.43	121.58	128.13
2	2	4597	UR3	O2-C2-N3	-3.42	116.52	121.34
2	2	4129	B8W	C4-C5-N7	-3.42	105.84	109.40
2	2	2297	E7G	C5-C4-N9	3.41	110.78	106.35
8	8	14	OMU	N3-C2-N1	3.41	119.42	114.89
2	2	2773	OMG	C5-C6-N1	3.40	119.96	113.95
2	2	2522	7MG	C5-C4-N3	-3.40	121.66	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4293	PSU	C6-N1-C2	-3.39	119.21	122.68
2	2	3899	BGH	C5-C4-N9	3.39	110.75	106.35
2	2	2424	OMG	C2-N1-C6	-3.38	118.88	125.10
2	2	1625	OMG	C2-N1-C6	-3.37	118.90	125.10
2	2	4083	5MU	C5M-C5-C6	-3.37	118.35	122.85
2	2	3887	OMC	O2-C2-N3	-3.36	116.87	122.33
2	2	4637	OMG	C2-N1-C6	-3.36	118.92	125.10
2	2	4196	OMG	C5-C6-N1	3.35	119.86	113.95
2	2	3715	PSU	C6-N1-C2	-3.33	119.28	122.68
2	2	4293	PSU	C4-N3-C2	-3.31	121.57	126.34
2	2	4355	E6G	O4'-C4'-C3'	-3.31	98.56	105.11
2	2	4370	OMG	C5-C6-N1	3.31	119.79	113.95
2	2	4872	2MG	C5-C6-N1	3.30	119.78	113.95
2	2	1605	7MG	N9-C8-N7	3.30	108.09	103.38
2	2	3897	B8K	C6-C5-C4	-3.29	115.84	122.62
2	2	3869	OMC	C6-C5-C4	3.28	122.80	117.50
2	2	4494	OMG	C2-N1-C6	-3.28	119.06	125.10
2	2	4306	OMU	C5-C4-N3	3.27	119.73	114.84
2	2	4083	5MU	O2-C2-N1	-3.27	118.44	122.79
2	2	4628	PSU	C6-N1-C2	-3.27	119.34	122.68
2	2	4371	MHG	C5-C4-N3	-3.26	121.92	128.13
2	2	1348	P4U	O2-C2-N3	-3.25	117.05	122.33
2	2	4623	OMG	C5-C6-N1	3.25	119.69	113.95
2	2	3869	OMC	O2-C2-N1	3.24	125.58	118.89
2	2	1677	PSU	C6-N1-C2	-3.23	119.38	122.68
2	2	1659	I4U	O2-C2-N3	-3.20	117.12	122.33
2	2	4129	B8W	C3'-C2'-C1'	3.19	105.79	100.98
2	2	4597	UR3	C6-N1-C2	-3.17	118.95	121.79
2	2	2364	OMG	C2-N1-C6	-3.16	119.27	125.10
2	2	2773	OMG	C2-N1-C6	-3.16	119.28	125.10
2	2	4335	5MC	CM5-C5-C6	-3.14	118.66	122.85
2	2	4371	MHG	N1-C2-N3	-3.12	119.13	123.95
2	2	4597	UR3	C3U-N3-C2	3.12	122.78	117.31
2	2	1316	OMG	C2-N1-C6	-3.10	119.40	125.10
2	2	4870	OMG	C2-N1-C6	-3.09	119.41	125.10
2	2	3909	OMC	C6-N1-C2	-3.08	115.14	120.49
2	2	4335	5MC	C5-C6-N1	-3.07	120.18	123.34
2	2	4529	B8W	C2'-C3'-C4'	-3.06	96.69	102.64
2	2	4196	OMG	C2-N1-C6	-3.06	119.47	125.10
2	2	4371	MHG	C2-N1-C6	-3.06	120.96	124.48
2	2	2786	B9H	C1'-N1-C6	3.05	127.50	120.84
2	2	2754	B9B	C1'-N9-C4	-3.05	121.28	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4628	PSU	O2-C2-N1	-3.04	119.44	122.79
2	2	4550	7MG	N9-C8-N7	3.03	107.71	103.38
2	2	2422	OMC	C1'-N1-C2	3.03	125.18	118.42
2	2	1522	OMG	C2-N1-C6	-3.02	119.55	125.10
2	2	2522	7MG	N9-C8-N7	3.00	107.67	103.38
2	2	4355	E6G	C2-N1-C6	3.00	120.90	116.08
2	2	1683	PSU	O2-C2-N1	-3.00	119.49	122.79
2	2	3899	BGH	C5-C4-N3	-2.99	122.43	128.13
2	2	978	2MG	CM2-N2-C2	-2.99	117.25	123.86
2	2	2786	B9H	O3'-C3'-C4'	2.99	119.70	111.05
2	2	4671	B8T	C6-C5-C4	2.98	120.61	116.96
2	2	4370	OMG	C2-N1-C6	-2.98	119.61	125.10
2	2	3729	PSU	C6-N1-C2	-2.98	119.64	122.68
2	2	3899	BGH	C6-C5-C4	-2.97	116.50	122.62
2	2	373	OMG	C2-N1-C6	-2.96	119.64	125.10
2	2	4129	B8W	C5-C6-N1	-2.96	117.63	123.26
2	2	2861	OMC	O2-C2-N3	-2.95	117.54	122.33
2	2	1683	PSU	C6-N1-C2	-2.94	119.68	122.68
2	2	4637	OMG	O6-C6-C5	-2.93	118.64	124.37
2	2	1524	A2M	O4'-C4'-C3'	-2.93	99.31	105.11
2	2	4472	B8W	O4'-C1'-C2'	-2.91	102.67	106.93
2	2	4623	OMG	C2-N1-C6	-2.90	119.75	125.10
2	2	2773	OMG	C8-N7-C5	2.90	108.52	102.99
2	2	4370	OMG	C8-N7-C5	2.89	108.50	102.99
2	2	978	2MG	O6-C6-C5	-2.89	118.73	124.37
2	2	4597	UR3	C3U-N3-C4	2.89	122.01	117.89
2	2	1797	E7G	N9-C8-N7	2.88	107.50	103.38
2	2	1517	2MG	CM2-N2-C2	-2.87	117.53	123.86
2	2	4637	OMG	C8-N7-C5	2.86	108.44	102.99
2	2	2364	OMG	C8-N7-C5	2.85	108.41	102.99
2	2	4870	OMG	C8-N7-C5	2.84	108.41	102.99
2	2	1456	B8Q	C31-N3-C2	2.84	121.91	117.79
2	2	3729	PSU	O2-C2-N1	-2.84	119.67	122.79
2	2	2522	7MG	C4-C5-N7	2.83	109.47	105.53
2	2	373	OMG	C8-N7-C5	2.83	108.38	102.99
2	2	4296	B8H	O4-C4-N3	-2.80	114.76	120.12
2	2	4494	OMG	O6-C6-C5	-2.80	118.91	124.37
2	2	4355	E6G	N2-C2-N1	-2.79	112.91	117.25
2	2	4472	B8W	C2-N1-C6	2.79	120.57	116.08
2	2	1677	PSU	O2-C2-N1	-2.78	119.73	122.79
2	2	4306	OMU	O4-C4-C5	-2.76	120.30	125.16
2	2	2804	OMC	O2-C2-N1	2.76	124.59	118.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1316	OMG	C8-N7-C5	2.76	108.25	102.99
2	2	1659	I4U	O4'-C1'-C2'	-2.75	100.65	106.64
2	2	4293	PSU	O4-C4-N3	-2.74	114.87	120.12
2	2	1582	PSU	C6-C5-C4	-2.73	116.29	118.20
2	2	4690	B8K	C5-C4-N3	-2.72	122.94	128.13
2	2	4620	OMU	O2-C2-N1	-2.71	119.18	122.79
2	2	1605	7MG	C2-N1-C6	-2.71	120.15	125.10
2	2	2050	OMG	C8-N7-C5	2.71	108.15	102.99
2	2	4185	B8W	C2-N1-C6	2.70	120.42	116.08
2	2	1605	7MG	C4-C5-N7	2.70	109.28	105.53
2	2	1322	1MA	C8-N7-C5	2.70	108.13	102.99
2	2	1860	B8H	O2-C2-N1	-2.69	119.84	122.87
2	2	1797	E7G	C2-N1-C6	-2.68	120.21	125.10
2	2	3897	B8K	C5-C4-N3	-2.67	123.04	128.13
2	2	1316	OMG	N2-C2-N1	2.67	122.40	116.71
2	2	1625	OMG	C8-N7-C5	2.65	108.04	102.99
2	2	4620	OMU	O4-C4-C5	-2.65	120.50	125.16
2	2	4690	B8K	C2-N1-C6	-2.63	120.30	125.10
2	2	4550	7MG	C4-C5-N7	2.63	109.18	105.53
2	2	4623	OMG	C8-N7-C5	2.63	108.00	102.99
2	2	3867	A2M	C3'-C2'-C1'	2.63	107.83	102.89
2	2	978	2MG	C8-N7-C5	2.62	107.98	102.99
2	2	4083	5MU	C6-N1-C2	-2.62	118.64	121.30
2	2	2297	E7G	C2-N1-C6	-2.61	120.35	125.10
2	2	1860	B8H	O4-C4-N3	-2.60	115.14	120.12
2	2	1534	A2M	O4'-C1'-C2'	-2.58	102.11	106.59
