



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 06:33 am GMT

PDB ID : 5FDU
Title : Crystal structure of the Metalnikowin I antimicrobial peptide bound to the *Thermus thermophilus* 70S ribosome
Authors : Seefeldt, A.C.; Graf, M.; Perebaskine, N.; Nguyen, F.; Arenz, S.; Mardirossian, M.; Scocchi, M.; Wilson, D.N.; Innis, C.A.
Deposited on : 2015-12-16
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

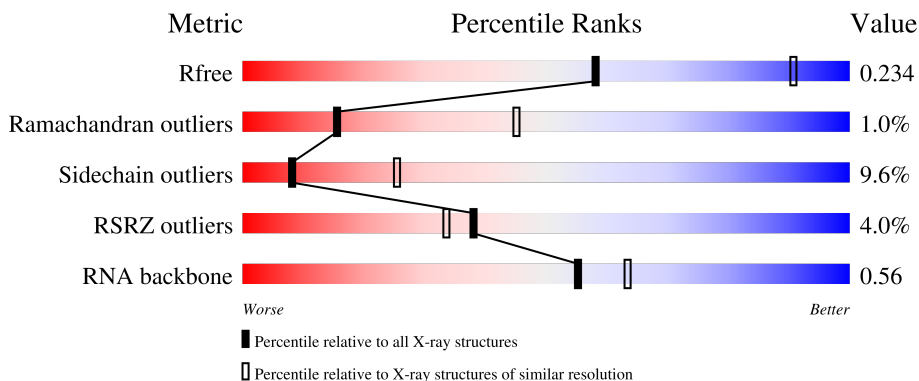
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	
1	2A	2915	
2	1B	120	
2	2B	120	
3	1D	275	


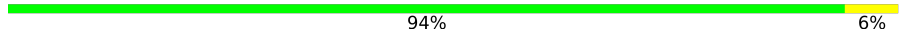



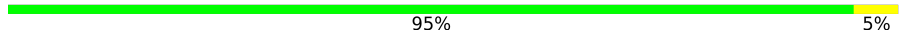
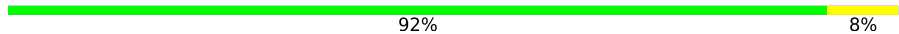
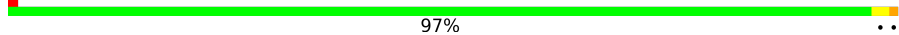





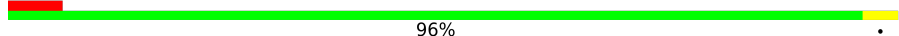


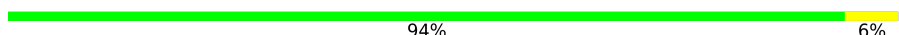

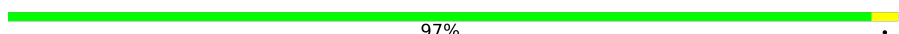






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Mol	Chain	Length	Quality of chain
3	2D	275	92% 7%
4	1E	204	89% 10%
4	2E	204	89% 11%
5	1F	203	85% 14%
5	2F	203	91% 9%
6	1G	181	88% 10%
6	2G	181	93% 6%
7	1H	174	93% 7%
7	2H	174	87% 13%
8	1I	147	88% 12%
8	2I	147	88% 10%
9	1N	140	89% 11%
9	2N	140	91% 9%
10	1O	122	90% 9%
10	2O	122	94% 6%
11	1P	149	93% 7%
11	2P	149	93% 7%
12	1Q	141	93% 5%
12	2Q	141	92% 7%
13	1R	118	86% 14%
13	2R	118	86% 13%
14	1S	110	90% 8%
14	2S	110	90% 10%
15	1T	131	92% 8%
15	2T	131	95% 5%

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Mol	Chain	Length	Quality of chain
16	1U	116	 84% 14%
16	2U	116	 94% 6%
17	1V	101	 85% 15%
17	2V	101	 89% 10%
18	1W	112	 90% 10%
18	2W	112	 95% 5%
19	1X	95	 92% 8%
19	2X	95	 97%
20	1Y	107	 91% 9%
20	2Y	107	 15% 91% 8%
21	1Z	203	 89% 11%
21	2Z	203	 3% 91% 8%
22	10	77	 92% 8%
22	20	77	 6% 96%
23	11	97	 91% 9%
23	21	97	 90% 9%
24	12	70	 94% 6%
24	22	70	 91% 9%
25	13	59	 97%
25	23	59	 10% 93% 7%
26	14	69	 14% 83% 16%
26	24	69	 25% 78% 22%
27	15	59	 83% 14%
27	25	59	 90% 10%
28	16	53	 89% 11%

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Mol	Chain	Length	Quality of chain
28	26	53	89% 11%
29	17	48	2% 83% 17%
29	27	48	90% 10%
30	18	64	88% 12%
30	28	64	89% 11%
31	19	37	92% 8%
31	29	37	5% 95% 5%
32	1a	1521	3% 55% 36% 7% .
32	2a	1521	4% 58% 35% 6% .
33	1b	231	7% 87% 11% .
33	2b	231	8% 84% 15% .
34	1c	206	6% 95% 5%
34	2c	206	3% 92% 8%
35	1d	208	2% 88% 12%
35	2d	208	92% 8%
36	1e	148	% 93% 7%
36	2e	148	% 95% 5%
37	1f	100	% 94% 6%
37	2f	100	96% .
38	1g	155	4% 93% 7%
38	2g	155	8% 94% 6%
39	1h	137	% 91% 8% .
39	2h	137	% 94% 6%
40	1i	127	9% 90% 10%
40	2i	127	17% 89% 9% ..

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Mol	Chain	Length	Quality of chain
41	1j	97	22% 90% 10%
41	2j	97	21% 90% 9%
42	1k	114	% 96%
42	2k	114	% 92% 8%
43	1l	122	2% 94% 6%
43	2l	122	93% 7%
44	1m	116	6% 90% 10%
44	2m	116	7% 88% 10%
45	1n	60	2% 90% 8%
45	2n	60	18% 93% 5%
46	1o	88	3% 93% 6%
46	2o	88	92% 8%
47	1p	82	7% 85% 13%
47	2p	82	4% 90% 10%
48	1q	99	% 92% 7%
48	2q	99	% 93% 7%
49	1r	68	4% 91% 9%
49	2r	68	4% 87% 13%
50	1s	83	12% 90% 10%
50	2s	83	42% 93% 7%
51	1t	98	3% 91% 7%
51	2t	98	% 94% 5%
52	1u	23	22% 87% 13%
52	2u	23	43% 87% 9%
53	1x	97	2% 95% 5%

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Mol	Chain	Length	Quality of chain
53	2x	97	
54	1y	10	
54	2y	10	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	18	3301	-	-	-	X
55	MG	1A	3071	-	-	-	X
55	MG	1A	3077	-	-	-	X
55	MG	1A	3084	-	-	-	X
55	MG	1A	3095	-	-	-	X
55	MG	1A	3106	-	-	-	X
55	MG	1A	3143	-	-	-	X
55	MG	1A	3173	-	-	-	X
55	MG	1A	3183	-	-	-	X
55	MG	1A	3193	-	-	-	X
55	MG	1A	3204	-	-	-	X
55	MG	1A	3220	-	-	-	X
55	MG	1A	3244	-	-	-	X
55	MG	1A	3396	-	-	-	X
55	MG	1A	3516	-	-	-	X
55	MG	1A	3611	-	-	-	X
55	MG	1A	3702	-	-	-	X
55	MG	1A	3725	-	-	-	X
55	MG	1A	3734	-	-	-	X
55	MG	1A	3758	-	-	-	X
55	MG	1A	3848	-	-	-	X
55	MG	1A	3895	-	-	-	X
55	MG	1A	3905	-	-	-	X
55	MG	1A	3913	-	-	-	X
55	MG	1A	3914	-	-	-	X
55	MG	1Q	204	-	-	-	X
55	MG	1V	201	-	-	-	X
55	MG	1a	3022	-	-	-	X
55	MG	1a	3038	-	-	-	X
55	MG	1a	3058	-	-	-	X
55	MG	1a	3063	-	-	-	X
55	MG	1a	3161	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1h	3001	-	-	-	X
55	MG	27	103	-	-	-	X
55	MG	28	101	-	-	-	X
55	MG	28	102	-	-	-	X
55	MG	2A	3047	-	-	-	X
55	MG	2A	3058	-	-	-	X
55	MG	2A	3074	-	-	-	X
55	MG	2A	3080	-	-	-	X
55	MG	2A	3090	-	-	-	X
55	MG	2A	3091	-	-	-	X
55	MG	2A	3109	-	-	-	X
55	MG	2A	3129	-	-	-	X
55	MG	2A	3136	-	-	-	X
55	MG	2A	3138	-	-	-	X
55	MG	2A	3142	-	-	-	X
55	MG	2A	3150	-	-	-	X
55	MG	2A	3154	-	-	-	X
55	MG	2A	3155	-	-	-	X
55	MG	2A	3163	-	-	-	X
55	MG	2A	3192	-	-	-	X
55	MG	2A	3257	-	-	-	X
55	MG	2A	3375	-	-	-	X
55	MG	2A	3455	-	-	-	X
55	MG	2A	3476	-	-	-	X
55	MG	2A	3485	-	-	-	X
55	MG	2A	3507	-	-	-	X
55	MG	2A	3553	-	-	-	X
55	MG	2A	3555	-	-	-	X
55	MG	2A	3563	-	-	-	X
55	MG	2A	3582	-	-	-	X
55	MG	2A	3643	-	-	-	X
55	MG	2A	3762	-	-	-	X
55	MG	2A	3765	-	-	-	X
55	MG	2A	3792	-	-	-	X
55	MG	2A	3813	-	-	-	X
55	MG	2D	302	-	-	-	X
55	MG	2H	201	-	-	-	X
55	MG	2P	202	-	-	-	X
55	MG	2Q	8004	-	-	-	X
55	MG	2X	102	-	-	-	X
55	MG	2a	1609	-	-	-	X
55	MG	2a	1614	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2a	1631	-	-	-	X
55	MG	2a	1636	-	-	-	X
55	MG	2a	1637	-	-	-	X
55	MG	2a	1653	-	-	-	X
55	MG	2a	1656	-	-	-	X
55	MG	2a	1710	-	-	-	X
55	MG	2a	1734	-	-	-	X
55	MG	2a	1742	-	-	-	X
55	MG	2n	502	-	-	-	X

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 293484 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2872	Total	C	N	O	P	0	0	0
			61862	27535	11569	19886	2872			
1	2A	2867	Total	C	N	O	P	0	0	0
			61751	27486	11547	19852	2866			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	Total	C	N	O	P	0	0	0
			2575	1145	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2571	1146	476	831	118			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1574	1004	294	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			880	554	171	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			877	553	171	151	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	2k	114	833	519	156	155	3	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	1l	122	932	586	185	159	2	0	0	0
43	2l	122	932	586	185	159	2	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1m	116	914	564	189	159	2	0	0	0
44	2m	114	895	550	186	157	2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	1n	60	492	312	104	72	4	0	0	0
45	2n	60	492	312	104	72	4	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	1o	88	728	456	144	126	2	0	0	0
46	2o	88	728	456	144	126	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	1p	82	681	433	134	113	1	0	0	0
47	2p	82	677	430	133	113	1	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	2r	68	Total	C	N	O		0	0	0
			555	355	108	92				

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
52	1u	23	Total	C	N	O		0	0	0
			199	122	48	29				
52	2u	23	Total	C	N	O		0	0	0
			199	122	48	29				

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1x	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2x	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is a protein called Metalnikowin I.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	1y	10	Total	C	N	O	0	0	0
			87	55	17	15			
54	2y	10	Total	C	N	O	0	0	0
			87	55	17	15			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1A	917	Total	Mg	0	0
			917	917		
55	1B	24	Total	Mg	0	0
			24	24		
55	1D	18	Total	Mg	0	0
			18	18		
55	1E	8	Total	Mg	0	0
			8	8		
55	1F	16	Total	Mg	0	0
			16	16		
55	1G	3	Total	Mg	0	0
			3	3		
55	1H	2	Total	Mg	0	0
			2	2		
55	1N	3	Total	Mg	0	0
			3	3		
55	1P	4	Total	Mg	0	0
			4	4		
55	1Q	5	Total	Mg	0	0
			5	5		
55	1R	5	Total	Mg	0	0
			5	5		
55	1S	1	Total	Mg	0	0
			1	1		
55	1T	1	Total	Mg	0	0
			1	1		
55	1U	7	Total	Mg	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1V	3	Total Mg 3 3	0	0
55	1W	3	Total Mg 3 3	0	0
55	1X	1	Total Mg 1 1	0	0
55	1Y	1	Total Mg 1 1	0	0
55	10	8	Total Mg 8 8	0	0
55	11	3	Total Mg 3 3	0	0
55	13	2	Total Mg 2 2	0	0
55	15	6	Total Mg 6 6	0	0
55	17	5	Total Mg 5 5	0	0
55	18	3	Total Mg 3 3	0	0
55	19	2	Total Mg 2 2	0	0
55	1a	223	Total Mg 223 223	0	0
55	1b	1	Total Mg 1 1	0	0
55	1d	5	Total Mg 5 5	0	0
55	1e	2	Total Mg 2 2	0	0
55	1f	1	Total Mg 1 1	0	0
55	1g	1	Total Mg 1 1	0	0
55	1h	2	Total Mg 2 2	0	0
55	1k	1	Total Mg 1 1	0	0
55	1l	1	Total Mg 1 1	0	0
55	1m	1	Total Mg 1 1	0	0

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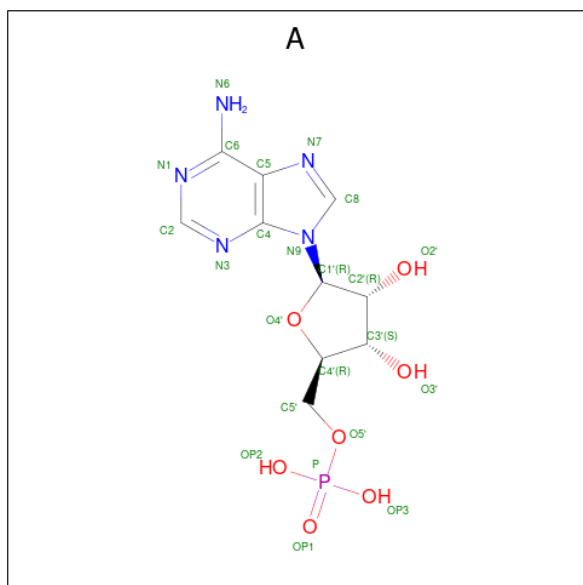
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1n	1	Total Mg 1 1	0	0
55	1o	1	Total Mg 1 1	0	0
55	1t	1	Total Mg 1 1	0	0
55	2A	821	Total Mg 821 821	0	0
55	2B	18	Total Mg 18 18	0	0
55	2D	11	Total Mg 11 11	0	0
55	2E	7	Total Mg 7 7	0	0
55	2F	10	Total Mg 10 10	0	0
55	2G	3	Total Mg 3 3	0	0
55	2H	1	Total Mg 1 1	0	0
55	2N	1	Total Mg 1 1	0	0
55	2P	2	Total Mg 2 2	0	0
55	2Q	5	Total Mg 5 5	0	0
55	2R	3	Total Mg 3 3	0	0
55	2S	1	Total Mg 1 1	0	0
55	2T	1	Total Mg 1 1	0	0
55	2U	4	Total Mg 4 4	0	0
55	2V	5	Total Mg 5 5	0	0
55	2W	1	Total Mg 1 1	0	0
55	2X	3	Total Mg 3 3	0	0
55	20	6	Total Mg 6 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	21	2	Total 2	Mg 2	0	0
55	23	1	Total 1	Mg 1	0	0
55	25	3	Total 3	Mg 3	0	0
55	27	4	Total 4	Mg 4	0	0
55	28	3	Total 3	Mg 3	0	0
55	2a	196	Total 196	Mg 196	0	0
55	2b	1	Total 1	Mg 1	0	0
55	2d	4	Total 4	Mg 4	0	0
55	2e	2	Total 2	Mg 2	0	0
55	2f	1	Total 1	Mg 1	0	0
55	2g	1	Total 1	Mg 1	0	0
55	2h	1	Total 1	Mg 1	0	0
55	2l	1	Total 1	Mg 1	0	0
55	2m	1	Total 1	Mg 1	0	0
55	2n	2	Total 2	Mg 2	0	0
55	2o	1	Total 1	Mg 1	0	0

- Molecule 56 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1B	1	Total C 1 1	0	0
56	2A	1	Total P 1 1	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

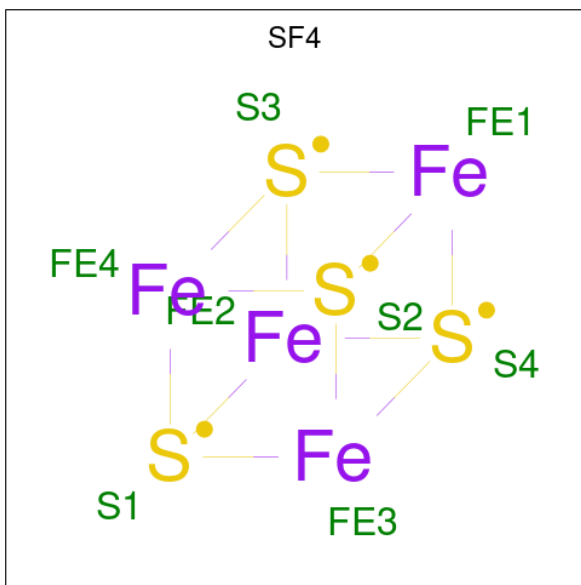
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1Y	1	Total Zn 1 1	0	0
57	14	1	Total Zn 1 1	0	0
57	15	1	Total Zn 1 1	0	0
57	16	1	Total Zn 1 1	0	0
57	19	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	2Y	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0
57	25	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	29	1	Total Zn 1 1	0	0
57	2n	1	Total Zn 1 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1d	1	Total Fe S 8 4 4	0	0
58	2d	1	Total Fe S 8 4 4	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1740	Total O 1740 1740	0	0
59	1B	42	Total O 42 42	0	0
59	1D	14	Total O 14 14	0	0
59	1E	18	Total O 18 18	0	0
59	1F	11	Total O 11 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1G	2	Total 2	O 2	0	0
59	1H	3	Total 3	O 3	0	0
59	1N	9	Total 9	O 9	0	0
59	1P	13	Total 13	O 13	0	0
59	1Q	5	Total 5	O 5	0	0
59	1R	3	Total 3	O 3	0	0
59	1T	5	Total 5	O 5	0	0
59	1U	6	Total 6	O 6	0	0
59	1V	4	Total 4	O 4	0	0
59	1W	2	Total 2	O 2	0	0
59	1X	1	Total 1	O 1	0	0
59	1Y	5	Total 5	O 5	0	0
59	10	4	Total 4	O 4	0	0
59	11	2	Total 2	O 2	0	0
59	13	1	Total 1	O 1	0	0
59	15	2	Total 2	O 2	0	0
59	16	3	Total 3	O 3	0	0
59	17	1	Total 1	O 1	0	0
59	18	7	Total 7	O 7	0	0
59	19	2	Total 2	O 2	0	0
59	1a	393	Total 393	O 393	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1d	10	Total O 10 10	0	0
59	1e	3	Total O 3 3	0	0
59	1f	1	Total O 1 1	0	0
59	1h	1	Total O 1 1	0	0
59	1j	1	Total O 1 1	0	0
59	1l	3	Total O 3 3	0	0
59	1m	2	Total O 2 2	0	0
59	1n	1	Total O 1 1	0	0
59	1o	1	Total O 1 1	0	0
59	1t	2	Total O 2 2	0	0
59	2A	1666	Total O 1666 1666	0	0
59	2B	35	Total O 35 35	0	0
59	2D	12	Total O 12 12	0	0
59	2E	17	Total O 17 17	0	0
59	2F	11	Total O 11 11	0	0
59	2G	2	Total O 2 2	0	0
59	2H	3	Total O 3 3	0	0
59	2N	1	Total O 1 1	0	0
59	2P	9	Total O 9 9	0	0
59	2Q	5	Total O 5 5	0	0
59	2R	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2T	3	Total O 3 3	0	0
59	2U	2	Total O 2 2	0	0
59	2V	2	Total O 2 2	0	0
59	2W	2	Total O 2 2	0	0
59	2X	6	Total O 6 6	0	0
59	2Y	3	Total O 3 3	0	0
59	20	6	Total O 6 6	0	0
59	21	3	Total O 3 3	0	0
59	23	1	Total O 1 1	0	0
59	25	2	Total O 2 2	0	0
59	26	2	Total O 2 2	0	0
59	27	1	Total O 1 1	0	0
59	28	5	Total O 5 5	0	0
59	29	1	Total O 1 1	0	0
59	2a	384	Total O 384 384	0	0
59	2c	1	Total O 1 1	0	0
59	2d	7	Total O 7 7	0	0
59	2e	4	Total O 4 4	0	0
59	2f	1	Total O 1 1	0	0
59	2h	1	Total O 1 1	0	0
59	2j	1	Total O 1 1	0	0