2	2	3887	OMC	C1'-N1-C2	2.58	124.18	118.42
2	2	4185	B8W	O4'-C1'-C2'	-2.58	103.16	106.93
2	2	1522	OMG	C8-N7-C5	2.55	107.84	102.99
2	2	2422	OMC	O2-C2-N1	2.53	124.12	118.89
2	2	1625	OMG	O6-C6-C5	-2.53	119.43	124.37
2	2	4370	OMG	O6-C6-C5	-2.53	119.44	124.37
2	2	1517	2MG	C3'-C2'-C1'	2.52	104.77	100.98
2	2	4371	MHG	C6-C5-C4	-2.51	117.44	122.62
2	2	1574	B9B	C2-N1-C6	2.51	120.11	116.08
2	2	2424	OMG	O6-C6-C5	-2.51	119.47	124.37
2	2	3899	BGH	N1-C2-N3	-2.50	118.65	123.32
2	2	1582	PSU	C6-N1-C2	-2.50	120.13	122.68
2	2	4529	B8W	O6-C6-C5	-2.49	112.45	116.01
2	2	4623	OMG	O6-C6-C5	-2.48	119.52	124.37
2	2	2522	7MG	C6-C5-C4	-2.48	117.51	122.62
2	2	1659	I4U	C6-N1-C2	-2.47	116.21	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4296	B8H	O2-C2-N1	-2.46	120.10	122.87
2	2	3880	P7G	C71-N7-C5	2.45	130.32	124.52
2	2	2297	E7G	N9-C8-N7	2.45	106.88	103.38
2	2	1574	B9B	C3'-C2'-C1'	2.43	104.64	100.98
2	2	4550	7MG	C6-C5-C4	-2.43	117.61	122.62
2	2	4472	B8W	C3'-C2'-C1'	2.43	104.63	100.98
2	2	237	B9B	C2-N1-C6	2.42	119.97	116.08
2	2	4494	OMG	C8-N7-C5	2.41	107.59	102.99
2	2	4690	B8K	O6-C6-N1	-2.41	115.51	120.12
2	2	4403	PSU	O4'-C1'-C2'	2.40	108.53	105.14
2	2	2508	PSU	C6-N1-C2	-2.40	120.23	122.68
2	2	2522	7MG	C2-N1-C6	-2.39	120.73	125.10
2	2	4530	UR3	C6-N1-C2	-2.39	119.65	121.79
2	2	3880	P7G	N9-C8-N7	2.39	106.79	103.38
2	2	2297	E7G	C6-C5-C4	-2.39	117.70	122.62
2	2	4536	OMC	O2-C2-N3	-2.39	118.45	122.33
2	2	4872	2MG	C8-N7-C5	2.39	107.54	102.99
2	2	3897	B8K	N2-C2-N1	2.39	121.80	116.71
2	2	2773	OMG	N2-C2-N1	2.39	121.79	116.71
2	2	1522	OMG	O6-C6-C5	-2.38	119.72	124.37
2	2	4403	PSU	C6-N1-C2	-2.36	120.27	122.68
2	2	4415	1MA	C8-N7-C5	2.36	107.49	102.99
2	2	4196	OMG	O6-C6-C5	-2.36	119.76	124.37
2	2	729	2MG	CM2-N2-C2	-2.35	118.66	123.86
2	2	729	2MG	C8-N7-C5	2.35	107.47	102.99
2	2	4564	M7A	C5-C4-N3	-2.35	121.12	126.62
2	2	4194	I4U	O4'-C1'-C2'	-2.34	101.53	106.64
2	2	1797	E7G	N9-C4-N3	2.34	128.97	125.47
2	2	3887	OMC	CM2-O2'-C2'	-2.34	108.39	114.52
2	2	3897	B8K	N1-C2-N3	-2.33	118.97	123.32
2	2	4872	2MG	O6-C6-C5	-2.33	119.82	124.37
2	2	2364	OMG	O6-C6-C5	-2.32	119.83	124.37
2	2	1883	OMG	N2-C2-N1	2.32	121.65	116.71
2	2	2297	E7G	N1-C2-N3	-2.31	119.02	123.32
2	2	1517	2MG	C8-N7-C5	2.29	107.36	102.99
2	2	1605	7MG	C6-C5-C4	-2.29	117.89	122.62
2	2	4550	7MG	N1-C2-N3	-2.29	119.05	123.32
2	2	4196	OMG	O2'-C2'-C1'	2.28	113.62	109.09
2	2	4196	OMG	C8-N7-C5	2.28	107.33	102.99
2	2	4597	UR3	C1'-N1-C2	2.27	120.83	116.99
2	2	4306	OMU	O2-C2-N1	-2.27	119.77	122.79
2	2	2365	OMC	O2-C2-N3	-2.27	118.64	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	3897	B8K	C2-N1-C6	-2.25	121.00	125.10
2	2	3887	OMC	O2-C2-N1	2.25	123.54	118.89
2	2	2050	OMG	O6-C6-C5	-2.25	119.98	124.37
2	2	4870	OMG	O6-C6-C5	-2.24	120.00	124.37
2	2	2773	OMG	O6-C6-C5	-2.23	120.01	124.37
2	2	1326	A2M	C3'-C2'-C1'	2.22	107.06	102.89
2	2	2754	B9B	N2-C2-N3	2.22	121.40	117.79
2	2	1909	P7G	N3-C2-N1	-2.21	119.20	123.32
2	2	2522	7MG	O6-C6-C5	-2.21	122.13	127.54
2	2	4690	B8K	N1-C2-N3	-2.21	119.20	123.32
2	2	3897	B8K	O3'-C3'-C2'	-2.20	104.70	111.82
2	2	4529	B8W	O4'-C4'-C5'	2.20	116.61	109.37
2	2	2861	OMC	C1'-N1-C2	2.20	123.32	118.42
2	2	3715	PSU	O2-C2-N1	-2.19	120.38	122.79
2	2	373	OMG	N1-C2-N3	-2.18	119.25	123.32
2	2	4690	B8K	O6-C6-C5	-2.17	122.21	127.54
2	2	4529	B8W	C2-N1-C6	2.17	119.56	116.08
2	2	4483	B8T	C5-C4-N3	-2.17	119.11	122.59
2	2	4083	5MU	C1'-N1-C6	2.16	124.72	121.12
2	2	4530	UR3	C3U-N3-C4	2.16	120.97	117.89
2	2	1348	P4U	C2-N3-C4	2.15	122.58	117.44
2	2	3869	OMC	C6-N1-C2	-2.15	116.77	120.49
2	2	4403	PSU	O2-C2-N1	-2.14	120.43	122.79
2	2	3897	B8K	O4'-C1'-C2'	-2.14	101.98	106.64
2	2	4483	B8T	O3'-C3'-C2'	2.13	118.72	111.82
2	2	4293	PSU	O2'-C2'-C1'	-2.13	106.15	111.23
2	2	4536	OMC	C6-N1-C2	-2.13	116.81	120.49
2	2	1348	P4U	C6-N1-C2	-2.12	116.81	120.49
2	2	2786	B9H	O2-C2-N1	-2.12	117.77	122.72
2	2	2522	7MG	N1-C2-N3	-2.11	119.38	123.32
2	2	237	B9B	N2-C2-N1	2.11	120.54	117.25
2	2	2380	B8W	C2-N1-C6	2.10	119.45	116.08
2	2	4623	OMG	N2-C2-N1	2.10	121.18	116.71
2	2	1683	PSU	O4-C4-N3	-2.09	116.10	120.12
2	2	729	2MG	O6-C6-C5	-2.09	120.28	124.37
2	2	4220	6MZ	C9-N6-C6	2.09	124.67	122.87
2	2	1797	E7G	O6-C6-C5	-2.09	122.42	127.54
2	2	4636	PSU	O2-C2-N1	-2.08	120.50	122.79
2	2	4529	B8W	O5'-C5'-C4'	2.07	116.05	108.99
2	2	1797	E7G	N1-C2-N3	-2.07	119.46	123.32
2	2	2804	OMC	C1'-N1-C2	2.06	123.02	118.42
2	2	2754	B9B	C2-N1-C6	2.05	119.38	116.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	4550	7MG	O6-C6-C5	-2.05	122.50	127.54
2	2	2508	PSU	O4-C4-N3	-2.04	116.20	120.12
2	2	1909	P7G	N2-C2-N3	2.04	121.05	116.71
8	8	14	OMU	CM2-O2'-C2'	2.04	119.87	114.52
2	2	3899	BGH	O6-C6-N1	-2.04	116.22	120.12
2	2	1316	OMG	N1-C2-N3	-2.03	119.52	123.32
2	2	4483	B8T	C6-C5-C4	2.03	119.45	116.96
2	2	4371	MHG	O6-C6-N1	-2.03	116.23	120.12
2	2	4550	7MG	C2-N1-C6	-2.03	121.40	125.10
2	2	1605	7MG	N1-C2-N3	-2.03	119.54	123.32
2	2	1866	UR3	O4'-C1'-N1	2.03	113.00	108.36
2	2	2297	E7G	O6-C6-C5	-2.02	122.58	127.54
2	2	3899	BGH	C2-N1-C6	-2.02	121.42	125.10
2	2	373	OMG	O6-C6-C5	-2.02	120.43	124.37
2	2	1677	PSU	O4'-C1'-C2'	2.02	107.99	105.14
2	2	1605	7MG	N2-C2-N1	2.01	120.99	116.71

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	8	14	OMU	C1'-C2'-O2'-CM2
2	2	237	B9B	C5-C6-O6-C61
2	2	237	B9B	N1-C6-O6-C61
2	2	237	B9B	C3'-C4'-C5'-O5'
2	2	237	B9B	C62-C61-O6-C6
2	2	1348	P4U	N3-C4-O4-C41
2	2	1574	B9B	C5-C6-O6-C61
2	2	1574	B9B	N1-C6-O6-C61
2	2	1582	PSU	C3'-C4'-C5'-O5'
2	2	1582	PSU	O4'-C4'-C5'-O5'
2	2	1797	E7G	O4'-C4'-C5'-O5'
2	2	1866	UR3	C3'-C4'-C5'-O5'
2	2	1871	A2M	O4'-C4'-C5'-O5'
2	2	1871	A2M	C3'-C4'-C5'-O5'
2	2	1883	OMG	C3'-C4'-C5'-O5'
2	2	2380	B8W	C5-C6-O6-C61
2	2	2754	B9B	C5-C6-O6-C61
2	2	2754	B9B	N1-C6-O6-C61
2	2	3701	OMC	C2'-C1'-N1-C2
2	2	3701	OMC	C2'-C1'-N1-C6
2	2	4129	B8W	C5-C6-O6-C61