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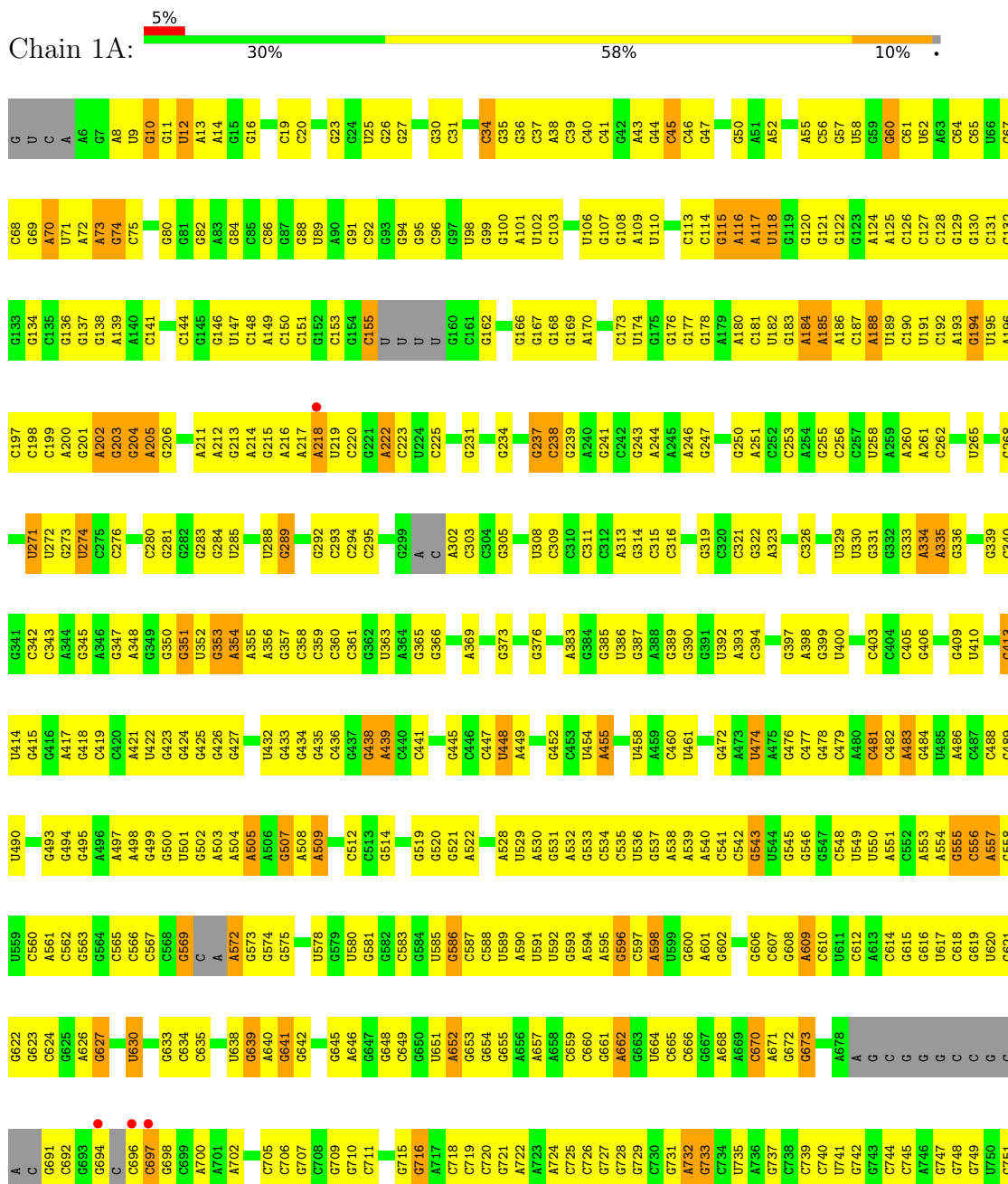
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2l	3	Total O 3 3	0	0
59	2m	3	Total O 3 3	0	0
59	2o	1	Total O 1 1	0	0
59	2p	1	Total O 1 1	0	0
59	2t	1	Total O 1 1	0	0

3 Residue-property plots

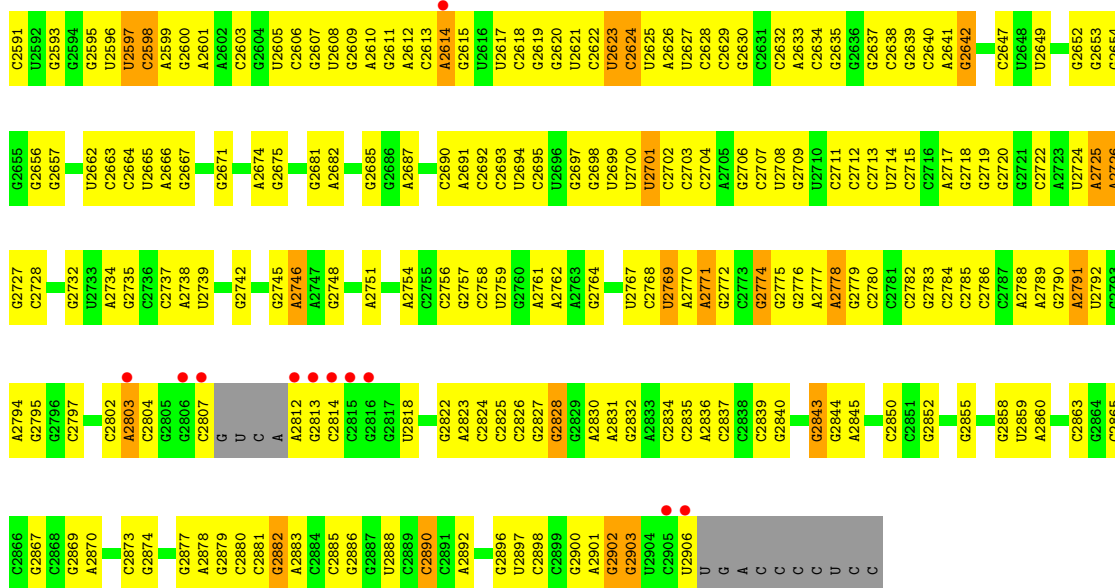
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: 23S ribosomal RNA

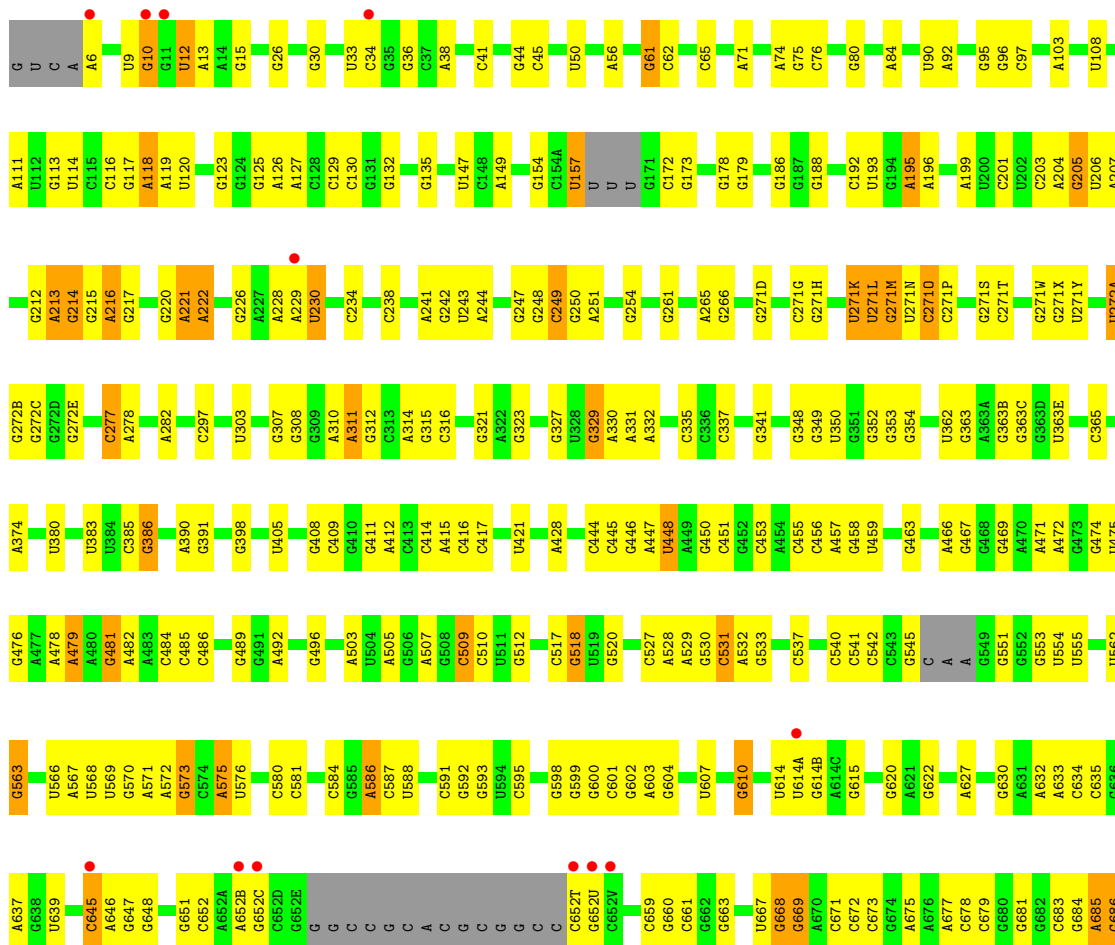


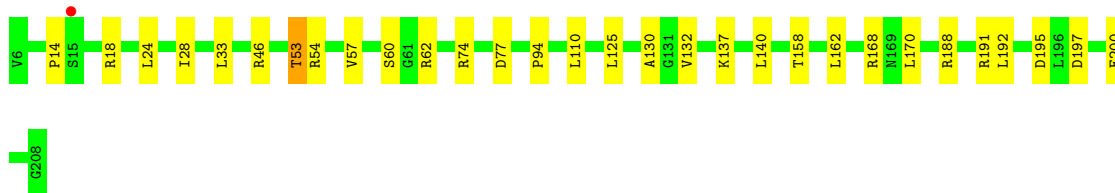
G1610	G1538	A1399	A1332	G1268	G1200	U1136	A1074	U1014	U953	C881	G817	A752
C1611	C1539	A1400	A1335	G1269	A1201	G1137	A1075	C1015	C954	A862	G818	A753
C1612	A1540	G1401	C1336	G1270	A1202	C1138	G1076	C1016	A955	C883		
A1613	A1541	G1402	C1337	G1271	G1203	G1139	G1077	G1017	A956	C884	A821	U756
A1614	A1542	G1403	C1338	G1272	G1204	U1140	U1078	G1018	A957	C885	G823	G757
G1615	A1543	G1404	U1340	A1273	U1205	A1141	U1079	G1019	C958	U886	G824	G758
A1616	C1544	G1405	C1341	G1274	G1206	A1142	G1080	C1020	U959	C887	G759	
A1617	A1406	A1406	G1342		G1207	U1143	U1081	G1021	C960	A888	G825	G760
A1618	G1407	C1343	G1343	G1277	G1208	A1144	U1082	G1022	C961	U889	U826	
A1619	A1408	C1344	C1344	G1278	G1209	G1145	G1083	G1023	C962	A890	G827	G762
G1620	G1409	G1345	G1345	C1279	G1210	U1146		G1024	A963	C891	G828	A763
A1621	G1410	U1346	U1346	G1280	C1211	U1147	G1087	G1025	A964	A829	A829	G764
C1622	A1411	A1347	A1347	G1281	C1212	U1148	C1088	A1026	G965	A830	A765	
U1623	A1412	A1348	A1348	G1282	U1213	U1149	C1089	A1027	G966	U894	A831	C766
U1624	A1413	G1349	G1349	A1283	G1214	C1150	U1090	C1028	U967	A895	G832	
U1625	G1414	G1284	G1284	G1284	G1215	U1151	A1091	A1029	G968	A896	G833	G770
A1626	G1415	U1285	U1285	G1285	G1216	G1152	A1092	A1030	C969	A897	U834	
A1627	A1416	U1286	U1286	G1286	G1217	G1153	A1093	C1031		U898	A835	G773
G1628	G1417	A1287	A1287	A1287	G1218	U1154	A1094	C1032	A972	U899	A836	A774
C1629	U1418				A1219	C1155	U1095	G1033	G973	G902	C837	G775
A1630	A1419	G1290	G1290	G1290	U1220	G1156	A1096	A1034	G974	G902	C838	G776
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• Molecule 1: 23S ribosomal RNA





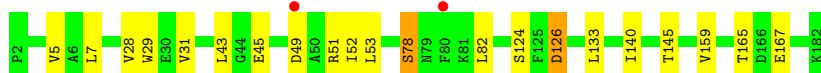
- Molecule 5: 50S ribosomal protein L4

Chain 2F: 91% 9%



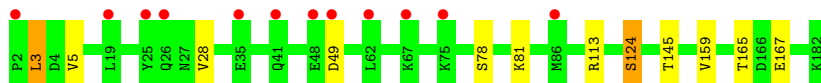
- Molecule 6: 50S ribosomal protein L5

Chain 1G: 88% 10% 2%



- Molecule 6: 50S ribosomal protein L5

Chain 2G: 93% 6% 7%



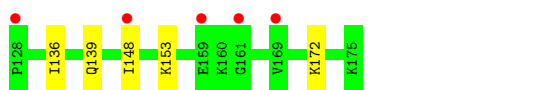
- Molecule 7: 50S ribosomal protein L6

Chain 1H: 93% 7% 2%



- Molecule 7: 50S ribosomal protein L6

Chain 2H: 87% 13% 16%

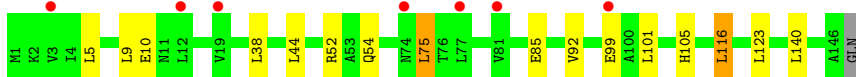
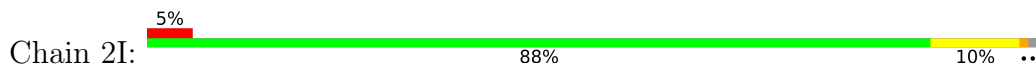


- Molecule 8: 50S ribosomal protein L9

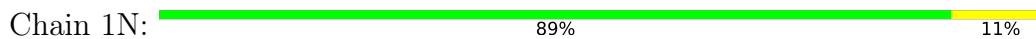
Chain 1I: 88% 12% 2%



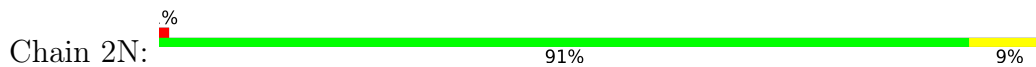
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



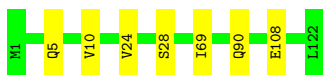
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15





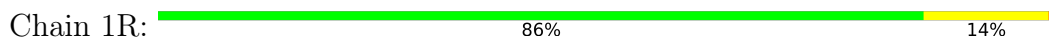
- Molecule 12: 50S ribosomal protein L16



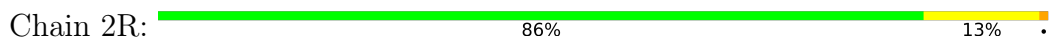
- Molecule 12: 50S ribosomal protein L16



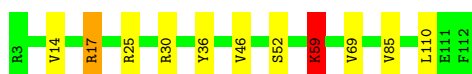
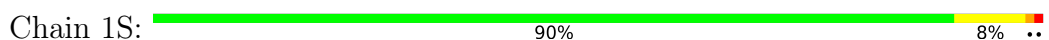
- Molecule 13: 50S ribosomal protein L17



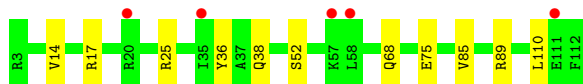
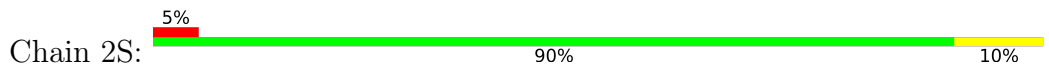
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

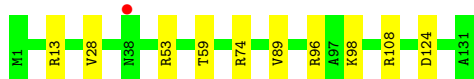


- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19

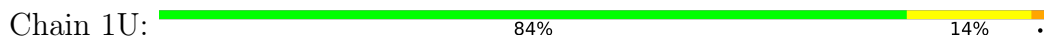




- Molecule 15: 50S ribosomal protein L19



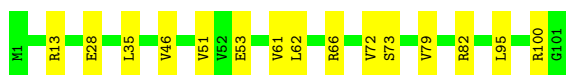
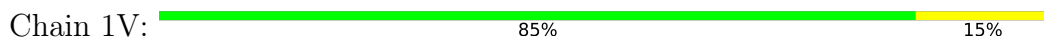
- Molecule 16: 50S ribosomal protein L20



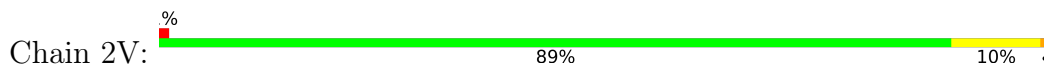
- Molecule 16: 50S ribosomal protein L20



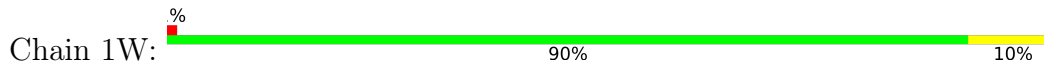
- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21

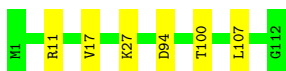


- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22





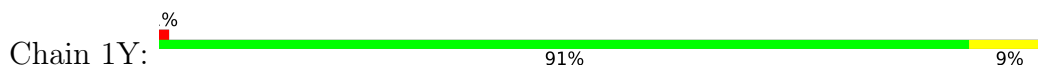
- Molecule 19: 50S ribosomal protein L23



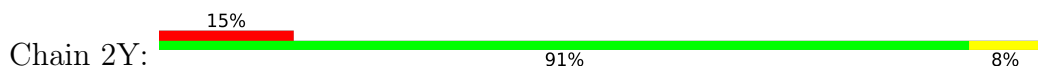
- Molecule 19: 50S ribosomal protein L23



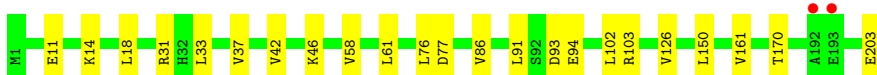
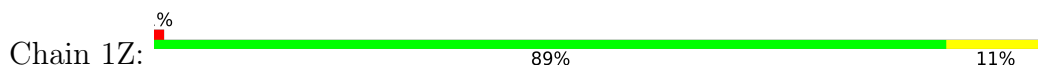
- Molecule 20: 50S ribosomal protein L24