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Mol	Chain	Res	Type	Atoms
2	2	4129	B8W	N1-C6-O6-C61
2	2	4185	B8W	C5-C6-O6-C61
2	2	4185	B8W	N1-C6-O6-C61
2	2	4196	OMG	C1'-C2'-O2'-CM2
2	2	4293	PSU	O4'-C4'-C5'-O5'
2	2	4355	E6G	C5-C6-O6-C61
2	2	4355	E6G	N1-C6-O6-C61
2	2	4403	PSU	O4'-C1'-C5-C6
2	2	4415	1MA	O4'-C4'-C5'-O5'
2	2	4472	B8W	C5-C6-O6-C61
2	2	4472	B8W	N1-C6-O6-C61
2	2	4529	B8W	C5-C6-O6-C61
2	2	4529	B8W	N1-C6-O6-C61
2	2	4529	B8W	O4'-C4'-C5'-O5'
2	2	4597	UR3	O4'-C4'-C5'-O5'
2	2	4597	UR3	C3'-C4'-C5'-O5'
2	2	4636	PSU	C3'-C4'-C5'-O5'
2	2	4637	OMG	O4'-C4'-C5'-O5'
2	2	4637	OMG	C3'-C4'-C5'-O5'
2	2	4870	OMG	O4'-C4'-C5'-O5'
2	2	4870	OMG	C3'-C4'-C5'-O5'
2	2	4872	2MG	O4'-C4'-C5'-O5'
2	2	4872	2MG	C3'-C4'-C5'-O5'
2	2	237	B9B	O4'-C4'-C5'-O5'
2	2	398	A2M	O4'-C4'-C5'-O5'
2	2	1797	E7G	C3'-C4'-C5'-O5'
2	2	1866	UR3	O4'-C4'-C5'-O5'
2	2	1883	OMG	O4'-C4'-C5'-O5'
2	2	2364	OMG	O4'-C4'-C5'-O5'
2	2	2380	B8W	O4'-C4'-C5'-O5'
2	2	3729	PSU	C3'-C4'-C5'-O5'
2	2	3729	PSU	O4'-C4'-C5'-O5'
2	2	3897	B8K	C3'-C4'-C5'-O5'
2	2	3897	B8K	O4'-C4'-C5'-O5'
2	2	4293	PSU	C3'-C4'-C5'-O5'
2	2	4371	MHG	O4'-C4'-C5'-O5'
2	2	4415	1MA	C3'-C4'-C5'-O5'
2	2	4636	PSU	O4'-C4'-C5'-O5'
2	2	237	B9B	O6-C61-C62-C63
2	2	1677	PSU	O4'-C4'-C5'-O5'
2	2	2364	OMG	C3'-C4'-C5'-O5'
2	2	4185	B8W	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	2	4196	OMG	O4'-C4'-C5'-O5'
2	2	4196	OMG	C3'-C4'-C5'-O5'
2	2	4220	6MZ	O4'-C4'-C5'-O5'
2	2	4220	6MZ	C3'-C4'-C5'-O5'
2	2	4371	MHG	C3'-C4'-C5'-O5'
2	2	4523	A2M	O4'-C4'-C5'-O5'
2	2	4523	A2M	C3'-C4'-C5'-O5'
2	2	4529	B8W	C3'-C4'-C5'-O5'
2	2	2380	B8W	N1-C6-O6-C61
2	2	2380	B8W	C3'-C4'-C5'-O5'
2	2	1677	PSU	C3'-C4'-C5'-O5'
2	2	4194	I4U	O4'-C4'-C5'-O5'
2	2	4371	MHG	C75-C73-C74-C76
2	2	4194	I4U	C3'-C4'-C5'-O5'
2	2	1326	A2M	C4'-C5'-O5'-P
2	2	1625	OMG	C3'-C4'-C5'-O5'
2	2	3869	OMC	O4'-C1'-N1-C2
2	2	2422	OMC	O4'-C4'-C5'-O5'
2	2	4355	E6G	O4'-C4'-C5'-O5'
2	2	3869	OMC	O4'-C1'-N1-C6
2	2	4371	MHG	C72-C73-C74-C76
2	2	2297	E7G	C72-C71-N7-C8
2	2	373	OMG	C4'-C5'-O5'-P
2	2	3867	A2M	C4'-C5'-O5'-P
2	2	4371	MHG	C2'-C1'-N9-C8
2	2	1871	A2M	C3'-C2'-O2'-CM'
2	2	4523	A2M	C3'-C2'-O2'-CM'
2	2	4523	A2M	C4'-C5'-O5'-P
2	2	2424	OMG	C3'-C4'-C5'-O5'
2	2	3701	OMC	O4'-C1'-N1-C6
2	2	1534	A2M	C4'-C5'-O5'-P
2	2	3897	B8K	C4'-C5'-O5'-P
2	2	1605	7MG	O4'-C4'-C5'-O5'
2	2	2363	A2M	O4'-C4'-C5'-O5'
2	2	4296	B8H	C3'-C4'-C5'-O5'
2	2	4296	B8H	O4'-C4'-C5'-O5'
2	2	1909	P7G	C72-C71-N7-C8
2	2	3887	OMC	C4'-C5'-O5'-P
2	2	4870	OMG	C4'-C5'-O5'-P
2	2	2401	A2M	C3'-C2'-O2'-CM'
2	2	3701	OMC	O4'-C1'-N1-C2
2	2	3867	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	2	1659	I4U	C42-C41-O4-C4
2	2	4194	I4U	C43-C41-O4-C4
2	2	1574	B9B	C62-C61-O6-C6
2	2	4403	PSU	O4'-C1'-C5-C4
2	2	1659	I4U	O4'-C4'-C5'-O5'
2	2	3718	A2M	O4'-C4'-C5'-O5'
2	2	398	A2M	C3'-C4'-C5'-O5'
2	2	3880	P7G	O4'-C4'-C5'-O5'
2	2	4371	MHG	O4'-C1'-N9-C8
2	2	1625	OMG	O4'-C4'-C5'-O5'
2	2	1677	PSU	O4'-C1'-C5-C6
2	2	4636	PSU	O4'-C1'-C5-C6
2	2	1866	UR3	C2'-C1'-N1-C2
2	2	729	2MG	O4'-C4'-C5'-O5'
2	2	1534	A2M	O4'-C4'-C5'-O5'
2	2	4371	MHG	C72-C71-N7-C8
2	2	4194	I4U	C42-C41-O4-C4
2	2	2424	OMG	O4'-C4'-C5'-O5'
2	2	3869	OMC	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 247 ligands modelled in this entry, 247 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