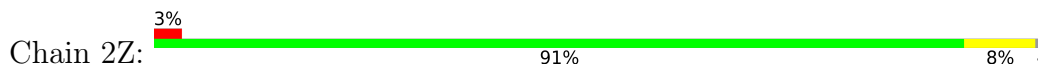
- Molecule 20: 50S ribosomal protein L24



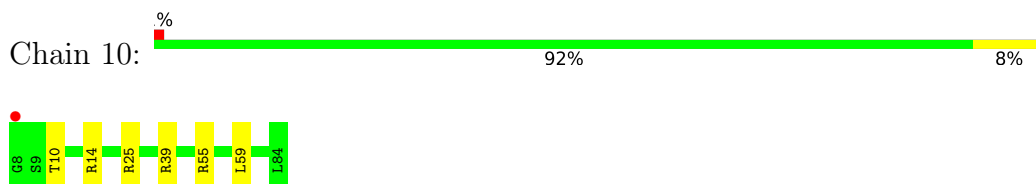
- Molecule 21: 50S ribosomal protein L25



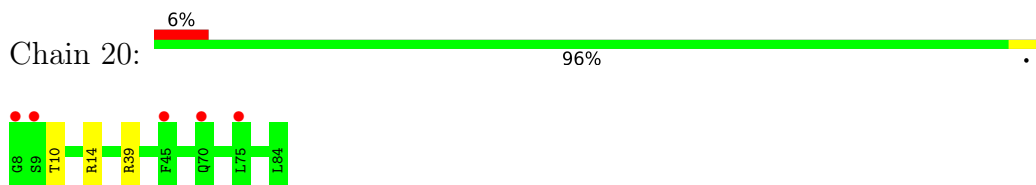
- Molecule 21: 50S ribosomal protein L25



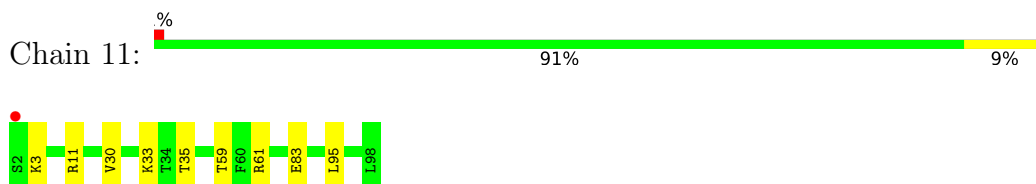
- Molecule 22: 50S ribosomal protein L27



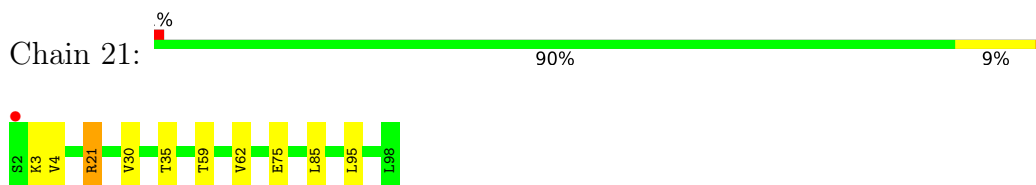
- Molecule 22: 50S ribosomal protein L27



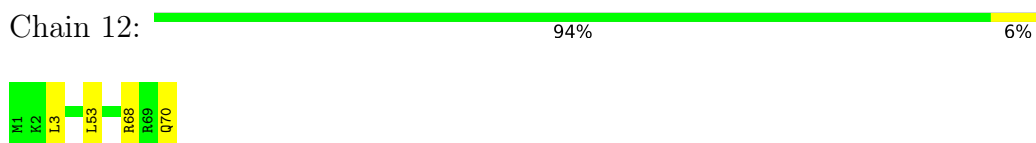
- Molecule 23: 50S ribosomal protein L28



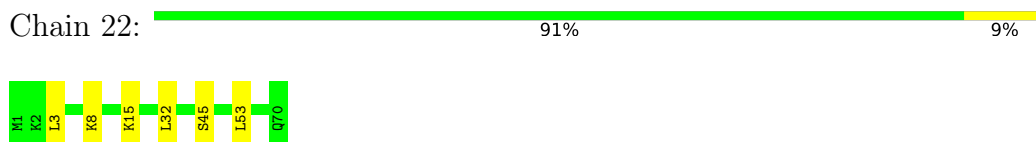
- Molecule 23: 50S ribosomal protein L28



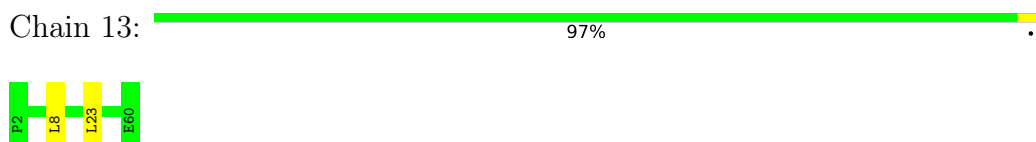
- Molecule 24: 50S ribosomal protein L29



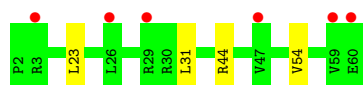
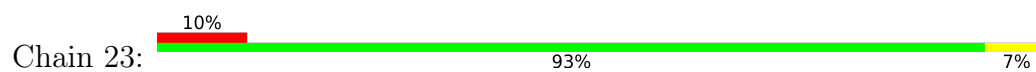
- Molecule 24: 50S ribosomal protein L29



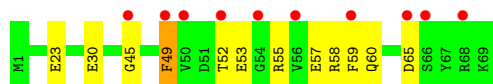
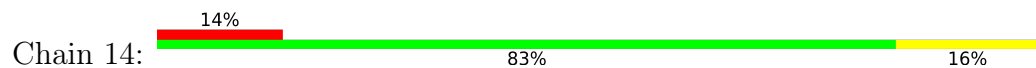
- Molecule 25: 50S ribosomal protein L30



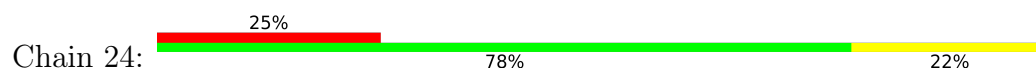
- Molecule 25: 50S ribosomal protein L30



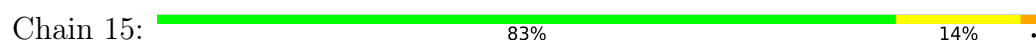
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



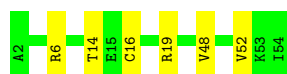
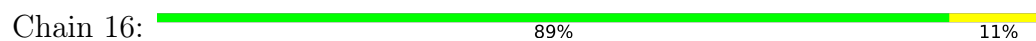
- Molecule 27: 50S ribosomal protein L32



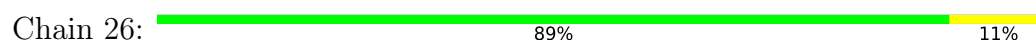
- Molecule 27: 50S ribosomal protein L32



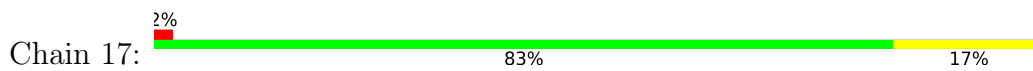
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



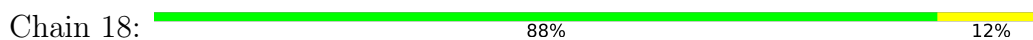
- Molecule 29: 50S ribosomal protein L34



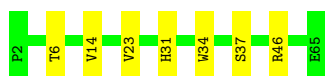
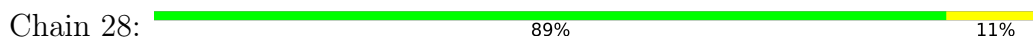
• Molecule 29: 50S ribosomal protein L34



• Molecule 30: 50S ribosomal protein L35



• Molecule 30: 50S ribosomal protein L35



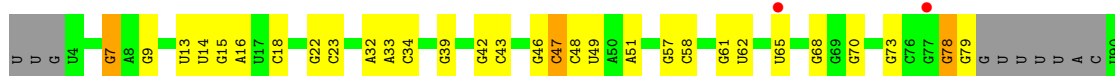
• Molecule 31: 50S ribosomal protein L36

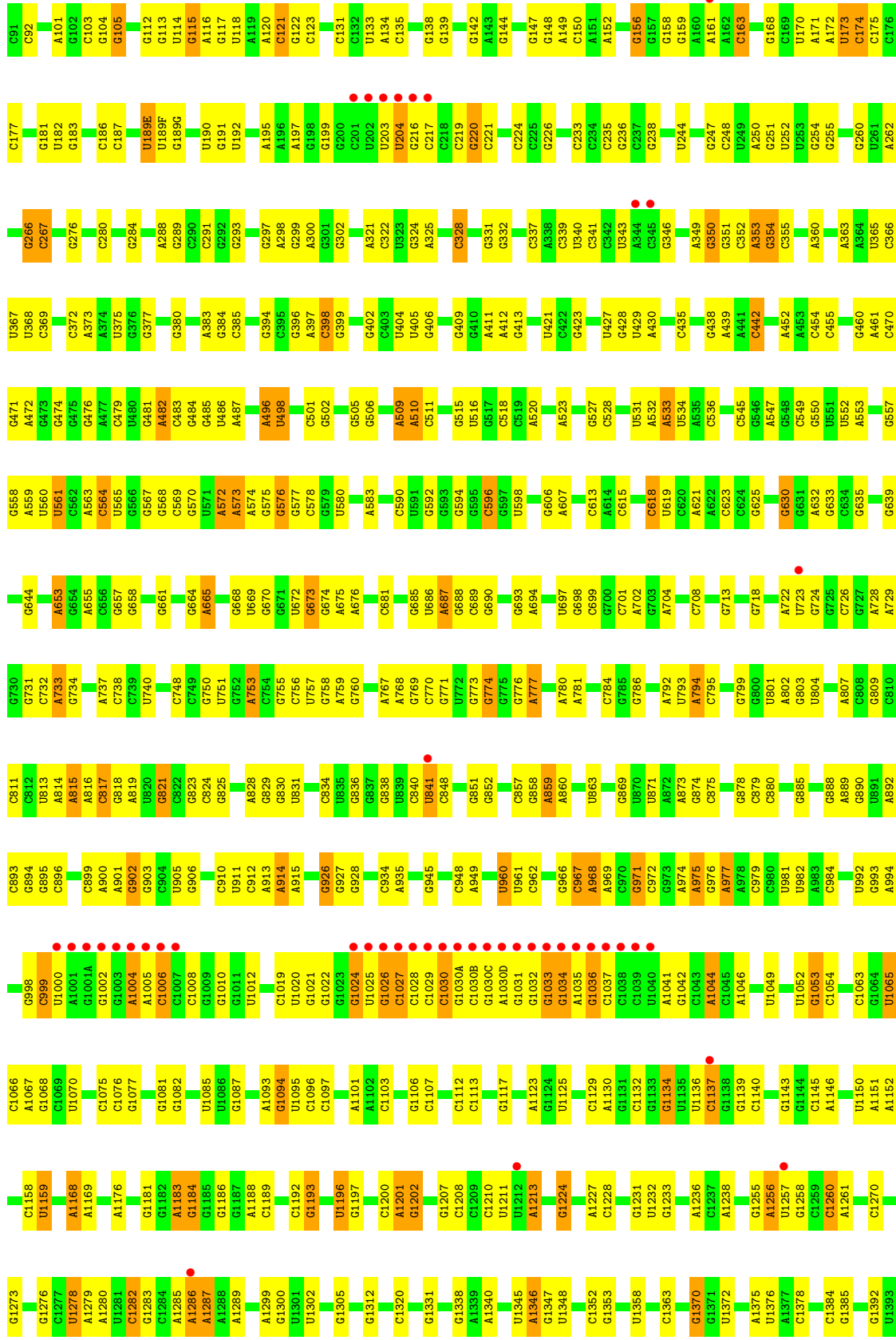


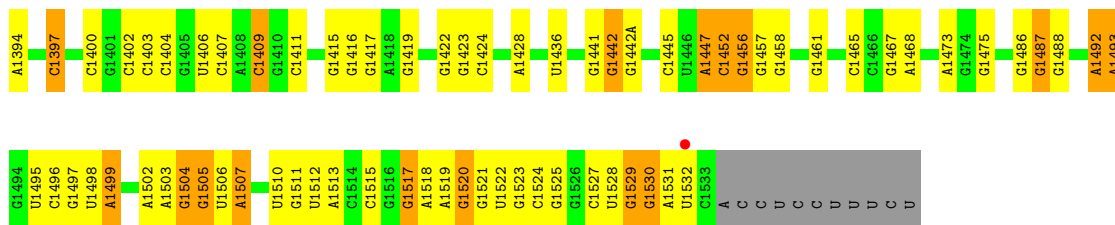
• Molecule 31: 50S ribosomal protein L36



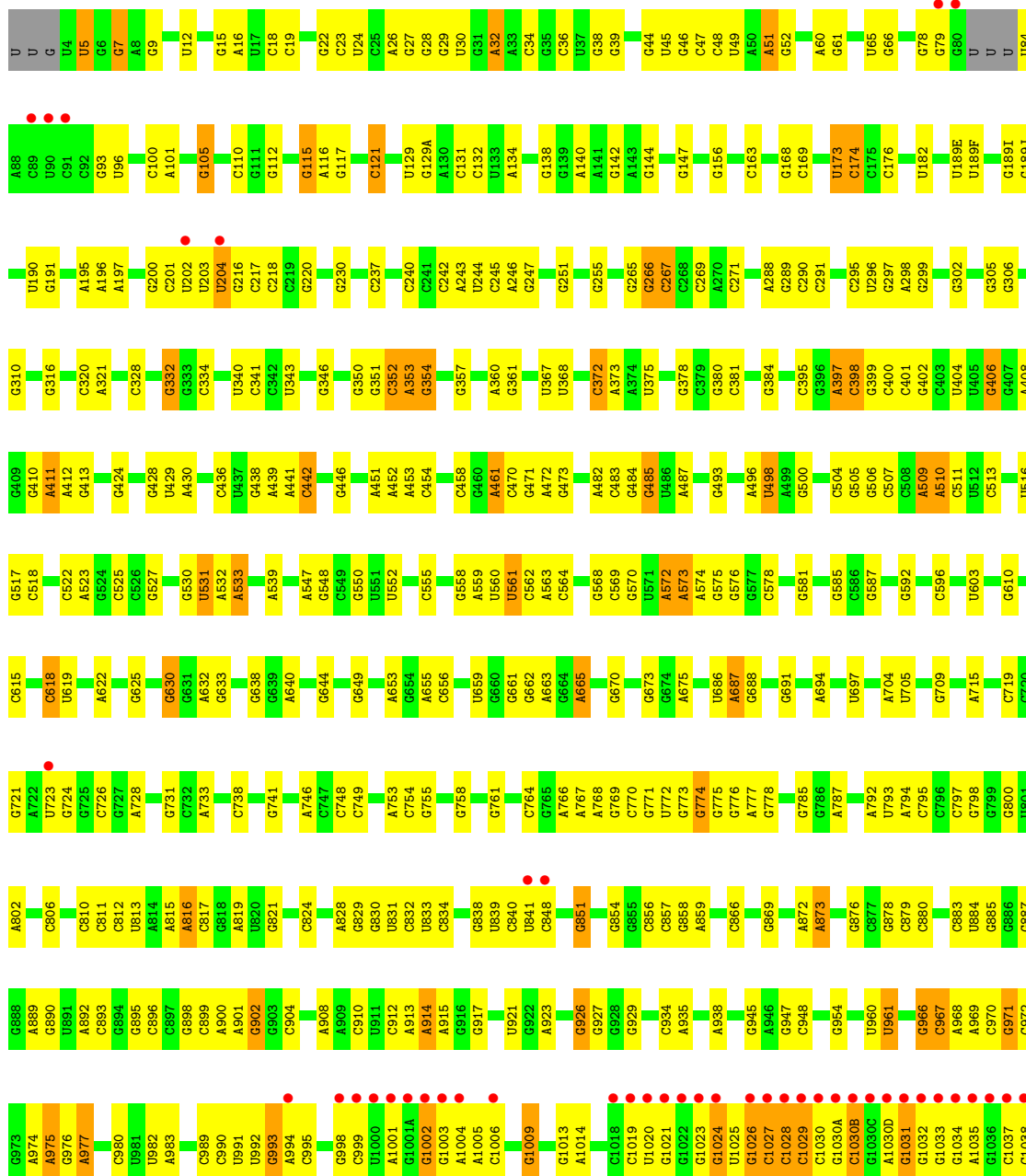
• Molecule 32: 16S ribosomal RNA

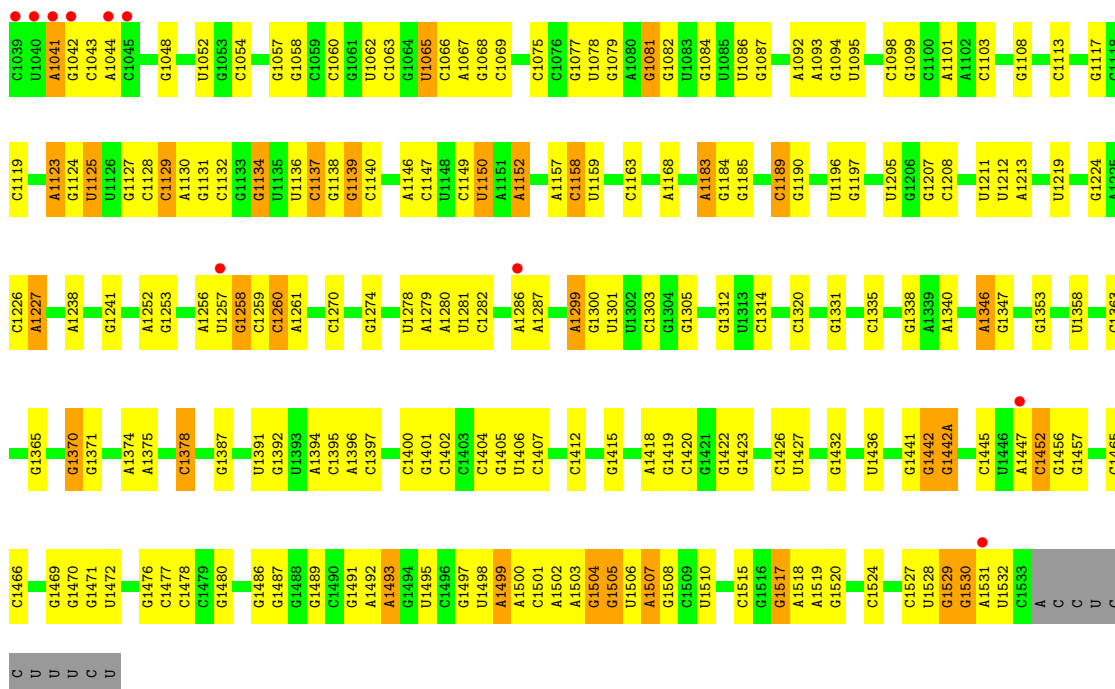




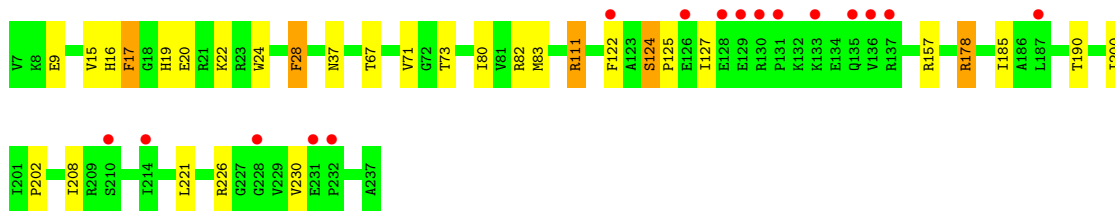
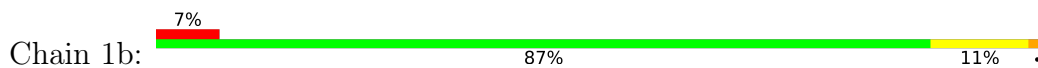


• Molecule 32: 16S ribosomal RNA

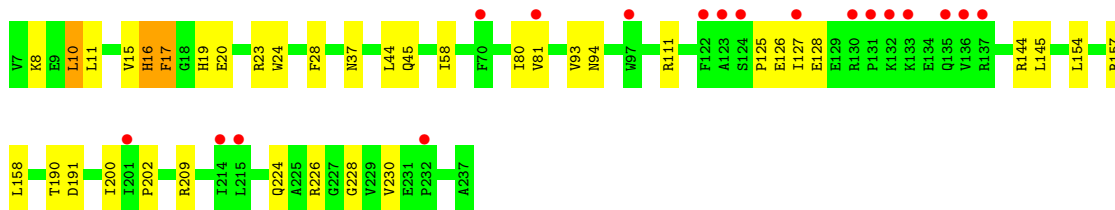
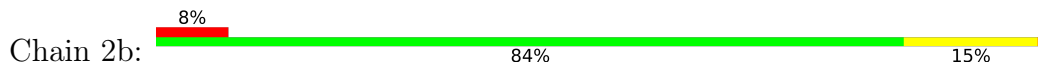




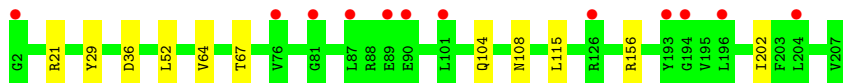
• Molecule 33: 30S ribosomal protein S2



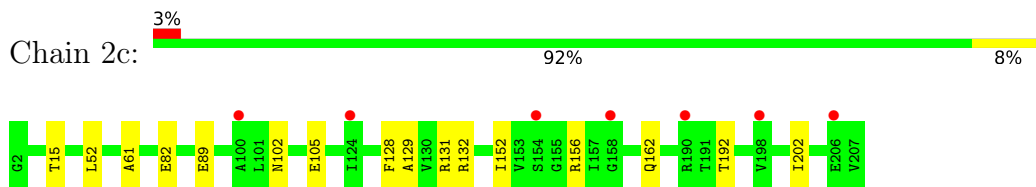
• Molecule 33: 30S ribosomal protein S2



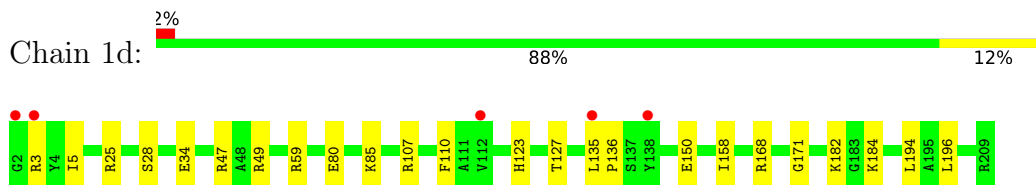
• Molecule 34: 30S ribosomal protein S3



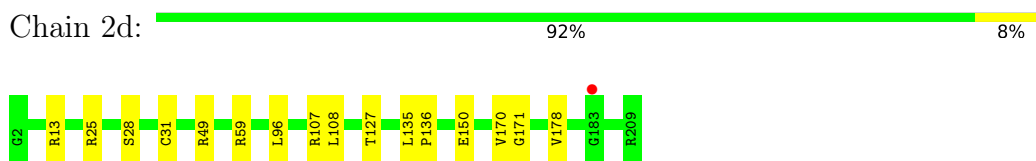
- Molecule 34: 30S ribosomal protein S3



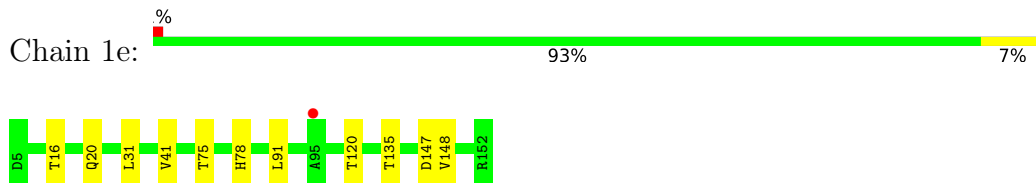
- Molecule 35: 30S ribosomal protein S4



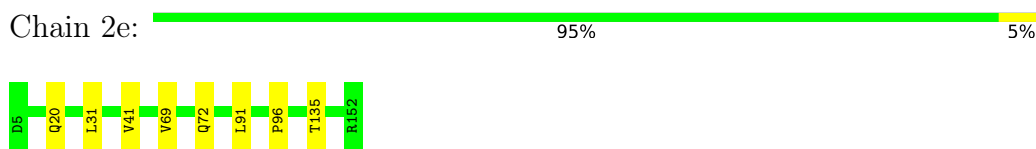
- Molecule 35: 30S ribosomal protein S4



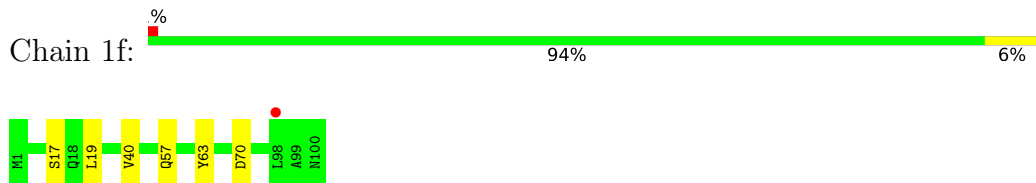
- Molecule 36: 30S ribosomal protein S5



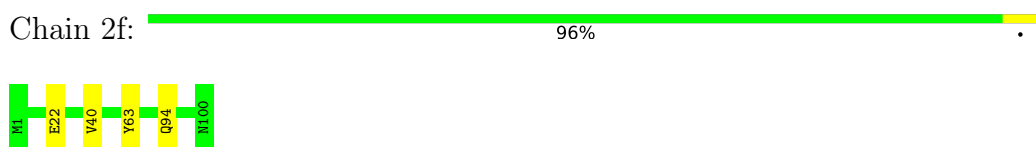
- Molecule 36: 30S ribosomal protein S5



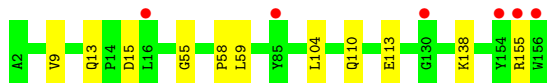
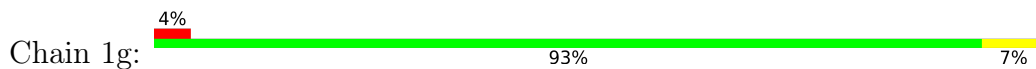
- Molecule 37: 30S ribosomal protein S6



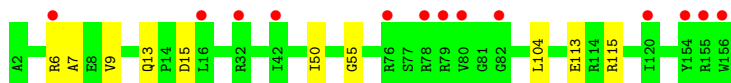
- Molecule 37: 30S ribosomal protein S6



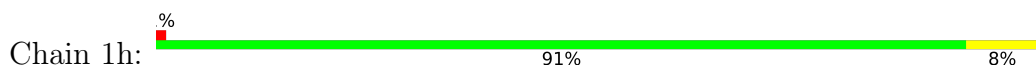
- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7



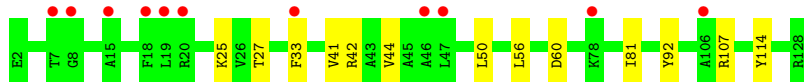
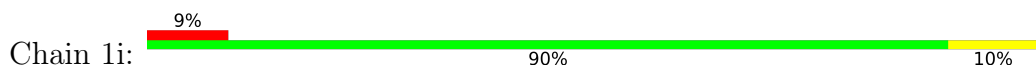
- Molecule 39: 30S ribosomal protein S8



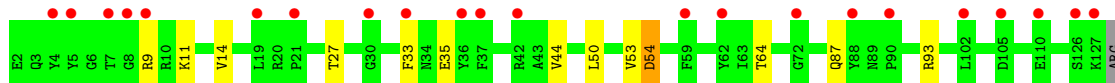
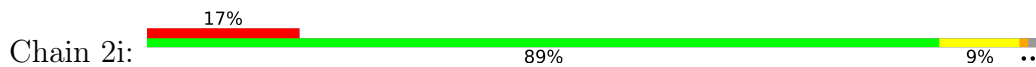
- Molecule 39: 30S ribosomal protein S8



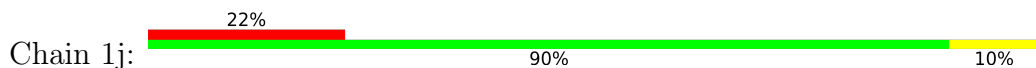
- Molecule 40: 30S ribosomal protein S9

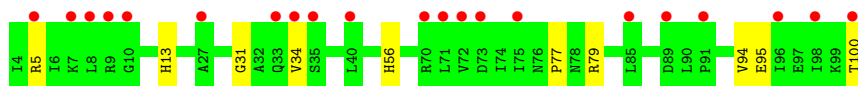


- Molecule 40: 30S ribosomal protein S9

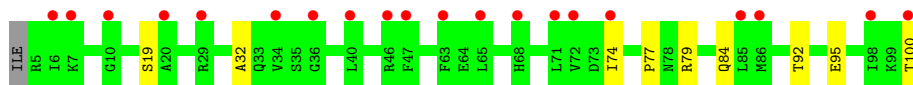
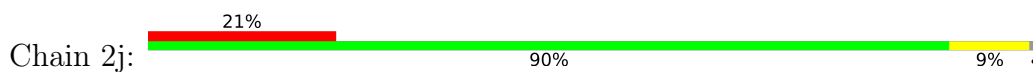


- Molecule 41: 30S ribosomal protein S10





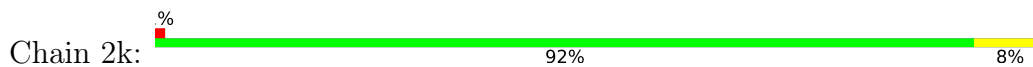
- Molecule 41: 30S ribosomal protein S10



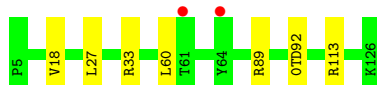
- Molecule 42: 30S ribosomal protein S11



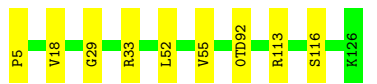
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



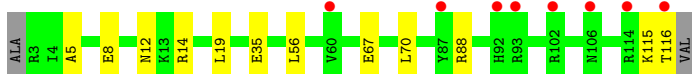
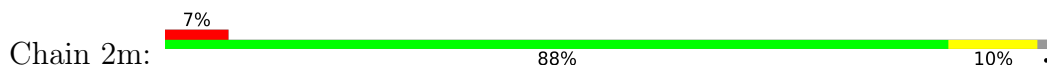
- Molecule 43: 30S ribosomal protein S12



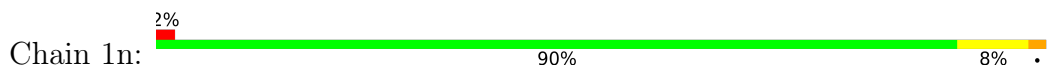
- Molecule 44: 30S ribosomal protein S13



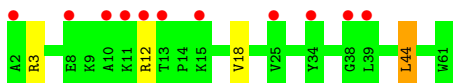
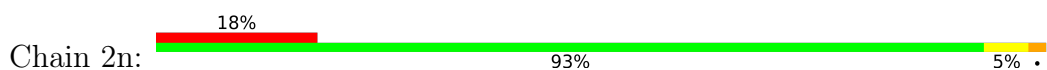
- Molecule 44: 30S ribosomal protein S13



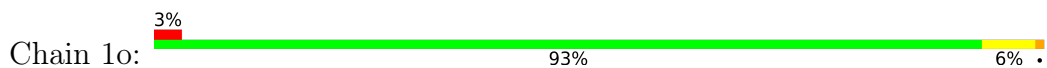
- Molecule 45: 30S ribosomal protein S14 type Z



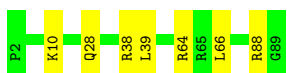
- Molecule 45: 30S ribosomal protein S14 type Z



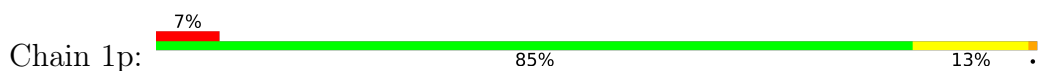
- Molecule 46: 30S ribosomal protein S15



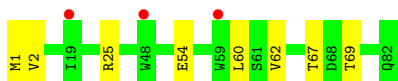
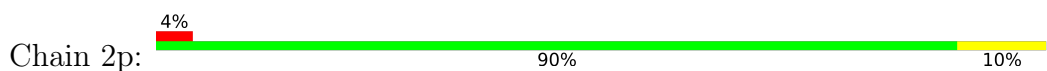
- Molecule 46: 30S ribosomal protein S15



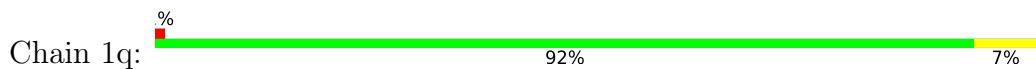
- Molecule 47: 30S ribosomal protein S16



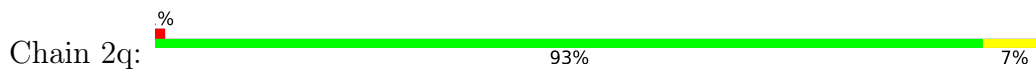
- Molecule 47: 30S ribosomal protein S16



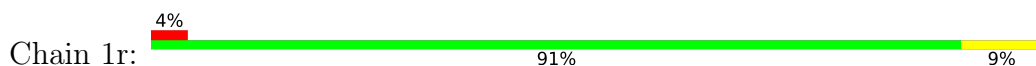
- Molecule 48: 30S ribosomal protein S17



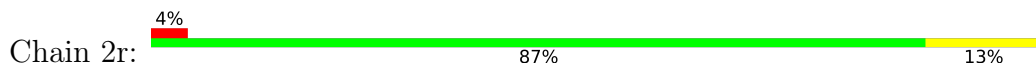
- Molecule 48: 30S ribosomal protein S17



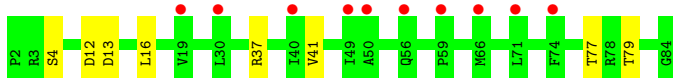
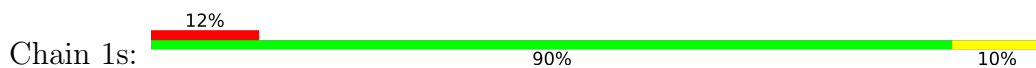
- Molecule 49: 30S ribosomal protein S18



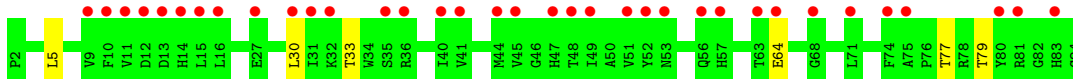
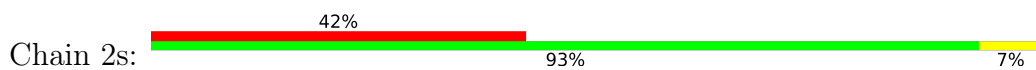
- Molecule 49: 30S ribosomal protein S18



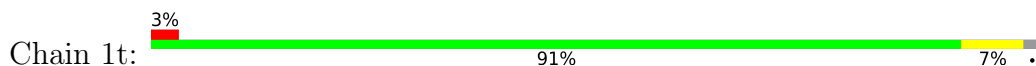
- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19

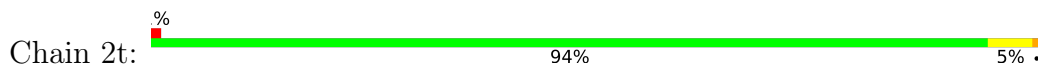


- Molecule 51: 30S ribosomal protein S20

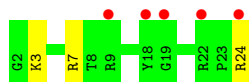




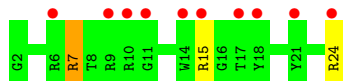
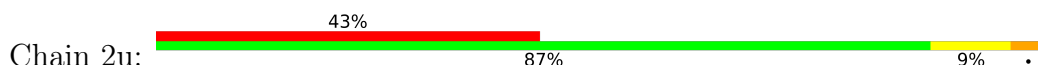
• Molecule 51: 30S ribosomal protein S20



• Molecule 52: 30S ribosomal protein Thx



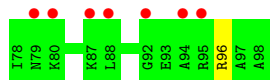
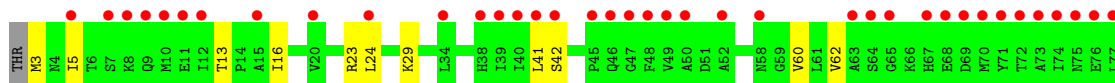
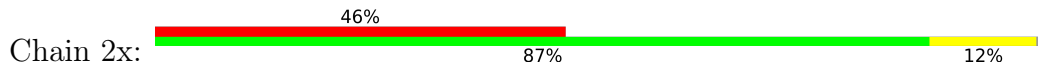
• Molecule 52: 30S ribosomal protein Thx