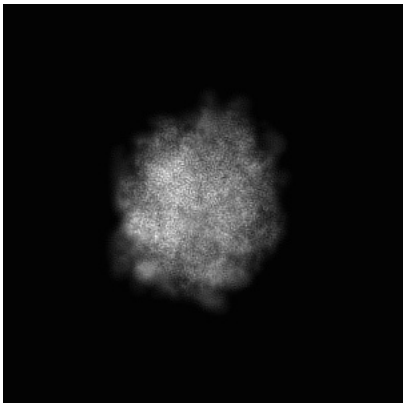
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0978. These allow visual inspection of the internal detail of the map and identification of artifacts.

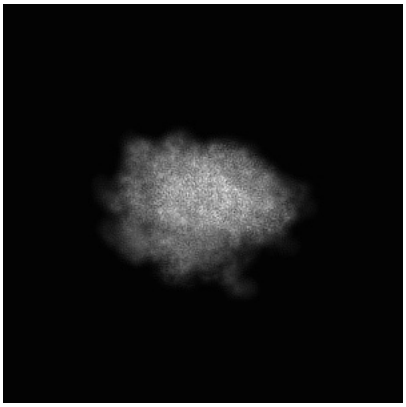
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

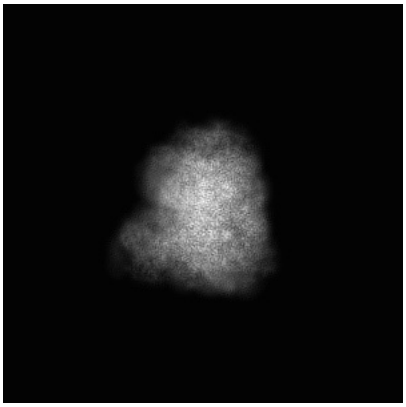
6.1.1 Primary map



X



Y

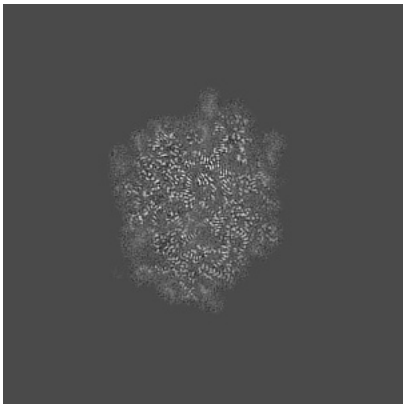


Z

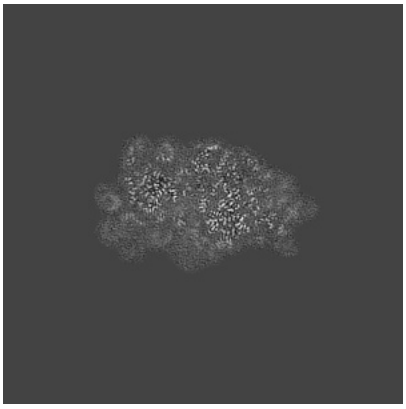
The images above show the map projected in three orthogonal directions.

6.2 Central slices

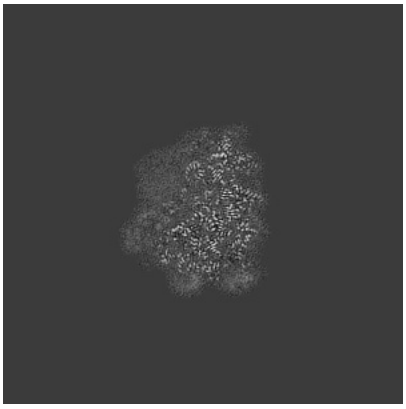
6.2.1 Primary map



X Index: 240



Y Index: 240

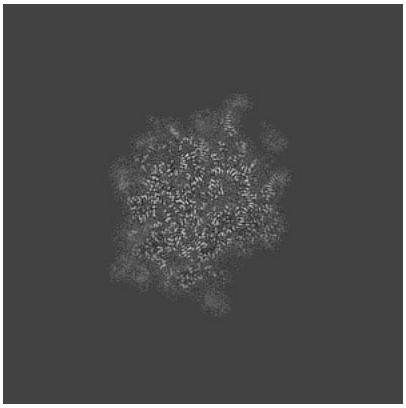


Z Index: 240

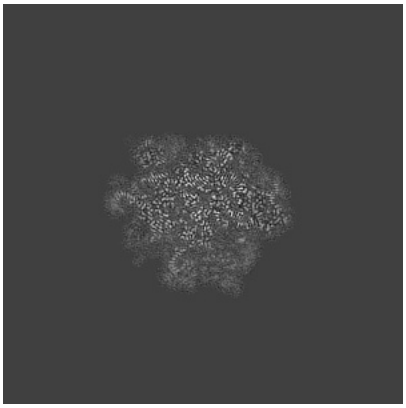
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

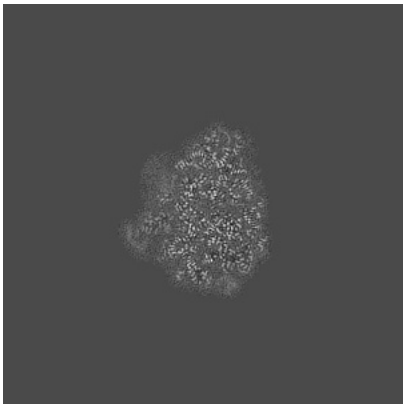
6.3.1 Primary map



X Index: 256



Y Index: 203

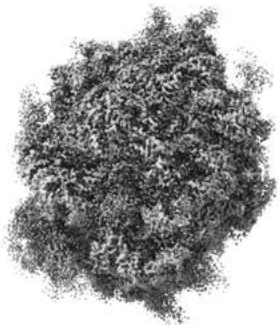


Z Index: 255

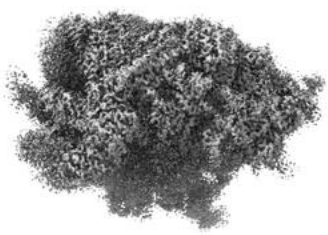
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