• Molecule 53: Ribosome-associated inhibitor A




• Molecule 53: Ribosome-associated inhibitor A



• Molecule 54: Metalnikowin I



- Molecule 54: Metalnikowin I

Chain 2y:  90% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.65Å 448.09Å 623.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 2.90 49.72 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.72-2.90) 99.1 (49.72-2.79)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.77Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.183 , 0.234 0.185 , 0.234	Depositor DCC
R_{free} test set	69999 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	293484	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, SF4, 0TD, 5MC, UR3, 7MG, M2G, 2MA, ZN, PSU, OMG, 4OC, 2MG, 5MU, OMU, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1A	1.58	593/69021 (0.9%)	2.13	4360/107735 (4.0%)
1	2A	1.20	117/68892 (0.2%)	1.77	2077/107529 (1.9%)
2	1B	1.24	7/2879 (0.2%)	2.02	149/4490 (3.3%)
2	2B	1.00	1/2874 (0.0%)	1.65	63/4482 (1.4%)
3	1D	0.99	2/2181 (0.1%)	1.03	6/2940 (0.2%)
3	2D	0.81	0/2186	0.95	3/2944 (0.1%)
4	1E	1.01	1/1592 (0.1%)	1.09	8/2149 (0.4%)
4	2E	0.78	0/1592	0.93	1/2149 (0.0%)
5	1F	0.99	0/1619	1.06	6/2193 (0.3%)
5	2F	0.73	0/1609	0.86	0/2181
6	1G	0.72	1/1451 (0.1%)	0.89	1/1961 (0.1%)
6	2G	0.69	1/1449 (0.1%)	0.83	1/1957 (0.1%)
7	1H	0.83	0/1356	0.95	1/1834 (0.1%)
7	2H	0.70	0/1350	0.82	0/1826
8	1I	0.75	2/1109 (0.2%)	0.87	1/1512 (0.1%)
8	2I	0.68	0/1091	0.87	2/1490 (0.1%)
9	1N	0.98	0/1148	0.97	2/1547 (0.1%)
9	2N	0.64	0/1144	0.82	0/1543
10	1O	1.08	1/943 (0.1%)	1.04	2/1269 (0.2%)
10	2O	0.79	0/943	0.87	0/1269
11	1P	0.88	0/1152	1.01	4/1533 (0.3%)
11	2P	0.69	0/1152	0.86	1/1533 (0.1%)
12	1Q	0.98	2/1143 (0.2%)	0.99	3/1527 (0.2%)
12	2Q	0.68	0/1143	0.83	0/1527
13	1R	0.96	0/982	1.10	5/1312 (0.4%)
13	2R	0.73	0/982	0.94	3/1312 (0.2%)
14	1S	0.80	0/887	0.99	3/1180 (0.3%)
14	2S	0.66	0/880	0.85	0/1172
15	1T	0.91	1/1105 (0.1%)	1.08	4/1477 (0.3%)
15	2T	0.73	0/1097	0.93	1/1468 (0.1%)
16	1U	1.10	5/977 (0.5%)	1.07	4/1301 (0.3%)
16	2U	0.76	0/977	0.83	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	1V	0.98	1/786 (0.1%)	1.01	2/1053 (0.2%)
17	2V	0.67	0/782	0.85	0/1049
18	1W	1.09	1/891 (0.1%)	1.06	2/1198 (0.2%)
18	2W	0.84	0/888	0.92	1/1194 (0.1%)
19	1X	0.95	0/764	0.98	1/1025 (0.1%)
19	2X	0.76	0/764	0.84	1/1025 (0.1%)
20	1Y	0.95	1/823 (0.1%)	1.07	3/1099 (0.3%)
20	2Y	0.77	0/823	0.95	1/1100 (0.1%)
21	1Z	0.77	0/1620	0.86	1/2200 (0.0%)
21	2Z	0.66	0/1590	0.84	0/2162
22	10	0.91	0/616	0.97	1/821 (0.1%)
22	20	0.67	0/616	0.88	0/821
23	11	0.98	0/761	0.99	1/1013 (0.1%)
23	21	0.82	0/766	1.03	2/1018 (0.2%)
24	12	0.88	0/590	0.92	0/781
24	22	0.81	0/594	0.86	0/785
25	13	0.94	0/474	1.02	0/635
25	23	0.66	0/469	0.82	0/630
26	14	0.85	0/559	0.86	0/754
26	24	0.92	0/549	0.91	1/741 (0.1%)
27	15	1.11	2/473 (0.4%)	1.19	4/639 (0.6%)
27	25	0.81	1/469 (0.2%)	0.96	2/635 (0.3%)
28	16	0.94	1/460 (0.2%)	0.97	0/613
28	26	0.76	1/456 (0.2%)	0.81	0/608
29	17	1.08	1/426 (0.2%)	1.14	3/561 (0.5%)
29	27	0.81	0/426	0.97	2/561 (0.4%)
30	18	1.00	1/525 (0.2%)	0.96	1/691 (0.1%)
30	28	0.72	0/525	0.83	0/691
31	19	0.90	1/310 (0.3%)	0.96	0/407
31	29	0.60	0/310	0.78	0/407
32	1a	1.09	48/35795 (0.1%)	1.70	858/55864 (1.5%)
32	2a	1.04	35/35890 (0.1%)	1.67	813/56012 (1.5%)
33	1b	0.71	0/1876	0.92	3/2533 (0.1%)
33	2b	0.73	0/1860	0.89	0/2518
34	1c	0.67	0/1582	0.80	0/2137
34	2c	0.73	0/1566	0.83	0/2119
35	1d	0.68	0/1695	0.84	0/2274
35	2d	0.70	0/1698	0.86	0/2277
36	1e	0.66	0/1149	0.84	0/1548
36	2e	0.66	0/1149	0.87	0/1548
37	1f	0.68	0/827	0.82	1/1120 (0.1%)
37	2f	0.69	0/829	0.82	0/1123
38	1g	0.67	0/1254	0.80	1/1683 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	2g	0.68	0/1248	0.79	0/1676
39	1h	0.66	0/1118	0.86	1/1506 (0.1%)
39	2h	0.62	0/1108	0.84	0/1494
40	1i	0.69	0/1005	0.82	0/1351
40	2i	0.75	0/985	0.87	1/1329 (0.1%)
41	1j	0.74	0/732	0.86	0/993
41	2j	0.73	0/723	0.81	0/984
42	1k	0.70	0/849	0.82	0/1150
42	2k	0.67	0/848	0.86	1/1149 (0.1%)
43	1l	0.69	0/937	0.84	0/1260
43	2l	0.68	0/937	0.89	1/1260 (0.1%)
44	1m	0.66	0/924	0.79	0/1242
44	2m	0.70	0/905	0.80	0/1217
45	1n	0.64	0/501	0.87	1/664 (0.2%)
45	2n	0.65	0/501	0.81	1/664 (0.2%)
46	1o	0.72	0/739	0.87	1/985 (0.1%)
46	2o	0.64	0/739	0.79	0/985
47	1p	0.63	0/697	0.86	0/939
47	2p	0.68	0/693	0.91	1/935 (0.1%)
48	1q	0.74	0/836	0.94	3/1117 (0.3%)
48	2q	0.68	0/836	0.92	1/1117 (0.1%)
49	1r	0.69	0/560	0.87	0/746
49	2r	0.70	0/560	0.81	0/746
50	1s	0.61	0/663	0.79	0/895
50	2s	0.72	0/660	0.81	1/893 (0.1%)
51	1t	0.67	0/734	0.88	0/969
51	2t	0.63	0/736	0.86	0/976
52	1u	0.57	0/203	0.73	0/266
52	2u	0.64	0/203	0.79	0/266
53	1x	0.67	0/776	0.78	0/1048
53	2x	0.67	0/761	0.77	0/1030
54	1y	1.01	0/90	1.06	0/122
54	2y	0.88	0/90	0.97	0/122
All	All	1.16	828/310078 (0.3%)	1.66	8429/463412 (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
19	1X	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	2X	0	1
33	1b	0	1
All	All	0	3