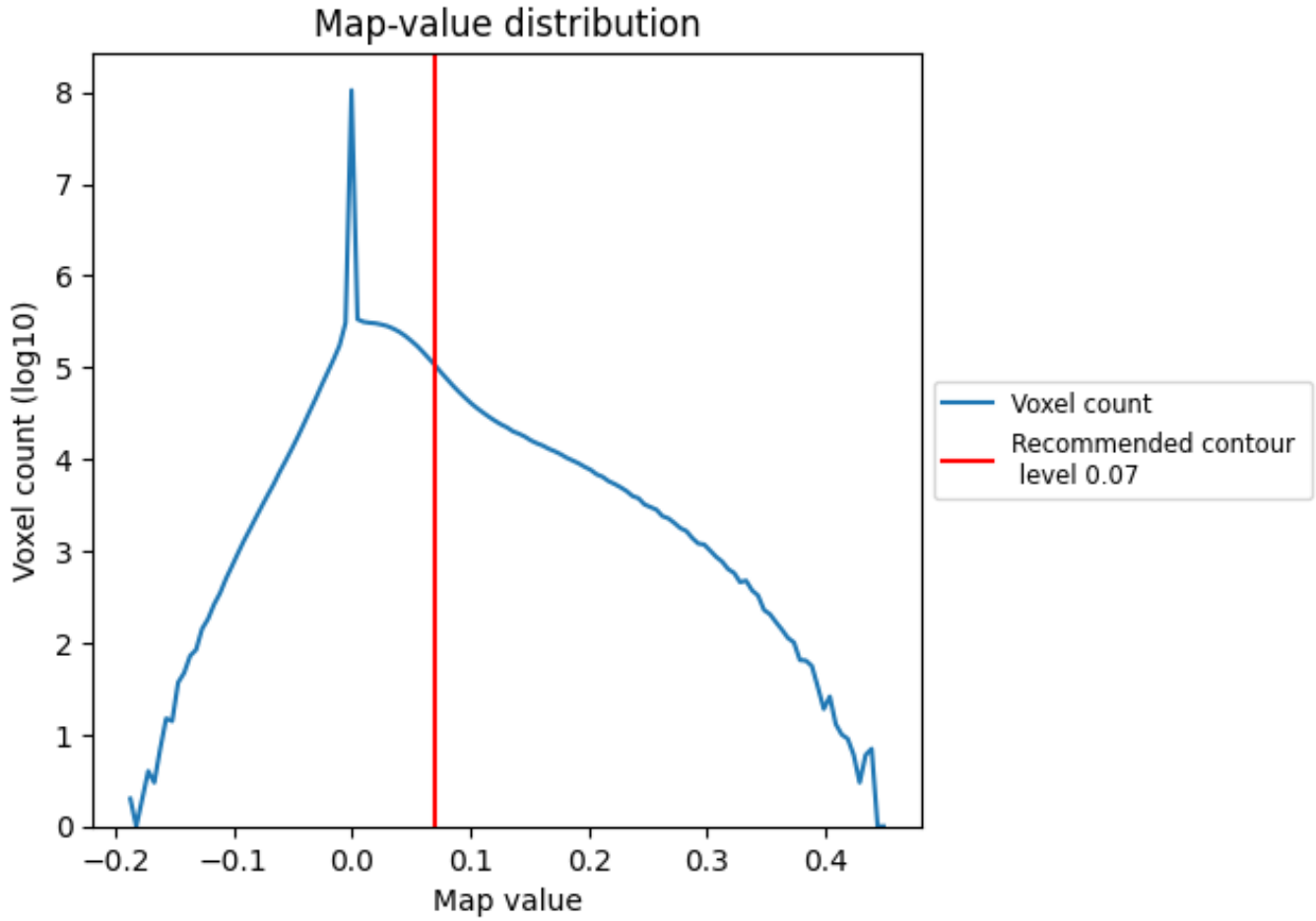
6.5 Mask visualisation (i)

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

7 Map analysis

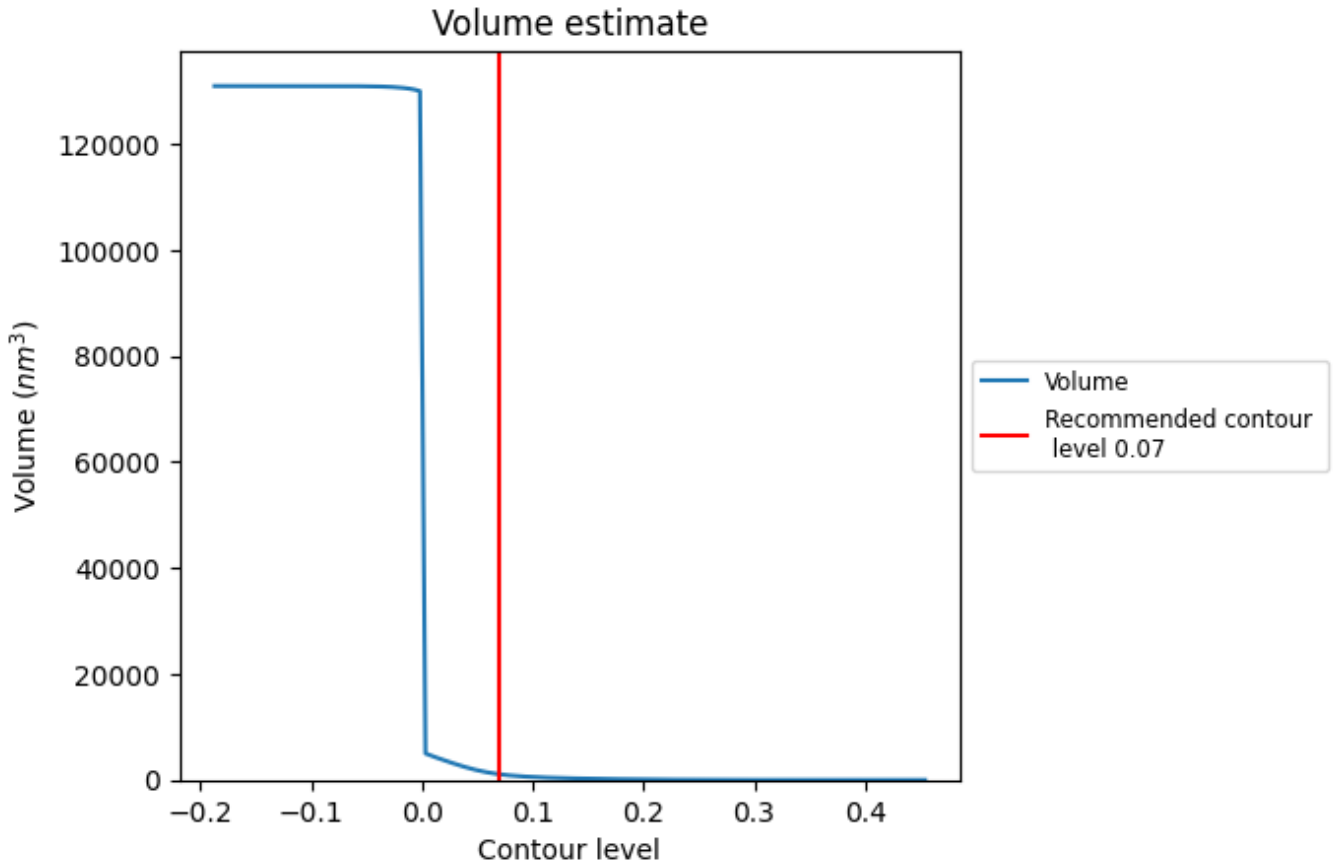
This section contains the results of statistical analysis of the map.

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.