All (828) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	354	A	N9-C4	-12.86	1.30	1.37
1	1A	2633	A	N7-C5	-9.63	1.33	1.39
1	1A	2026	G	N7-C5	-9.47	1.33	1.39
1	2A	1046	A	N9-C4	9.45	1.43	1.37
1	1A	2037	A	N3-C4	-9.27	1.29	1.34
1	1A	1377	A	N3-C4	-9.01	1.29	1.34
1	1A	218	A	N9-C4	8.82	1.43	1.37
1	1A	840	A	C5-C6	-8.81	1.33	1.41
1	1A	2069	U	C4-O4	-8.80	1.16	1.23
1	1A	854	U	C2-N3	8.75	1.43	1.37
1	1A	1035	G	C5-C4	-8.69	1.32	1.38
1	1A	1820	A	N9-C4	-8.45	1.32	1.37
1	1A	495	G	N9-C8	-8.44	1.31	1.37
32	1a	1492	A	N9-C4	8.36	1.42	1.37
1	1A	1026	A	N9-C4	-8.28	1.32	1.37
1	1A	251	A	N9-C4	-8.10	1.32	1.37
32	2a	1030(D)	A	N9-C4	8.09	1.42	1.37
1	1A	2082	A	N9-C4	-8.08	1.32	1.37
1	1A	1724	A	N9-C4	-8.06	1.33	1.37
1	2A	573	G	N7-C5	-7.97	1.34	1.39
1	1A	354	A	C5-C6	-7.96	1.33	1.41
32	2a	1034	G	N9-C4	7.96	1.44	1.38
1	1A	2331	G	N3-C4	-7.96	1.29	1.35
32	1a	250	A	N9-C4	7.95	1.42	1.37
1	1A	1235	G	N7-C5	-7.94	1.34	1.39
1	1A	557	A	N9-C4	-7.85	1.33	1.37
1	1A	839	G	C6-N1	-7.85	1.34	1.39
1	1A	752	A	C5-C6	-7.82	1.34	1.41
1	1A	1144	A	N9-C4	7.80	1.42	1.37
1	1A	351	G	N9-C8	-7.80	1.32	1.37
1	1A	1395	A	N3-C4	7.79	1.39	1.34
1	1A	1261	G	N9-C8	-7.77	1.32	1.37
1	1A	1239	A	N7-C5	-7.76	1.34	1.39
1	1A	1959	A	N9-C4	-7.76	1.33	1.37
1	1A	2093	A	N7-C5	-7.76	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1994	A	N9-C4	-7.75	1.33	1.37
1	1A	2601	A	N9-C4	-7.75	1.33	1.37
1	1A	839	G	N1-C2	-7.74	1.31	1.37
1	2A	741	G	N3-C4	-7.72	1.30	1.35
1	2A	1091	G	N9-C4	7.72	1.44	1.38
1	1A	1822	A	N3-C4	-7.71	1.30	1.34
1	1A	2738	A	N3-C4	-7.71	1.30	1.34
1	1A	2257	U	C4-O4	-7.71	1.17	1.23
1	1A	782	A	N3-C4	-7.69	1.30	1.34
1	1A	36	G	N7-C5	-7.58	1.34	1.39
1	1A	823	G	N7-C5	-7.57	1.34	1.39
1	1A	495	G	N7-C5	-7.51	1.34	1.39
1	1A	1177	G	C6-N1	-7.50	1.34	1.39
1	1A	835	A	N7-C5	-7.45	1.34	1.39
1	1A	2777	A	N9-C4	-7.44	1.33	1.37
1	1A	2084	A	N3-C4	7.44	1.39	1.34
1	1A	2724	U	N1-C6	-7.39	1.31	1.38
1	1A	1092	A	N9-C4	7.30	1.42	1.37
1	1A	1301	U	N1-C6	-7.29	1.31	1.38
1	1A	2376	C	N1-C6	-7.26	1.32	1.37
1	1A	2081	A	N3-C4	-7.24	1.30	1.34
32	2a	343	U	C2-N3	-7.24	1.32	1.37
1	1A	1405	A	N7-C5	7.22	1.43	1.39
1	2A	776	G	N7-C5	-7.20	1.34	1.39
1	1A	1272	A	N9-C4	-7.20	1.33	1.37
1	1A	1119	A	N9-C4	7.16	1.42	1.37
1	1A	2441	G	N7-C5	-7.14	1.34	1.39
1	1A	2037	A	N9-C4	-7.13	1.33	1.37
32	1a	148	G	N9-C4	7.13	1.43	1.38
1	1A	561	A	N3-C4	-7.10	1.30	1.34
1	2A	587	C	N1-C6	-7.10	1.32	1.37
1	1A	2068	G	N7-C5	-7.10	1.34	1.39
1	1A	1135	G	N9-C4	7.08	1.43	1.38
1	1A	2663	C	N1-C6	-7.04	1.32	1.37
1	2A	529	A	N9-C4	-7.04	1.33	1.37
1	1A	1455	C	N1-C6	-7.04	1.32	1.37
1	1A	2331	G	N9-C4	-7.04	1.32	1.38
1	1A	1283	A	N3-C4	-7.00	1.30	1.34
1	1A	2081	A	C5-C4	-6.97	1.33	1.38
32	2a	1034	G	C2-N3	6.96	1.38	1.32
10	1O	21	CYS	CB-SG	-6.94	1.70	1.82
1	1A	1307	C	C4-N4	-6.92	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	554	A	N9-C8	6.89	1.43	1.37
1	1A	2405	A	N7-C5	-6.89	1.35	1.39
1	1A	2803	A	N9-C4	6.89	1.42	1.37
1	1A	1054	C	N1-C6	-6.88	1.33	1.37
1	1A	1222	A	N9-C4	6.88	1.42	1.37
1	2A	2805	G	N9-C4	6.86	1.43	1.38
1	2A	2621	A	N9-C4	-6.83	1.33	1.37
1	1A	835	A	N9-C8	-6.83	1.32	1.37
1	1A	553	A	N9-C4	6.82	1.42	1.37
1	1A	101	A	C6-N6	6.78	1.39	1.33
1	1A	356	A	N9-C4	-6.75	1.33	1.37
1	1A	2738	A	N9-C4	-6.74	1.33	1.37
1	1A	1347	A	N9-C4	-6.74	1.33	1.37
1	1A	1809	U	C4-C5	-6.73	1.37	1.43
1	1A	2251	G	N1-C2	-6.73	1.32	1.37
1	1A	519	G	C6-N1	-6.72	1.34	1.39
1	1A	2331	G	N9-C8	6.71	1.42	1.37
32	1a	1034	G	C6-N1	6.71	1.44	1.39
1	1A	1190	G	N1-C2	-6.70	1.32	1.37
1	1A	560	C	C4-N4	-6.70	1.27	1.33
1	1A	840	A	C6-N1	-6.70	1.30	1.35
1	1A	609	A	N3-C4	-6.68	1.30	1.34
1	1A	1816	A	C5-C6	-6.68	1.35	1.41
1	1A	553	A	N7-C5	-6.67	1.35	1.39
1	1A	1648	U	C2-N3	-6.66	1.33	1.37
1	1A	354	A	N9-C8	6.64	1.43	1.37
1	1A	2562	G	N7-C5	-6.63	1.35	1.39
1	1A	2465	A	C6-N6	-6.62	1.28	1.33
32	1a	346	G	C6-N1	6.62	1.44	1.39
1	1A	1014	U	C4-O4	-6.61	1.18	1.23
1	1A	2358	A	N7-C5	-6.60	1.35	1.39
1	1A	1175	A	C6-N1	-6.60	1.30	1.35
1	1A	187	C	N3-C4	-6.59	1.29	1.33
1	1A	1296	G	N1-C2	-6.58	1.32	1.37
1	1A	1127	U	C2-N3	6.58	1.42	1.37
1	1A	1054	C	N3-C4	-6.57	1.29	1.33
1	1A	724	A	N7-C5	-6.57	1.35	1.39
1	1A	550	U	N1-C2	-6.57	1.32	1.38
1	1A	1926	G	N7-C5	-6.57	1.35	1.39
1	1A	476	G	C6-O6	-6.56	1.18	1.24
1	1A	1305	G	C6-N1	-6.56	1.34	1.39
32	2a	1034	G	N3-C4	6.54	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	811	A	N3-C4	-6.53	1.30	1.34
1	1A	596	G	N7-C5	-6.51	1.35	1.39
32	2a	1436	U	C2-N3	6.51	1.42	1.37
1	1A	872	C	N1-C6	-6.50	1.33	1.37
1	1A	795	G	C6-N1	-6.49	1.35	1.39
1	1A	2256	U	C2-N3	-6.49	1.33	1.37
1	1A	1310	G	C6-N1	-6.48	1.35	1.39
1	2A	2821	A	N9-C4	-6.47	1.33	1.37
1	1A	700	A	N3-C4	6.46	1.38	1.34
1	1A	1708	G	C5-C4	-6.46	1.33	1.38
1	1A	1280	U	C2-N3	-6.46	1.33	1.37
32	2a	767	A	N9-C4	-6.45	1.33	1.37
1	1A	1724	A	N3-C4	-6.44	1.30	1.34
1	1A	200	A	C5-C4	-6.43	1.34	1.38
1	1A	484	G	C5-C4	-6.43	1.33	1.38
1	1A	1796	C	N3-C4	-6.42	1.29	1.33
1	1A	1382	A	N3-C4	-6.41	1.31	1.34
32	1a	1493	A	N9-C4	6.41	1.41	1.37
1	1A	2446	A	N7-C5	-6.40	1.35	1.39
1	1A	505	A	N3-C4	-6.40	1.31	1.34
1	1A	2627	U	C2-N3	-6.39	1.33	1.37
1	2A	1378	A	N9-C4	-6.38	1.34	1.37
1	1A	2014	G	C2-N3	-6.37	1.27	1.32
1	1A	2073	A	N7-C5	-6.37	1.35	1.39
1	1A	800	C	N3-C4	-6.36	1.29	1.33
2	1B	1	U	C2-N3	6.36	1.42	1.37
1	1A	218	A	N3-C4	6.35	1.38	1.34
1	1A	829	A	C5-C6	-6.35	1.35	1.41
1	1A	1809	U	C4-O4	-6.35	1.18	1.23
1	1A	2627	U	C2-O2	-6.35	1.16	1.22
1	1A	2879	G	N7-C5	-6.34	1.35	1.39
1	1A	1507	A	N3-C4	6.34	1.38	1.34
1	1A	1112	U	N1-C2	6.34	1.44	1.38
1	1A	2605	U	C2-N3	-6.34	1.33	1.37
1	1A	2277	U	N1-C6	-6.33	1.32	1.38
1	1A	1359	U	C4-O4	-6.33	1.18	1.23
1	2A	675	A	N9-C4	-6.33	1.34	1.37
1	2A	1533	G	C5-C4	6.33	1.42	1.38
1	1A	572	A	N9-C4	6.32	1.41	1.37
1	1A	1666	G	C6-N1	-6.32	1.35	1.39
1	1A	720	C	C2-N3	6.31	1.40	1.35
1	1A	841	G	N9-C8	-6.31	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	598	A	N3-C4	-6.30	1.31	1.34
1	2A	2014	A	N3-C4	-6.30	1.31	1.34
1	1A	710	G	C5-C4	-6.29	1.33	1.38
1	2A	1091	G	N3-C4	6.29	1.39	1.35
1	1A	1993	A	C6-N6	-6.28	1.28	1.33
1	1A	1200	G	N1-C2	-6.28	1.32	1.37
1	1A	2056	U	N3-C4	-6.27	1.32	1.38
1	1A	198	C	N1-C6	-6.27	1.33	1.37
1	1A	1611	C	N3-C4	-6.27	1.29	1.33
1	1A	218	A	C5-C4	6.27	1.43	1.38
1	1A	1667	U	N1-C6	-6.26	1.32	1.38
4	1E	123	ALA	CA-CB	-6.26	1.39	1.52
1	1A	886	U	C4-O4	-6.25	1.18	1.23
1	2A	1269	A	N9-C4	-6.25	1.34	1.37
1	1A	705	C	N1-C6	-6.24	1.33	1.37
32	2a	1003	G	N9-C4	6.24	1.43	1.38
1	1A	1298	G	N9-C4	-6.23	1.32	1.38
1	1A	2803	A	N3-C4	6.23	1.38	1.34
1	1A	884	C	N3-C4	-6.22	1.29	1.33
1	1A	1422	C	N3-C4	-6.22	1.29	1.33
1	1A	199	C	N1-C2	-6.21	1.33	1.40
1	2A	2249	U	C2-N3	-6.21	1.33	1.37
1	1A	828	A	C5-C4	-6.20	1.34	1.38
1	1A	1116	A	N9-C4	6.20	1.41	1.37
1	1A	1027	A	N9-C4	-6.20	1.34	1.37
1	1A	2106	C	N3-C4	-6.20	1.29	1.33
1	2A	1652	A	N9-C4	-6.20	1.34	1.37
1	1A	225	C	C2-N3	-6.19	1.30	1.35
1	1A	1829	U	C2-N3	-6.19	1.33	1.37
1	1A	2691	A	C6-N6	-6.19	1.28	1.33
1	1A	1317	G	N3-C4	6.18	1.39	1.35
1	1A	1356	G	C6-N1	-6.18	1.35	1.39
1	1A	557	A	C6-N1	-6.18	1.31	1.35
1	2A	2207	G	N9-C8	-6.18	1.33	1.37
1	2A	1076	C	N1-C2	6.17	1.46	1.40
1	2A	1670	C	N1-C6	-6.17	1.33	1.37
1	1A	1113	A	N9-C4	6.17	1.41	1.37
32	1a	144	G	N9-C4	6.16	1.42	1.38
1	1A	2037	A	C5-C4	-6.16	1.34	1.38
1	1A	2055	A	N3-C4	-6.15	1.31	1.34
1	2A	528	A	N7-C5	-6.14	1.35	1.39
32	1a	780	A	N9-C4	-6.13	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	670	C	N1-C6	6.13	1.40	1.37
1	1A	2526	U	C2-N3	-6.13	1.33	1.37
1	1A	2277	U	N1-C2	-6.13	1.33	1.38
1	1A	808	A	N7-C5	-6.13	1.35	1.39
1	1A	2403	G	C6-N1	-6.13	1.35	1.39
1	1A	1130	A	C5-C6	6.12	1.46	1.41
1	1A	2453	C	C4-N4	-6.12	1.28	1.33
1	1A	1988	A	C5-C4	-6.12	1.34	1.38
1	1A	2785	C	N3-C4	-6.12	1.29	1.33
1	1A	1708	G	C2-N3	-6.12	1.27	1.32
32	2a	569	C	N1-C6	-6.12	1.33	1.37
1	1A	590	A	C8-N7	6.11	1.35	1.31
1	1A	848	G	C6-N1	-6.11	1.35	1.39
1	1A	2457	G	N9-C8	-6.11	1.33	1.37
1	2A	2014	A	N9-C4	-6.11	1.34	1.37
1	1A	848	G	N9-C8	-6.11	1.33	1.37
1	1A	528	A	N3-C4	-6.11	1.31	1.34
1	1A	537	G	N7-C5	-6.10	1.35	1.39
1	1A	1613	A	N3-C4	6.10	1.38	1.34
1	1A	2062	C	C4-C5	-6.10	1.38	1.43
1	1A	594	A	C5-C4	-6.10	1.34	1.38
1	1A	2139	A	N9-C4	6.10	1.41	1.37
1	2A	944	G	N9-C8	-6.10	1.33	1.37
1	1A	1822	A	C6-N1	-6.09	1.31	1.35
1	1A	488	C	N1-C6	-6.08	1.33	1.37
1	2A	2441	C	N3-C4	-6.08	1.29	1.33
1	2A	2177	C	N1-C6	6.07	1.40	1.37
1	1A	1727	U	C4-O4	-6.07	1.18	1.23
32	1a	204	U	N1-C2	6.07	1.44	1.38
1	1A	1202	A	N9-C4	-6.06	1.34	1.37
1	1A	720	C	N3-C4	6.05	1.38	1.33
1	1A	1833	A	N7-C5	-6.04	1.35	1.39
1	1A	1130	A	N7-C5	6.04	1.42	1.39
1	1A	2526	U	N3-C4	-6.04	1.33	1.38
1	1A	1838	G	N9-C4	-6.04	1.33	1.38
1	2A	1972	A	N9-C4	-6.04	1.34	1.37
1	1A	555	G	N1-C2	-6.03	1.32	1.37
1	1A	1035	G	N9-C8	-6.03	1.33	1.37
32	2a	1027	C	N1-C2	6.01	1.46	1.40
1	1A	2619	G	N7-C5	-6.01	1.35	1.39
1	1A	1537	G	N9-C8	-6.00	1.33	1.37
1	1A	2134	G	C2-N3	6.00	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1177	G	N1-C2	-6.00	1.32	1.37
1	1A	1249	A	C5-C6	-6.00	1.35	1.41
1	1A	168	G	N3-C4	-5.99	1.31	1.35
1	1A	919	A	N3-C4	-5.99	1.31	1.34
32	1a	1044	A	N9-C4	5.99	1.41	1.37
1	1A	178	G	N7-C5	-5.99	1.35	1.39
1	1A	351	G	N7-C5	-5.98	1.35	1.39
2	1B	98	G	N7-C5	-5.98	1.35	1.39
32	1a	1436	U	C2-N3	5.98	1.42	1.37
1	1A	2057	G	N9-C4	-5.98	1.33	1.38
1	2A	1070	A	N9-C4	5.98	1.41	1.37
12	1Q	35	VAL	CB-CG1	-5.97	1.40	1.52
1	1A	554	A	C6-N1	5.97	1.39	1.35
1	1A	2054	G	N3-C4	-5.97	1.31	1.35
1	1A	731	G	C5-C4	-5.97	1.34	1.38
1	1A	1080	G	C5-C4	-5.96	1.34	1.38
32	1a	1256	A	N9-C4	5.96	1.41	1.37
1	1A	187	C	N1-C6	-5.96	1.33	1.37
1	2A	2114	A	C5-C4	5.95	1.43	1.38
1	1A	996	C	N3-C4	-5.95	1.29	1.33
1	2A	1308	A	N3-C4	-5.95	1.31	1.34
1	1A	2407	C	C4-N4	-5.94	1.28	1.33
1	1A	167	G	N3-C4	-5.93	1.31	1.35
1	2A	6	A	N9-C4	5.93	1.41	1.37
30	18	56	GLU	CG-CD	5.93	1.60	1.51
1	1A	199	C	N1-C6	-5.93	1.33	1.37
1	1A	1244	U	C2-N3	-5.92	1.33	1.37
1	1A	13	A	N7-C5	-5.92	1.35	1.39
1	1A	883	G	C6-N1	-5.91	1.35	1.39
1	1A	2283	G	N7-C5	-5.91	1.35	1.39
32	1a	161	A	N9-C4	5.91	1.41	1.37
1	1A	124	A	N3-C4	-5.91	1.31	1.34
1	1A	474	U	N3-C4	-5.90	1.33	1.38
1	1A	1679	A	N7-C5	-5.90	1.35	1.39
1	1A	1031	C	N1-C6	5.90	1.40	1.37
32	1a	1493	A	N3-C4	5.90	1.38	1.34
1	1A	1304	C	N1-C6	-5.89	1.33	1.37
1	1A	1983	C	N1-C6	-5.89	1.33	1.37
32	1a	814	A	N9-C4	-5.89	1.34	1.37
1	1A	1507	A	N9-C4	5.89	1.41	1.37
1	1A	2187	G	N7-C5	5.89	1.42	1.39
1	1A	1075	A	N7-C5	-5.88	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	439	A	N9-C4	-5.88	1.34	1.37
1	2A	2117	A	N9-C4	5.88	1.41	1.37
1	1A	590	A	N9-C4	-5.88	1.34	1.37
1	1A	785	G	N3-C4	-5.88	1.31	1.35
1	1A	2584	A	C5-C4	-5.87	1.34	1.38
1	1A	2261	U	C2-N3	-5.87	1.33	1.37
1	1A	122	G	C5-C6	-5.87	1.36	1.42
1	1A	1911	A	N9-C4	-5.87	1.34	1.37
1	1A	716	G	C2-N3	-5.87	1.28	1.32
32	1a	1026	G	N7-C5	5.87	1.42	1.39
1	1A	2538	G	C5-C4	-5.86	1.34	1.38
1	1A	811	A	C6-N1	-5.85	1.31	1.35
1	1A	1394	G	C5-C4	-5.85	1.34	1.38
1	1A	1640	G	N3-C4	-5.85	1.31	1.35
1	1A	2520	G	N9-C8	-5.84	1.33	1.37
1	1A	795	G	C6-O6	-5.84	1.18	1.24
1	1A	1102	G	N3-C4	5.84	1.39	1.35
1	1A	1472	G	C5-C6	-5.83	1.36	1.42
16	1U	4	ALA	CA-CB	-5.82	1.40	1.52
1	1A	2258	G	N9-C8	-5.82	1.33	1.37
1	1A	2595	G	N9-C8	-5.82	1.33	1.37
1	1A	1235	G	N9-C8	-5.81	1.33	1.37
16	1U	69	CYS	CB-SG	-5.81	1.72	1.81
1	1A	173	C	N1-C6	-5.81	1.33	1.37
32	1a	1021	G	N9-C4	5.81	1.42	1.38
1	1A	829	A	N7-C5	-5.80	1.35	1.39
1	1A	622	G	C5-C4	-5.80	1.34	1.38
1	1A	1232	G	C6-O6	-5.80	1.19	1.24
1	1A	353	G	C8-N7	-5.80	1.27	1.30
1	1A	2717	A	N9-C4	-5.80	1.34	1.37
1	1A	2451	A	N3-C4	5.79	1.38	1.34
1	1A	2271	G	C5-C4	-5.79	1.34	1.38
1	1A	1840	A	C6-N6	-5.78	1.29	1.33
1	2A	2007	C	N3-C4	-5.78	1.29	1.33
1	1A	2134	G	N9-C4	5.77	1.42	1.38
1	1A	2443	U	C2-N3	-5.77	1.33	1.37
1	1A	811	A	C5-C4	-5.77	1.34	1.38
1	1A	1816	A	C6-N1	-5.77	1.31	1.35
32	1a	1033	G	N3-C4	5.76	1.39	1.35
1	1A	494	G	C6-N1	-5.76	1.35	1.39
1	1A	841	G	N3-C4	5.76	1.39	1.35
1	2A	2805	G	C5-C6	5.76	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1034	G	C6-N1	5.75	1.43	1.39
2	1B	38	C	N3-C4	-5.75	1.29	1.33
6	1G	29	TRP	CB-CG	-5.75	1.40	1.50
1	1A	2652	G	N3-C4	-5.74	1.31	1.35
1	1A	1424	A	N9-C4	-5.74	1.34	1.37
32	1a	804	U	C2-O2	-5.74	1.17	1.22
1	1A	1723	A	C5-C6	-5.74	1.35	1.41
1	1A	521	G	N7-C5	-5.73	1.35	1.39
1	1A	1237	G	N3-C4	-5.73	1.31	1.35
1	1A	1321	A	N7-C5	-5.73	1.35	1.39
1	1A	1112	U	C2-N3	5.73	1.41	1.37
1	1A	2898	C	N3-C4	-5.73	1.29	1.33
1	1A	751	G	N3-C4	-5.73	1.31	1.35
32	1a	163	C	N1-C6	5.72	1.40	1.37
32	2a	764	C	N3-C4	-5.72	1.29	1.33
1	1A	882	A	N3-C4	-5.72	1.31	1.34
1	1A	2454	C	C5-C6	-5.72	1.29	1.34
1	2A	459	U	C2-N3	-5.72	1.33	1.37
1	1A	2405	A	N9-C8	-5.71	1.33	1.37
1	1A	499	G	N1-C2	-5.71	1.33	1.37
1	2A	2160	G	N9-C4	5.71	1.42	1.38
1	1A	2074	G	N7-C5	-5.70	1.35	1.39
1	1A	1037	C	N3-C4	-5.70	1.29	1.33
1	1A	1822	A	N9-C4	-5.69	1.34	1.37
1	1A	1447	G	C6-O6	5.69	1.29	1.24
1	2A	1794	U	C2-N3	-5.69	1.33	1.37
1	1A	2157	A	N9-C4	5.69	1.41	1.37
27	15	35	GLU	CG-CD	5.69	1.60	1.51
1	1A	798	A	N3-C4	-5.69	1.31	1.34
1	1A	182	U	C2-N3	-5.68	1.33	1.37
32	2a	346	G	C6-N1	5.68	1.43	1.39
1	1A	1349	G	C2-N3	-5.67	1.28	1.32
1	2A	12	U	N1-C2	5.67	1.43	1.38
1	1A	2514	G	C6-N1	-5.67	1.35	1.39
1	1A	668	A	N9-C8	-5.67	1.33	1.37
1	1A	1679	A	N3-C4	-5.67	1.31	1.34
32	1a	732	C	N3-C4	-5.67	1.29	1.33
1	1A	2561	G	N3-C4	-5.67	1.31	1.35
1	2A	1296	G	N1-C2	-5.67	1.33	1.37
1	1A	825	G	N7-C5	-5.66	1.35	1.39
1	1A	1132	A	N9-C4	5.66	1.41	1.37
1	1A	710	G	C6-N1	-5.66	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	888	A	N7-C5	-5.65	1.35	1.39
1	1A	569	G	N9-C8	5.65	1.41	1.37
1	1A	1741	C	N1-C6	-5.65	1.33	1.37
8	1I	10	GLU	CB-CG	5.65	1.62	1.52
1	1A	1801	G	N3-C4	-5.65	1.31	1.35
2	1B	57	A	N7-C5	-5.64	1.35	1.39
1	2A	639	U	C2-N3	-5.64	1.33	1.37
1	2A	1082	U	N1-C2	5.64	1.43	1.38
1	1A	398	A	N9-C4	-5.63	1.34	1.37
1	1A	184	A	N9-C4	-5.63	1.34	1.37
2	1B	108	U	C2-N3	-5.62	1.33	1.37
1	1A	1026	A	C6-N6	-5.62	1.29	1.33
1	1A	865	G	C6-N1	-5.62	1.35	1.39
1	1A	1281	G	N1-C2	-5.62	1.33	1.37
1	1A	1707	C	N3-C4	-5.62	1.30	1.33
32	1a	1530	G	C6-N1	5.62	1.43	1.39
1	1A	1475	G	N1-C2	-5.61	1.33	1.37
32	2a	1499	A	N9-C4	-5.61	1.34	1.37
1	1A	196	A	C5-C6	-5.61	1.36	1.41
1	1A	2469	U	C4-C5	-5.61	1.38	1.43
1	1A	2579	G	C5-C4	-5.61	1.34	1.38
1	2A	747	U	N1-C2	-5.61	1.33	1.38
1	1A	2784	C	N3-C4	-5.61	1.30	1.33
1	2A	126	A	N9-C4	-5.61	1.34	1.37
1	1A	1202	A	N3-C4	-5.60	1.31	1.34
1	1A	2042	A	C6-N6	-5.60	1.29	1.33
1	1A	840	A	C6-N6	-5.60	1.29	1.33
1	1A	1683	C	N1-C6	-5.60	1.33	1.37
1	1A	2129	C	N1-C6	5.60	1.40	1.37
1	1A	2828	G	C6-N1	-5.59	1.35	1.39
32	1a	250	A	C5-C4	5.59	1.42	1.38
32	2a	1227	A	N9-C4	-5.59	1.34	1.37
1	1A	2024	G	C8-N7	-5.59	1.27	1.30
1	1A	729	G	C6-N1	-5.59	1.35	1.39
1	1A	1117	G	N9-C4	5.59	1.42	1.38
1	1A	2465	A	C6-N1	-5.59	1.31	1.35
1	1A	1720	U	N1-C2	-5.58	1.33	1.38
1	1A	2014	G	N1-C2	-5.58	1.33	1.37
1	1A	2234	G	N9-C8	-5.58	1.33	1.37
32	1a	1417	G	C6-O6	-5.58	1.19	1.24
1	2A	1537	G	N9-C4	5.58	1.42	1.38
1	1A	1660	A	N7-C5	-5.58	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	190	C	N1-C6	-5.58	1.33	1.37
1	1A	813	C	N1-C6	-5.58	1.33	1.37
1	1A	403	C	N3-C4	-5.57	1.30	1.33
1	1A	1795	G	N7-C5	-5.57	1.35	1.39
1	1A	2780	C	N3-C4	-5.57	1.30	1.33
1	2A	1067	A	N9-C4	5.57	1.41	1.37
32	1a	70	G	C5-C4	5.57	1.42	1.38
1	1A	1321	A	C2-N3	-5.57	1.28	1.33
1	1A	2075	G	N3-C4	-5.56	1.31	1.35
1	1A	2251	G	C6-N1	-5.55	1.35	1.39
1	2A	2177	C	N1-C2	5.55	1.45	1.40
1	1A	2687	A	C5-C4	-5.55	1.34	1.38
1	1A	1417	G	N7-C5	-5.55	1.35	1.39
1	1A	2707	C	C4-N4	-5.54	1.28	1.33
1	1A	859	C	C4-N4	-5.54	1.28	1.33
27	15	59	GLU	CG-CD	5.54	1.60	1.51
1	1A	1456	G	N3-C4	-5.54	1.31	1.35
1	1A	773	G	C5-C6	-5.54	1.36	1.42
1	1A	2026	G	C5-C6	-5.54	1.36	1.42
1	2A	1803	A	N3-C4	-5.54	1.31	1.34
32	1a	1512	U	C2-N3	-5.54	1.33	1.37
1	2A	807	U	C2-N3	5.54	1.41	1.37
1	1A	1282	G	C5-C4	-5.53	1.34	1.38
1	1A	2234	G	N9-C4	-5.53	1.33	1.38
1	1A	645	G	N9-C8	-5.53	1.33	1.37
32	2a	1149	C	N1-C6	5.53	1.40	1.37
1	1A	409	G	C6-N1	-5.53	1.35	1.39
1	2A	2087	G	C5-C4	-5.53	1.34	1.38
1	1A	20	C	N3-C4	-5.53	1.30	1.33
1	1A	747	G	N9-C8	-5.53	1.33	1.37
1	1A	1656	A	N9-C4	-5.52	1.34	1.37
18	1W	20	VAL	CB-CG2	-5.52	1.41	1.52
1	1A	1075	A	C5-C6	-5.52	1.36	1.41
1	1A	1021	G	C2-N3	-5.52	1.28	1.32
1	1A	1707	C	C2-O2	-5.52	1.19	1.24
1	1A	2629	C	N1-C2	-5.52	1.34	1.40
1	1A	539	A	N9-C8	-5.51	1.33	1.37
1	1A	1048	G	C2-N3	-5.51	1.28	1.32
3	1D	221	VAL	CB-CG2	-5.51	1.41	1.52
1	1A	1314	A	N7-C5	-5.51	1.35	1.39
1	1A	1718	U	C4-O4	-5.51	1.19	1.23
1	2A	2454	G	C6-N1	-5.51	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2607	G	N1-C2	-5.50	1.33	1.37
1	1A	817	G	C6-N1	-5.50	1.35	1.39
1	2A	1963	U	N1-C2	5.50	1.43	1.38
1	1A	178	G	N9-C4	-5.50	1.33	1.38
1	1A	1299	A	N7-C5	-5.50	1.35	1.39
1	1A	2506	G	C6-N1	-5.49	1.35	1.39
1	1A	1672	G	N9-C8	-5.49	1.34	1.37
1	2A	126	A	N3-C4	-5.49	1.31	1.34
1	1A	1026	A	C5-C6	-5.49	1.36	1.41
1	1A	1076	G	C5-C4	-5.49	1.34	1.38
1	1A	1518	A	N9-C4	5.49	1.41	1.37
1	1A	2184	G	N9-C4	5.49	1.42	1.38
1	1A	2789	A	C6-N1	-5.49	1.31	1.35
1	1A	2791	A	N9-C8	-5.49	1.33	1.37
8	1I	10	GLU	CG-CD	5.49	1.60	1.51
1	2A	2801(A)	A	N9-C4	5.48	1.41	1.37
1	2A	1353	A	N9-C4	-5.48	1.34	1.37
1	1A	1280	U	C2-O2	-5.48	1.17	1.22
32	1a	300	A	C5-C6	-5.47	1.36	1.41
1	1A	652	A	C5-C4	-5.47	1.34	1.38
1	1A	836	A	N7-C5	-5.47	1.35	1.39
1	1A	733	G	C5-C6	-5.47	1.36	1.42
1	1A	1181	G	N9-C8	-5.47	1.34	1.37
1	1A	1347	A	N3-C4	-5.46	1.31	1.34
1	1A	2415	C	N1-C6	-5.46	1.33	1.37
1	2A	1142(A)	A	N7-C5	-5.46	1.35	1.39
1	1A	2724	U	C4-C5	-5.46	1.38	1.43
1	1A	1721	G	N9-C8	-5.46	1.34	1.37
1	1A	323	A	C6-N1	-5.45	1.31	1.35
1	1A	2076	A	N7-C5	-5.45	1.35	1.39
1	1A	2024	G	C5-C4	-5.45	1.34	1.38
1	2A	1721	G	N3-C4	5.45	1.39	1.35
1	2A	2207	G	N7-C5	-5.45	1.35	1.39
1	1A	1834	A	N7-C5	-5.45	1.35	1.39
1	1A	1336	C	C2-O2	-5.44	1.19	1.24
1	1A	1055	A	C5-C6	-5.44	1.36	1.41
1	1A	1371	G	N9-C8	-5.44	1.34	1.37
1	2A	2589	A	N9-C4	-5.44	1.34	1.37
1	1A	2622	C	N1-C6	-5.44	1.33	1.37
28	16	16	CYS	CB-SG	-5.44	1.73	1.81
1	2A	789	A	N7-C5	-5.43	1.35	1.39
1	2A	1353	A	N3-C4	-5.43	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2251	G	C5-C4	-5.43	1.34	1.38
1	1A	1087	C	N1-C6	5.43	1.40	1.37
1	1A	1690	G	C5-C4	-5.43	1.34	1.38
1	1A	2187	G	C5-C6	5.43	1.47	1.42
1	1A	2579	G	N7-C5	5.43	1.42	1.39
1	1A	806	G	N3-C4	-5.43	1.31	1.35
32	1a	1024	G	N3-C4	5.43	1.39	1.35
1	1A	1043	G	C6-N1	-5.42	1.35	1.39
1	1A	1656	A	C5-C6	-5.42	1.36	1.41
1	1A	1310	G	C6-O6	-5.42	1.19	1.24
1	1A	2634	C	C4-N4	-5.42	1.29	1.33
1	1A	1707	C	C4-N4	-5.42	1.29	1.33
1	2A	1108	U	C2-N3	5.42	1.41	1.37
1	1A	607	C	C4-C5	-5.41	1.38	1.43
1	1A	792	G	C5-C6	-5.41	1.36	1.42
1	1A	885	C	C4-N4	-5.41	1.29	1.33
32	1a	1024	G	N9-C4	5.41	1.42	1.38
6	2G	167	GLU	CG-CD	5.41	1.60	1.51
1	1A	2635	G	N3-C4	-5.41	1.31	1.35
1	2A	2148	G	N9-C4	5.41	1.42	1.38
2	1B	76	G	N9-C8	-5.41	1.34	1.37
1	1A	239	G	N3-C4	-5.40	1.31	1.35
1	1A	2256	U	N3-C4	-5.40	1.33	1.38
1	1A	1313	U	P-OP1	-5.40	1.39	1.49
1	2A	1051	G	C6-N1	5.40	1.43	1.39
1	1A	1402	G	N9-C8	-5.40	1.34	1.37
1	1A	2048	C	N1-C6	-5.39	1.33	1.37
1	1A	2289	G	N9-C8	-5.39	1.34	1.37
1	1A	2775	G	C5-C4	-5.39	1.34	1.38
1	1A	729	G	C5-C4	-5.39	1.34	1.38
1	1A	979	G	C5-C4	-5.39	1.34	1.38
1	1A	2082	A	C6-N1	-5.39	1.31	1.35
1	2A	1091	G	P-O5'	5.39	1.65	1.59
17	1V	53	GLU	CG-CD	5.39	1.60	1.51
32	1a	1021	G	N3-C4	5.38	1.39	1.35
1	1A	722	A	C6-N6	-5.38	1.29	1.33
1	1A	1640	G	C2-N3	-5.38	1.28	1.32
1	1A	2835	C	N1-C6	-5.38	1.33	1.37
3	1D	199	ALA	CA-CB	-5.38	1.41	1.52
1	2A	2454	G	N3-C4	-5.38	1.31	1.35
32	2a	190	U	C2-N3	5.38	1.41	1.37
1	1A	896	A	N9-C8	-5.37	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1833	A	N9-C4	-5.37	1.34	1.37
32	2a	1035	A	N9-C4	5.37	1.41	1.37
1	1A	1830	G	C5-C4	-5.37	1.34	1.38
32	1a	156	G	N9-C8	5.37	1.41	1.37
1	1A	117	A	N9-C4	-5.36	1.34	1.37
1	2A	733	G	N7-C5	-5.36	1.36	1.39
1	1A	957	A	C6-N1	-5.36	1.31	1.35
1	1A	2693	C	N1-C6	-5.36	1.33	1.37
1	1A	1347	A	P-O5'	-5.36	1.54	1.59
1	2A	1901	A	N3-C4	-5.36	1.31	1.34
1	1A	2395	G	N3-C4	-5.36	1.31	1.35
1	1A	2102	G	N9-C8	-5.36	1.34	1.37
32	1a	1041	A	N3-C4	5.35	1.38	1.34
1	1A	737	G	C5-C4	-5.35	1.34	1.38
1	1A	864	C	N1-C6	-5.35	1.33	1.37
1	1A	1639	G	C5-C4	-5.35	1.34	1.38
1	1A	1655	A	C5-C6	-5.35	1.36	1.41
1	1A	2818	U	C2-N3	5.35	1.41	1.37
1	2A	2805	G	C5-C4	5.35	1.42	1.38
1	1A	780	G	C6-N1	-5.35	1.35	1.39
1	1A	1294	G	C6-O6	5.34	1.28	1.24
1	1A	361	C	N1-C6	-5.34	1.33	1.37
1	1A	833	C	N3-C4	-5.34	1.30	1.33
1	2A	678	C	N3-C4	-5.34	1.30	1.33
1	2A	776	G	C5-C6	-5.34	1.37	1.42
1	2A	2087	G	N3-C4	-5.34	1.31	1.35
1	1A	619	G	N1-C2	-5.34	1.33	1.37
1	1A	722	A	C5-C6	-5.34	1.36	1.41
1	1A	1172	A	N9-C4	-5.34	1.34	1.37
1	1A	700	A	C6-N1	5.33	1.39	1.35
1	1A	2341	G	C5-C4	-5.33	1.34	1.38
1	1A	2403	G	N1-C2	-5.33	1.33	1.37
32	1a	1417	G	C5-C6	-5.33	1.37	1.42
1	2A	591	C	N1-C6	-5.33	1.33	1.37
32	2a	1370	G	N3-C4	5.32	1.39	1.35
1	1A	724	A	N9-C8	-5.32	1.33	1.37
32	2a	1157	A	N9-C4	5.32	1.41	1.37
1	1A	598	A	N9-C4	-5.32	1.34	1.37
1	1A	2882	G	C2-N3	5.32	1.37	1.32
1	1A	1106	U	C2-N3	5.32	1.41	1.37
1	1A	1716	A	N3-C4	-5.31	1.31	1.34
1	1A	483	A	N9-C8	-5.31	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2119	A	N9-C4	5.31	1.41	1.37
1	1A	1316	C	C4-N4	-5.31	1.29	1.33
1	1A	1617	A	C5-C6	-5.31	1.36	1.41
32	1a	1035	A	N3-C4	5.31	1.38	1.34
1	2A	1846	G	N9-C4	-5.31	1.33	1.38
1	2A	1597	A	N9-C4	-5.31	1.34	1.37
1	1A	225	C	C2-O2	-5.30	1.19	1.24
1	1A	966	G	N7-C5	-5.30	1.36	1.39
1	1A	2625	U	C2-N3	-5.30	1.34	1.37
1	2A	1088	A	N9-C4	5.30	1.41	1.37
1	1A	1846	A	N3-C4	-5.30	1.31	1.34
1	1A	2450	U	C4-O4	-5.30	1.19	1.23
1	2A	479	A	N3-C4	-5.30	1.31	1.34
1	1A	519	G	N1-C2	-5.29	1.33	1.37
1	1A	822	G	N9-C4	-5.29	1.33	1.38
1	1A	831	A	N9-C4	-5.29	1.34	1.37
1	1A	1706	U	C2-O2	-5.29	1.17	1.22
1	1A	2628	C	N3-C4	-5.29	1.30	1.33
1	1A	38	A	C5-C4	-5.28	1.35	1.38
1	1A	2014	G	C5-C4	-5.28	1.34	1.38
1	1A	118	U	N1-C2	-5.28	1.33	1.38
1	1A	2469	U	C4-O4	-5.28	1.19	1.23
1	1A	2472	U	C2-N3	-5.28	1.34	1.37
32	1a	346	G	N9-C4	5.28	1.42	1.38
1	2A	1074	G	N3-C4	5.28	1.39	1.35
1	1A	560	C	C4-C5	-5.28	1.38	1.43
1	2A	2775	A	N9-C4	-5.27	1.34	1.37
32	2a	204	U	N1-C2	5.27	1.43	1.38
32	2a	1001	A	C5-C6	5.27	1.45	1.41
1	1A	1007	G	N1-C2	-5.27	1.33	1.37
32	2a	993	G	N9-C4	5.27	1.42	1.38
1	2A	1563	G	N7-C5	-5.26	1.36	1.39
1	1A	2611	G	N1-C2	-5.26	1.33	1.37
1	1A	833	C	C4-N4	-5.26	1.29	1.33
1	1A	1597	C	N1-C6	-5.26	1.33	1.37
1	2A	1036	G	C6-N1	5.26	1.43	1.39
1	1A	1386	U	C4-O4	-5.26	1.19	1.23
32	1a	1169	A	N9-C4	5.26	1.41	1.37
32	2a	1026	G	C5-C4	5.26	1.42	1.38
32	2a	1027	C	N1-C6	5.26	1.40	1.37
1	1A	1135	G	C5-C4	5.25	1.42	1.38
1	1A	2778	A	N7-C5	-5.25	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	821	A	N1-C2	-5.25	1.29	1.34
1	2A	1264	G	N9-C8	-5.25	1.34	1.37
1	1A	55	A	C5-C6	-5.25	1.36	1.41
1	1A	601	A	N7-C5	-5.25	1.36	1.39
1	1A	707	G	C5-C4	-5.25	1.34	1.38
32	1a	346	G	N7-C5	5.24	1.42	1.39
1	1A	460	C	N3-C4	-5.24	1.30	1.33
1	1A	610	C	C2-N3	-5.24	1.31	1.35
1	1A	773	G	C6-N1	-5.24	1.35	1.39
1	1A	801	C	N3-C4	5.24	1.37	1.33
1	1A	2041	A	C6-N6	-5.24	1.29	1.33
32	1a	1513	A	C5-C4	-5.24	1.35	1.38
1	1A	2358	A	N9-C8	-5.24	1.33	1.37
1	2A	1091	G	C5-C4	5.23	1.42	1.38
1	1A	1674	G	N1-C2	-5.23	1.33	1.37
1	1A	2051	G	N9-C8	-5.23	1.34	1.37
1	1A	1727	U	C4-C5	-5.23	1.38	1.43
1	1A	1960	A	N9-C4	-5.23	1.34	1.37
1	1A	2467	G	N7-C5	-5.23	1.36	1.39
1	1A	69	G	C6-N1	-5.22	1.35	1.39
1	1A	2254	G	N7-C5	-5.22	1.36	1.39
1	2A	2510	C	N3-C4	-5.22	1.30	1.33
1	1A	1417	G	N9-C8	-5.22	1.34	1.37
1	1A	2279	A	C8-N7	-5.22	1.27	1.31
32	1a	349	A	N9-C4	5.22	1.41	1.37
1	1A	477	C	N1-C6	-5.22	1.34	1.37
1	1A	802	C	C4-N4	-5.22	1.29	1.33
1	1A	1803	G	N9-C8	-5.22	1.34	1.37
1	1A	2530	A	N7-C5	-5.22	1.36	1.39
1	2A	2160	G	C5-C4	5.21	1.42	1.38
1	1A	1361	C	C2-O2	-5.21	1.19	1.24
32	2a	51	A	N7-C5	-5.21	1.36	1.39
1	1A	836	A	N9-C4	-5.20	1.34	1.37
1	1A	1025	G	N1-C2	-5.20	1.33	1.37
1	1A	1786	A	N7-C5	-5.20	1.36	1.39
32	1a	299	G	C6-O6	-5.20	1.19	1.24
27	25	49	CYS	CB-SG	-5.20	1.73	1.81
1	2A	1932	A	N9-C4	-5.20	1.34	1.37
1	1A	1104	G	N3-C4	5.20	1.39	1.35
1	1A	554	A	N3-C4	-5.19	1.31	1.34
1	1A	1370	G	N1-C2	-5.19	1.33	1.37
1	1A	2464	C	N1-C6	-5.19	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2697	G	N9-C8	-5.19	1.34	1.37
29	17	5	TRP	CB-CG	-5.19	1.41	1.50
1	1A	354	A	N7-C5	-5.19	1.36	1.39
1	1A	1672	G	C5-C4	-5.18	1.34	1.38
32	2a	1033	G	C6-N1	5.18	1.43	1.39
1	1A	1282	G	N1-C2	-5.18	1.33	1.37
1	2A	2143	C	N1-C2	5.18	1.45	1.40
1	1A	1204	C	N3-C4	-5.18	1.30	1.33
1	2A	586	A	N3-C4	-5.18	1.31	1.34
1	2A	2106	G	N9-C4	5.18	1.42	1.38
1	1A	271	U	N1-C6	5.18	1.42	1.38
1	1A	1312	G	C5-C6	-5.18	1.37	1.42
1	1A	2061	C	C4-C5	-5.18	1.38	1.43
1	1A	2850	C	N1-C6	-5.18	1.34	1.37
1	2A	472	A	N3-C4	-5.17	1.31	1.34
1	2A	2434	A	C5-C4	-5.17	1.35	1.38
32	2a	1014	A	N9-C4	5.17	1.41	1.37
1	1A	319	G	N7-C5	-5.17	1.36	1.39
1	1A	2081	A	C6-N1	-5.17	1.31	1.35
32	2a	908	A	N9-C4	-5.17	1.34	1.37
1	1A	1092	A	N3-C4	5.17	1.38	1.34
1	1A	1672	G	C2-N3	-5.17	1.28	1.32
1	1A	1957	G	C2-N3	-5.17	1.28	1.32
1	1A	2585	C	C4-C5	-5.16	1.38	1.43
1	1A	1092	A	C5-C4	5.16	1.42	1.38
1	2A	2805	G	N3-C4	5.16	1.39	1.35
1	1A	2264	G	C5-C4	-5.15	1.34	1.38
32	1a	1276	G	C5-C4	5.15	1.42	1.38
1	2A	2143	C	N1-C6	5.15	1.40	1.37
1	1A	1019	G	C6-N1	-5.15	1.35	1.39
1	1A	1261	G	C5-C4	-5.15	1.34	1.38
32	2a	1452	C	N1-C2	5.15	1.45	1.40
1	1A	1112	U	N1-C6	5.15	1.42	1.38
1	2A	1678	G	N7-C5	-5.15	1.36	1.39
1	1A	821	A	N3-C4	-5.14	1.31	1.34
1	1A	2709	G	N7-C5	-5.14	1.36	1.39
1	1A	2075	G	C5-C4	-5.14	1.34	1.38
1	1A	933	C	N1-C6	5.14	1.40	1.37
32	1a	1507	A	N7-C5	-5.14	1.36	1.39
1	2A	2805	G	N7-C5	5.13	1.42	1.39
1	1A	2398	C	C4-C5	-5.13	1.38	1.43
1	1A	1690	G	N1-C2	-5.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1054	C	C4-C5	-5.12	1.38	1.43
1	1A	2476	C	C4-C5	-5.12	1.38	1.43
1	2A	1335	U	C4-O4	-5.12	1.19	1.23
1	2A	2140	C	N1-C6	5.12	1.40	1.37
1	1A	1986	G	C5-C6	-5.12	1.37	1.42
1	2A	1767	C	N3-C4	-5.12	1.30	1.33
1	1A	1831	C	N3-C4	-5.11	1.30	1.33
1	1A	787	U	C4-O4	-5.11	1.19	1.23
1	1A	110	U	N1-C2	-5.11	1.33	1.38
1	1A	2289	G	N7-C5	-5.11	1.36	1.39
1	1A	2436	C	N1-C2	-5.11	1.35	1.40
1	1A	215	G	C2-N3	-5.11	1.28	1.32
1	1A	1043	G	N1-C2	-5.11	1.33	1.37
1	1A	1790	A	C5-C6	-5.11	1.36	1.41
1	1A	2580	C	N1-C6	-5.11	1.34	1.37
1	1A	2582	G	N9-C8	-5.11	1.34	1.37
20	1Y	34	LYS	CD-CE	5.11	1.64	1.51
1	1A	1148	C	N1-C2	5.10	1.45	1.40
1	2A	1046	A	N3-C4	5.10	1.38	1.34
1	1A	1692	G	N9-C4	5.10	1.42	1.38
1	2A	1047	G	N9-C4	5.10	1.42	1.38
1	2A	1244	G	N9-C4	-5.10	1.33	1.38
1	1A	1926	G	N9-C8	-5.10	1.34	1.37
1	2A	2572	A	N9-C4	-5.10	1.34	1.37
32	2a	1465	C	C2-N3	5.10	1.39	1.35
1	1A	2254	G	C5-C4	-5.10	1.34	1.38
16	1U	9	VAL	CB-CG1	-5.10	1.42	1.52
1	1A	1059	C	C4-N4	-5.09	1.29	1.33
1	1A	1661	C	C2-O2	-5.09	1.19	1.24
32	1a	144	G	N3-C4	5.09	1.39	1.35
32	1a	1035	A	N9-C4	5.09	1.41	1.37
1	1A	1414	G	N1-C2	-5.09	1.33	1.37
1	2A	1460	A	N9-C4	5.09	1.41	1.37
1	1A	1103	A	N7-C5	5.09	1.42	1.39
16	1U	15	LYS	CE-NZ	5.09	1.61	1.49
1	1A	560	C	N3-C4	-5.08	1.30	1.33
1	1A	957	A	C5-C6	-5.08	1.36	1.41
16	1U	59	ARG	CG-CD	5.08	1.64	1.51
1	1A	1257	G	N9-C8	-5.08	1.34	1.37
1	1A	1258	A	N3-C4	-5.08	1.31	1.34
1	2A	2173	A	N9-C4	5.08	1.40	1.37
32	1a	78	G	C6-N1	5.08	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1062	G	N1-C2	-5.08	1.33	1.37
1	1A	1421	C	N1-C6	-5.08	1.34	1.37
1	1A	2046	G	N7-C5	5.08	1.42	1.39
1	1A	2250	G	N9-C8	-5.07	1.34	1.37
1	2A	1696	G	C5-C4	-5.07	1.34	1.38
1	1A	47	G	C8-N7	5.07	1.33	1.30
1	2A	1041	C	N1-C6	5.07	1.40	1.37
1	1A	1875	C	C4-N4	-5.07	1.29	1.33
1	1A	505	A	C2-N3	-5.06	1.28	1.33
32	1a	1447	A	N9-C4	5.06	1.40	1.37
1	1A	897	C	N3-C4	-5.06	1.30	1.33
1	1A	979	G	N9-C8	-5.06	1.34	1.37
1	1A	1981	G	C2-N3	-5.06	1.28	1.32
1	2A	1253	A	N7-C5	-5.06	1.36	1.39
1	2A	1702	G	C5-C4	-5.06	1.34	1.38
1	2A	2148	G	N3-C4	5.06	1.39	1.35
1	1A	2550	C	C4-N4	-5.05	1.29	1.33
1	1A	125	A	C6-N6	-5.05	1.29	1.33
1	2A	414	C	N3-C4	-5.05	1.30	1.33
1	1A	2593	G	N1-C2	-5.05	1.33	1.37
1	2A	509	C	N1-C6	-5.05	1.34	1.37
1	2A	1384	A	N3-C4	-5.05	1.31	1.34
32	2a	1129	C	N3-C4	5.05	1.37	1.33
1	1A	2415	C	N3-C4	-5.05	1.30	1.33
1	1A	1474	C	C4-C5	5.05	1.47	1.43
1	1A	1831	C	N1-C6	-5.05	1.34	1.37
1	1A	2610	A	C5-C4	-5.04	1.35	1.38
1	1A	2794	A	N9-C4	-5.04	1.34	1.37
15	1T	96	ARG	CB-CG	-5.04	1.39	1.52
1	1A	2501	G	C8-N7	-5.04	1.27	1.30
1	1A	753	A	N9-C4	-5.04	1.34	1.37
1	1A	1382	A	N7-C5	-5.04	1.36	1.39
1	1A	2055	A	C5-C4	-5.04	1.35	1.38
1	2A	471	A	N9-C4	-5.04	1.34	1.37
1	2A	2100	G	N3-C4	5.04	1.39	1.35
1	2A	2153	G	N3-C4	5.04	1.39	1.35
1	1A	589	U	C4-O4	-5.04	1.19	1.23
1	1A	1978	U	N1-C2	-5.04	1.34	1.38
1	1A	1728	G	N9-C4	-5.03	1.33	1.38
31	19	11	CYS	CB-SG	-5.03	1.73	1.81
32	2a	395	C	N3-C4	-5.03	1.30	1.33
32	2a	1124	G	N9-C4	5.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1986	G	N7-C5	-5.03	1.36	1.39
1	1A	1781	G	N7-C5	5.03	1.42	1.39
1	1A	2785	C	N1-C6	-5.03	1.34	1.37
2	1B	100	A	N3-C4	-5.03	1.31	1.34
12	1Q	96	VAL	CB-CG2	-5.03	1.42	1.52
1	1A	2004	C	N3-C4	-5.03	1.30	1.33
1	1A	2818	U	N3-C4	5.03	1.43	1.38
1	1A	421	A	C6-N1	-5.03	1.32	1.35
1	1A	560	C	N1-C6	-5.03	1.34	1.37
1	1A	1409	C	N3-C4	-5.02	1.30	1.33
1	1A	2041	A	C6-N1	-5.02	1.32	1.35
1	1A	1091	A	N3-C4	5.02	1.37	1.34
1	1A	1121	C	N1-C2	5.02	1.45	1.40
32	1a	1021	G	C2-N3	5.02	1.36	1.32
1	1A	2181	G	N9-C4	5.02	1.42	1.38
1	1A	2579	G	C6-N1	-5.02	1.36	1.39
32	1a	1143	G	C6-N1	5.02	1.43	1.39
32	2a	1021	G	C6-N1	5.02	1.43	1.39
1	2A	2009	G	N3-C4	-5.01	1.31	1.35
1	1A	865	G	N1-C2	-5.01	1.33	1.37
28	26	40	CYS	CB-SG	-5.01	1.73	1.81
1	1A	434	G	N7-C5	-5.01	1.36	1.39
1	1A	1074	A	N3-C4	-5.01	1.31	1.34
1	1A	1282	G	C2-N3	-5.01	1.28	1.32
1	1A	1986	G	N1-C2	-5.01	1.33	1.37
1	1A	505	A	C6-N1	-5.01	1.32	1.35
1	1A	1030	A	C8-N7	-5.01	1.28	1.31
1	1A	1831	C	C2-N3	-5.01	1.31	1.35
1	1A	199	C	C2-N3	-5.00	1.31	1.35
1	1A	321	C	N1-C6	-5.00	1.34	1.37
1	1A	602	G	C6-N1	-5.00	1.36	1.39
1	1A	1143	U	C2-N3	5.00	1.41	1.37
1	1A	2100	C	C2-N3	-5.00	1.31	1.35
1	2A	38	A	N7-C5	-5.00	1.36	1.39
1	1A	369	A	C6-N6	-5.00	1.29	1.33
1	1A	572	A	C5-C6	5.00	1.45	1.41
2	2B	45	A	N9-C4	5.00	1.40	1.37