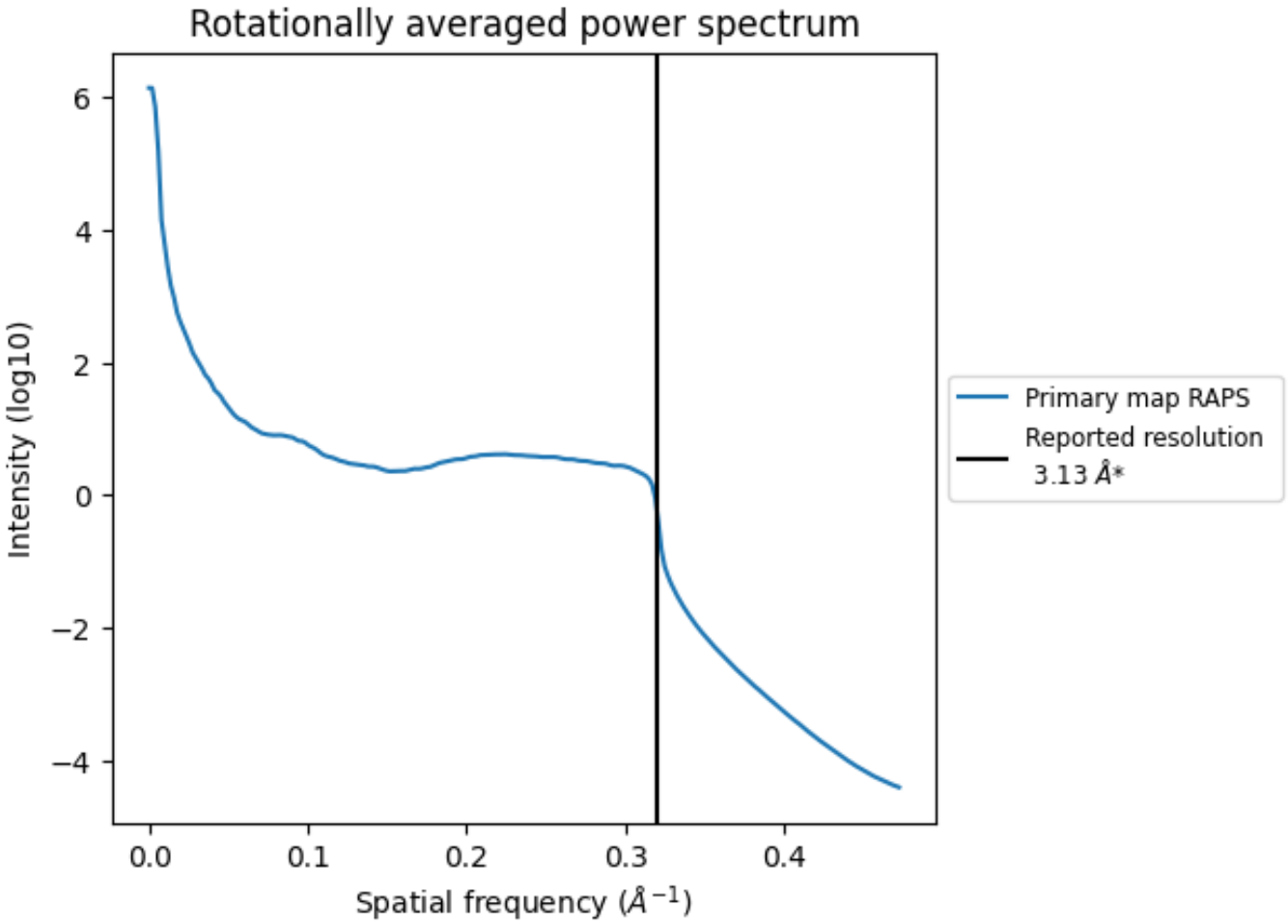
7.2 Volume estimate



The volume at the recommended contour level is 1075 nm^3; this corresponds to an approximate mass of 971 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 0.319 $Å^{-1}$

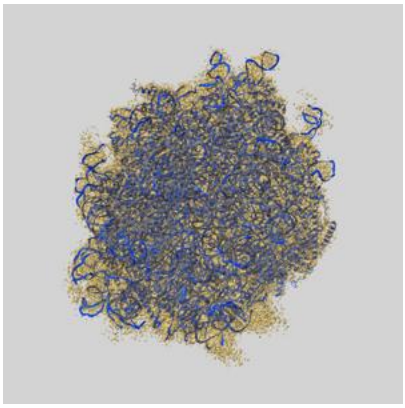
8 Fourier-Shell correlation

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

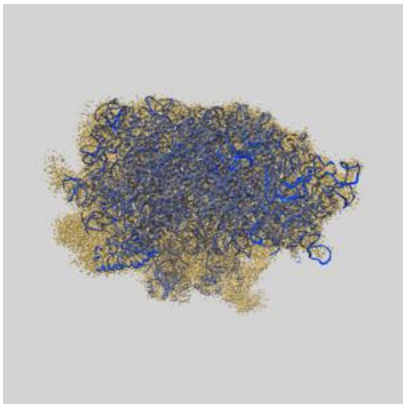
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0978 and PDB model 6LU8. Per-residue inclusion information can be found in section 3 on page 14.

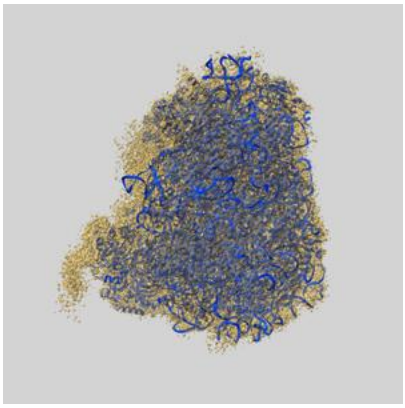
9.1 Map-model overlay



X



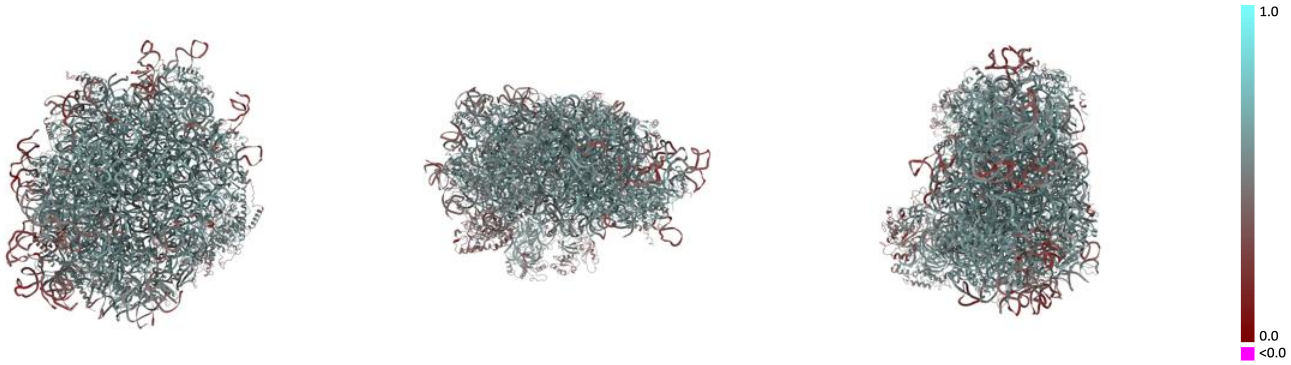
Y



Z

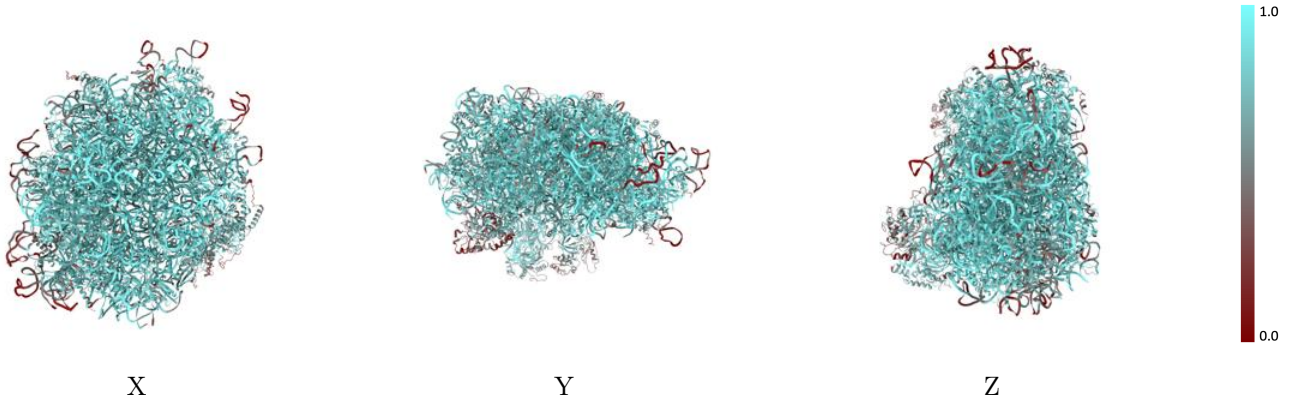
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



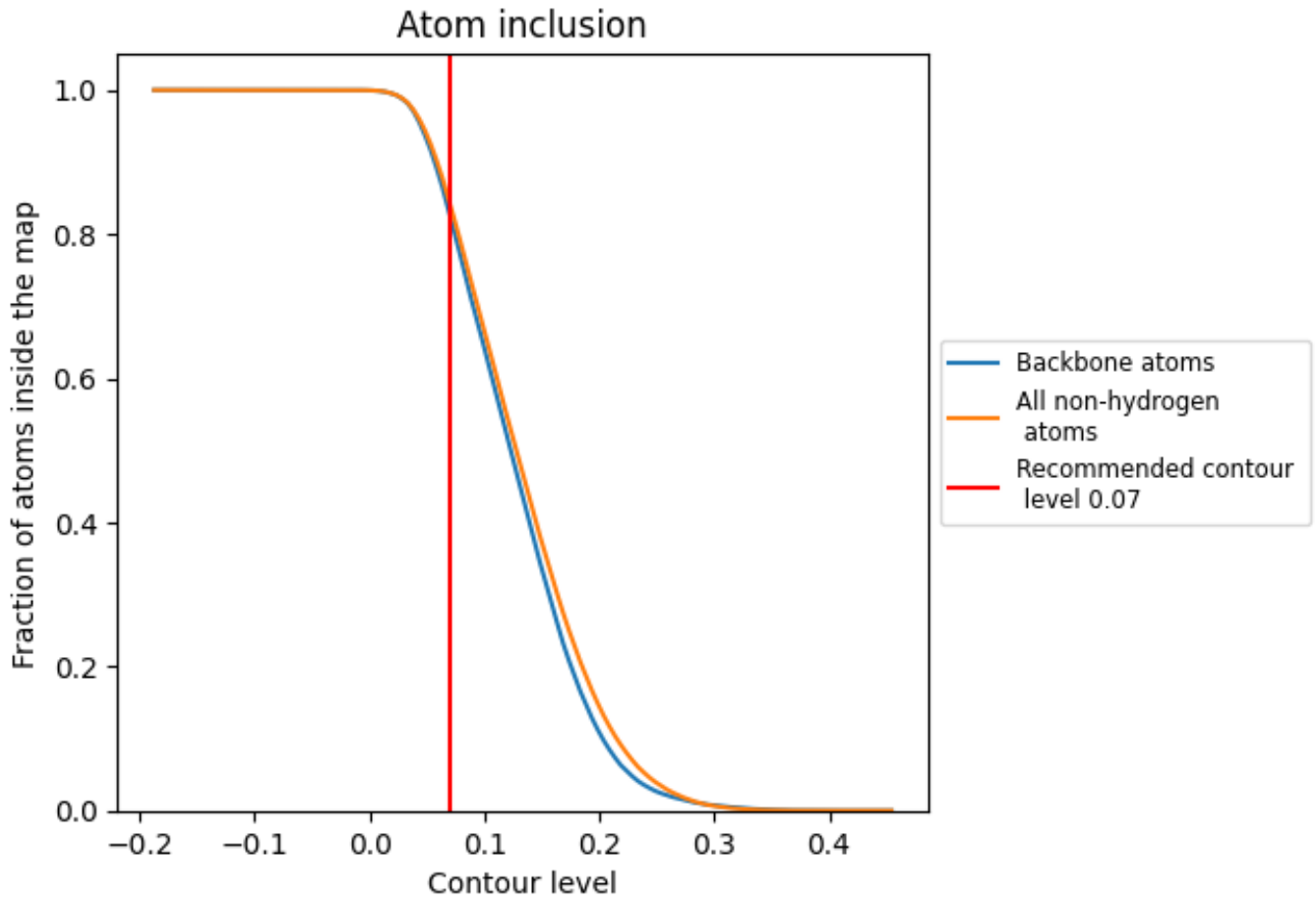
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (i)



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 84% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8424	0.5400
1	0.2517	0.3670
2	0.8672	0.5310
3	0.7708	0.5010
4	0.6456	0.4800
5	0.9336	0.5570
6	0.7356	0.5280
7	0.8126	0.5550
8	0.9226	0.5670
9	0.7570	0.5340
A	0.4020	0.3520
B	0.8821	0.5790
C	0.8073	0.5320
D	0.8986	0.5870
E	0.7902	0.5490
F	0.9014	0.5820
G	0.7428	0.5350
H	0.8624	0.5730
I	0.7757	0.5400
K	0.8340	0.5530
L	0.9284	0.6040
M	0.9421	0.5900
N	0.6438	0.4660
O	0.7379	0.5460
P	0.9338	0.5880
Q	0.8317	0.5600
R	0.3803	0.4050
S	0.8722	0.5680
U	0.9605	0.6110
V	0.8904	0.5840
W	0.8517	0.5700
X	0.8614	0.5670
Y	0.9038	0.5890
Z	0.9372	0.6030
a	0.8862	0.5840

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Chain	Atom inclusion	Q-score
b	0.9304	0.5950
c	0.9032	0.5780
d	0.7695	0.5410
e	0.8673	0.5670
g	0.8702	0.5750
h	0.8646	0.5780
i	0.8276	0.5600
j	0.8390	0.5660
k	0.9273	0.5940
l	0.8785	0.5830
m	0.9156	0.5920
n	0.9419	0.6070
o	0.8135	0.5460
p	0.8933	0.5790
r	0.7245	0.5170
z	0.7326	0.5280