All (8429) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1208	C	O5'-P-OP1	-35.12	68.56	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1520	G	O5'-P-OP1	-30.95	73.56	110.70
32	1a	1520	G	O5'-P-OP2	27.90	144.18	110.70
32	2a	1208	C	OP1-P-OP2	-24.71	82.53	119.60
32	1a	1520	G	OP1-P-OP2	-23.77	83.94	119.60
1	1A	354	A	C2-N3-C4	-20.18	100.51	110.60
1	1A	1045	U	O5'-P-OP2	-19.05	87.84	110.70
1	1A	1442	U	O5'-P-OP1	-16.79	90.55	110.70
1	1A	1270	C	C6-N1-C2	16.65	126.96	120.30
32	2a	1208	C	O5'-P-OP2	16.47	130.47	110.70
1	1A	991	G	O5'-P-OP1	-16.01	91.29	105.70
1	1A	2331	G	N3-C4-N9	-15.92	116.45	126.00
1	1A	720	C	C2-N3-C4	-15.74	112.03	119.90
1	2A	800	A	O5'-P-OP1	-15.71	91.56	105.70
1	1A	1316	C	C6-N1-C2	15.68	126.57	120.30
1	1A	1743	G	O5'-P-OP2	-15.68	91.59	105.70
32	2a	438	G	O5'-P-OP2	-15.64	91.62	105.70
1	1A	876	A	O5'-P-OP2	-15.64	91.63	105.70
1	1A	2045	G	O5'-P-OP1	-15.44	91.80	105.70
1	1A	2080	A	O5'-P-OP2	-15.36	91.88	105.70
1	1A	82	G	N9-C4-C5	-15.19	99.32	105.40
32	1a	558	G	O5'-P-OP1	-15.10	92.11	105.70
32	1a	533	A	N1-C6-N6	15.09	127.65	118.60
1	1A	1695	C	O5'-P-OP1	-14.96	92.23	105.70
32	1a	1530	G	C5-C6-O6	-14.86	119.68	128.60
1	2A	751	A	O5'-P-OP1	-14.81	92.37	105.70
1	1A	1021	G	O5'-P-OP2	-14.77	92.41	105.70
32	2a	343	U	C2-N1-C1'	-14.74	100.01	117.70
32	1a	1137	C	C6-N1-C2	-14.73	114.41	120.30
32	1a	1530	G	N1-C6-O6	14.63	128.68	119.90
32	2a	1207	2MG	OP1-P-O3'	14.62	137.37	105.20
1	1A	918	U	C5-C4-O4	-14.55	117.17	125.90
32	2a	343	U	N3-C4-O4	-14.40	109.32	119.40
1	1A	598	A	O5'-P-OP1	-14.17	92.95	105.70
32	1a	343	U	C2-N1-C1'	-14.14	100.73	117.70
1	2A	2608	G	O5'-P-OP2	-14.00	93.10	105.70
1	1A	2019	G	O5'-P-OP2	-13.98	93.12	105.70
1	1A	2639	G	C5-C6-O6	-13.96	120.22	128.60
1	1A	2566	U	O5'-P-OP1	-13.87	93.22	105.70
1	1A	2331	G	N3-C4-C5	13.71	135.45	128.60
1	2A	1071	G	C8-N9-C4	-13.61	100.96	106.40
32	2a	30	U	O5'-P-OP2	-13.60	93.46	105.70
1	1A	592	U	N1-C2-O2	-13.57	113.30	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1177	G	C5-C6-O6	13.53	136.72	128.60
1	1A	354	A	N3-C4-C5	13.45	136.22	126.80
1	2A	2699	C	C5-C6-N1	-13.43	114.29	121.00
1	2A	774	A	O5'-P-OP2	-13.40	93.64	105.70
32	1a	343	U	N3-C4-O4	-13.12	110.22	119.40
1	1A	1382	A	O5'-P-OP2	-13.01	93.99	105.70
1	1A	2425	G	O5'-P-OP2	-12.99	94.01	105.70
1	1A	121	G	O5'-P-OP2	-12.99	94.01	105.70
1	2A	1298	C	O5'-P-OP2	-12.98	94.02	105.70
1	2A	1079	C	C6-N1-C2	-12.95	115.12	120.30
1	1A	61	C	O5'-P-OP2	-12.95	94.05	105.70
32	2a	1207	2MG	OP2-P-O3'	-12.90	76.82	105.20
1	2A	2467	C	C6-N1-C2	-12.87	115.15	120.30
1	2A	2597	G	O5'-P-OP2	-12.86	94.13	105.70
32	2a	404	U	N1-C2-O2	12.85	131.79	122.80
1	1A	799	A	C2-N3-C4	-12.78	104.21	110.60
1	1A	847	A	O5'-P-OP1	-12.77	94.21	105.70
1	2A	807	U	C2-N3-C4	-12.74	119.36	127.00
1	2A	2023	G	O5'-P-OP1	-12.73	94.24	105.70
2	1B	108	U	O5'-P-OP2	-12.71	94.26	105.70
1	1A	720	C	N1-C2-O2	-12.71	111.27	118.90
1	1A	1312	G	C5-C6-O6	-12.70	120.98	128.60
1	1A	1750	G	O5'-P-OP2	-12.65	94.31	105.70
1	1A	1725	G	N1-C6-O6	12.62	127.47	119.90
32	1a	404	U	N1-C2-O2	12.60	131.62	122.80
2	1B	56	G	O5'-P-OP2	-12.59	94.37	105.70
1	2A	467	G	C8-N9-C4	12.59	111.44	106.40
1	1A	184	A	C5-N7-C8	-12.56	97.62	103.90
1	1A	2383	G	C5-C6-O6	-12.55	121.07	128.60
1	1A	2257	U	N3-C4-C5	12.53	122.12	114.60
1	1A	354	A	C5-N7-C8	-12.51	97.65	103.90
1	1A	2257	U	C2-N3-C4	-12.51	119.50	127.00
1	1A	1060	U	O5'-P-OP2	-12.49	94.46	105.70
1	1A	2608	U	N1-C2-O2	-12.46	114.08	122.80
1	1A	1007	G	O5'-P-OP1	-12.46	94.49	105.70
1	2A	2430	A	O5'-P-OP2	-12.45	94.50	105.70
32	2a	1003	G	C8-N9-C4	-12.39	101.44	106.40
32	1a	902	G	O5'-P-OP2	-12.38	94.56	105.70
1	1A	2194	U	C5-C4-O4	12.36	133.31	125.90
1	1A	2550	C	N3-C4-C5	12.35	126.84	121.90
1	1A	2443	U	C5-C6-N1	-12.34	116.53	122.70
1	1A	1263	C	O5'-P-OP2	-12.26	94.67	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	598	A	O5'-P-OP2	12.19	125.33	110.70
1	1A	1270	C	C5-C6-N1	-12.19	114.91	121.00
1	1A	2512	U	C5-C6-N1	-12.18	116.61	122.70
1	1A	2331	G	C2-N3-C4	-12.14	105.83	111.90
1	2A	1783	A	O5'-P-OP2	-12.11	94.80	105.70
1	2A	1272	A	O5'-P-OP2	-12.07	94.83	105.70
1	2A	1071	G	N7-C8-N9	12.05	119.12	113.10
1	1A	447	C	C6-N1-C2	12.01	125.10	120.30
1	1A	749	G	O5'-P-OP2	-12.01	94.89	105.70
1	1A	1177	G	N1-C6-O6	-11.95	112.73	119.90
1	1A	1301	U	N3-C4-O4	11.93	127.75	119.40
1	2A	529	A	C5-N7-C8	-11.93	97.94	103.90
2	1B	13	A	O5'-P-OP2	-11.92	94.97	105.70
1	1A	2405	A	O5'-P-OP2	-11.86	95.03	105.70
1	1A	1237	G	C8-N9-C4	11.84	111.13	106.40
1	2A	1079	C	O4'-C1'-N1	11.82	117.66	108.20
1	1A	543	G	O5'-P-OP2	-11.81	95.07	105.70
32	2a	1003	G	N3-C4-C5	-11.78	122.71	128.60
1	1A	553	A	C8-N9-C4	-11.77	101.09	105.80
1	2A	2549	G	O5'-P-OP2	-11.76	95.11	105.70
1	1A	2640	C	C6-N1-C2	11.76	125.00	120.30
1	1A	354	A	C4-C5-N7	11.75	116.58	110.70
1	1A	1318	A	O5'-P-OP2	-11.72	95.16	105.70
1	2A	2378	A	N1-C6-N6	11.71	125.62	118.60
32	2a	343	U	C5-C4-O4	11.69	132.91	125.90
1	1A	1720	U	N1-C2-O2	-11.65	114.65	122.80
1	1A	537	G	O4'-C1'-N9	11.63	117.50	108.20
1	1A	82	G	C8-N9-C4	11.57	111.03	106.40
1	1A	2331	G	C5-N7-C8	-11.57	98.51	104.30
1	1A	581	G	N1-C6-O6	-11.55	112.97	119.90
1	1A	2386	C	C6-N1-C2	11.55	124.92	120.30
5	1F	54	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	1A	2735	G	C8-N9-C4	11.52	111.01	106.40
1	1A	1232	G	O5'-P-OP2	-11.51	95.34	105.70
32	1a	42	G	O5'-P-OP1	-11.50	95.35	105.70
1	1A	2346	G	C4-C5-N7	11.48	115.39	110.80
1	1A	1725	G	C5-C6-O6	-11.46	121.73	128.60
1	1A	2609	G	O5'-P-OP2	-11.44	95.41	105.70
1	1A	561	A	O5'-P-OP2	-11.43	95.42	105.70
1	1A	181	C	N1-C2-O2	-11.43	112.04	118.90
1	1A	592	U	C2-N3-C4	-11.42	120.15	127.00
1	2A	484	C	O5'-P-OP2	-11.39	95.45	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1647	G	C5-C6-O6	-11.38	121.77	128.60
1	1A	1358	U	C5-C4-O4	11.38	132.73	125.90
1	2A	1063	G	C8-N9-C4	-11.33	101.87	106.40
1	1A	2593	G	N3-C2-N2	11.32	127.82	119.90
1	2A	1638	C	O5'-P-OP2	-11.32	95.51	105.70
1	1A	2272	C	C5-C6-N1	-11.28	115.36	121.00
32	2a	266	G	C8-N9-C4	-11.27	101.89	106.40
1	1A	1042	A	O5'-P-OP1	-11.26	95.56	105.70
32	2a	1528	U	O5'-P-OP2	-11.26	95.57	105.70
1	1A	1232	G	O5'-P-OP1	11.25	124.20	110.70
1	1A	2059	G	N3-C2-N2	11.24	127.77	119.90
1	1A	1666	G	N1-C6-O6	-11.24	113.16	119.90
1	1A	2057	G	C5-N7-C8	-11.23	98.68	104.30
1	2A	2699	C	C6-N1-C2	11.23	124.79	120.30
1	1A	1057	G	O5'-P-OP2	-11.23	95.59	105.70
1	2A	1673	U	O5'-P-OP1	-11.20	95.62	105.70
1	1A	2259	A	C8-N9-C4	11.20	110.28	105.80
1	2A	1904	G	N1-C6-O6	-11.19	113.19	119.90
32	2a	770	C	O5'-P-OP2	-11.13	95.68	105.70
32	1a	533	A	C5-C6-N6	-11.12	114.81	123.70
1	1A	1316	C	C5-C6-N1	-11.11	115.44	121.00
1	1A	2735	G	N9-C4-C5	-11.11	100.96	105.40
1	2A	906	G	C5-C6-O6	11.10	135.26	128.60
1	1A	2627	U	O5'-P-OP1	-11.09	95.72	105.70
2	2B	6	C	C6-N1-C2	11.09	124.73	120.30
1	1A	2092	G	N1-C2-N2	-11.07	106.24	116.20
1	1A	1237	G	N7-C8-N9	-11.06	107.57	113.10
1	2A	1097	U	C2-N1-C1'	11.05	130.96	117.70
1	1A	1359	U	O5'-P-OP1	-11.04	95.77	105.70
1	1A	1030	A	C8-N9-C4	11.01	110.20	105.80
32	2a	697	U	O5'-P-OP2	-11.00	95.80	105.70
32	2a	343	U	C6-N1-C1'	11.00	136.60	121.20
1	2A	1076	C	N1-C2-O2	10.99	125.50	118.90
1	2A	2611	U	O5'-P-OP1	-10.99	95.81	105.70
1	1A	1995	G	C4-C5-N7	-10.98	106.41	110.80
1	1A	2421	G	O5'-P-OP2	-10.98	95.82	105.70
1	1A	1995	G	C5-C6-O6	10.97	135.19	128.60
32	2a	1495	U	N1-C2-O2	10.96	130.47	122.80
32	1a	1417	G	C5-C6-O6	-10.95	122.03	128.60
1	1A	1811	A	C8-N9-C4	-10.94	101.42	105.80
1	1A	82	G	C2-N3-C4	-10.94	106.43	111.90
1	1A	581	G	C5-C6-O6	10.93	135.16	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	375	U	O5'-P-OP1	-10.92	95.87	105.70
32	1a	1137	C	C5-C6-N1	10.92	126.46	121.00
1	1A	1282	G	C8-N9-C4	10.90	110.76	106.40
1	1A	2439	C	C6-N1-C2	10.89	124.66	120.30
32	1a	590	C	O5'-P-OP2	-10.88	95.91	105.70
1	1A	2049	G	C5-C6-O6	10.88	135.13	128.60
1	1A	2453	C	C2-N3-C4	-10.87	114.46	119.90
1	1A	2475	C	N3-C4-C5	10.86	126.24	121.90
32	2a	404	U	N3-C2-O2	-10.85	114.60	122.20
1	1A	592	U	N1-C2-N3	10.85	121.41	114.90
1	1A	1216	G	C8-N9-C4	-10.85	102.06	106.40
32	2a	1125	U	C5-C4-O4	10.84	132.41	125.90
32	2a	1530	G	C8-N9-C4	10.84	110.74	106.40
1	2A	1992	G	C8-N9-C4	-10.84	102.07	106.40
32	2a	1034	G	N3-C4-C5	-10.84	123.18	128.60
1	1A	196	A	C5-C6-N6	-10.81	115.05	123.70
1	1A	2102	G	O5'-P-OP2	-10.80	95.97	105.70
1	1A	2627	U	N3-C2-O2	-10.79	114.64	122.20
32	1a	343	U	C5-C4-O4	10.77	132.36	125.90
1	2A	2523	G	O5'-P-OP2	-10.76	96.02	105.70
1	1A	418	G	C6-N1-C2	-10.75	118.65	125.10
1	1A	2019	G	O5'-P-OP1	10.75	123.60	110.70
1	1A	82	G	C4-C5-N7	10.75	115.10	110.80
32	1a	533	A	C6-C5-N7	-10.74	124.78	132.30
1	1A	1006	C	O5'-P-OP2	-10.72	96.06	105.70
1	1A	1648	U	O5'-P-OP2	10.71	123.55	110.70
1	1A	1030	A	N9-C4-C5	-10.71	101.52	105.80
32	1a	1436	U	C2-N3-C4	-10.69	120.58	127.00
32	2a	1098	C	O5'-P-OP1	-10.69	96.08	105.70
1	1A	580	U	O5'-P-OP2	-10.68	96.09	105.70
1	1A	2511	C	N3-C4-C5	-10.66	117.64	121.90
1	1A	1167	C	C6-N1-C2	-10.65	116.04	120.30
32	2a	558	G	O5'-P-OP1	-10.63	96.13	105.70
1	2A	203	C	O5'-P-OP2	-10.63	96.13	105.70
1	1A	398	A	N1-C6-N6	10.63	124.98	118.60
1	2A	2318	G	O4'-C1'-N9	10.61	116.69	108.20
1	1A	2858	G	O4'-C1'-N9	10.61	116.69	108.20
1	2A	529	A	C4-C5-N7	10.61	116.00	110.70
32	2a	297	G	O5'-P-OP2	-10.59	96.17	105.70
23	21	21	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	1A	2802	C	C2-N1-C1'	-10.58	107.16	118.80
1	1A	2497	G	C2-N3-C4	-10.57	106.62	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1757	C	C6-N1-C2	10.57	124.53	120.30
1	1A	2460	A	C5-C6-N6	-10.56	115.25	123.70
1	1A	196	A	N1-C6-N6	10.56	124.94	118.60
1	1A	352	U	N3-C2-O2	-10.55	114.82	122.20
1	1A	2587	C	N1-C2-O2	10.54	125.22	118.90
1	2A	1074	G	O5'-P-OP2	-10.51	96.24	105.70
1	1A	2624	C	O5'-P-OP2	-10.51	96.24	105.70
1	1A	745	C	O5'-P-OP2	-10.48	96.26	105.70
1	1A	2376	C	C6-N1-C2	10.48	124.49	120.30
1	1A	2335	G	C4-C5-N7	10.47	114.99	110.80
1	1A	2518	U	O5'-P-OP2	-10.47	96.27	105.70
1	1A	1026	A	C8-N9-C4	10.47	109.99	105.80
1	1A	2464	C	N1-C2-O2	-10.47	112.62	118.90
1	1A	2258	G	C8-N9-C4	10.46	110.59	106.40
1	1A	2387	G	C8-N9-C4	10.46	110.58	106.40
1	1A	1316	C	N3-C4-C5	10.46	126.08	121.90
32	1a	1417	G	C4-C5-N7	10.44	114.97	110.80
1	2A	718	A	N1-C6-N6	10.44	124.86	118.60
1	1A	1291	G	O5'-P-OP1	-10.43	96.32	105.70
1	1A	1354	A	O5'-P-OP2	-10.42	96.32	105.70
1	2A	467	G	N7-C8-N9	-10.42	107.89	113.10
32	2a	1034	G	N3-C4-N9	10.41	132.25	126.00
1	2A	752	A	C8-N9-C4	-10.41	101.64	105.80
1	1A	2346	G	C6-C5-N7	-10.41	124.16	130.40
1	2A	2145	C	C6-N1-C2	-10.41	116.14	120.30
1	2A	1639	U	O5'-P-OP2	-10.40	96.34	105.70
1	1A	1817	A	O5'-P-OP2	-10.39	96.35	105.70
1	2A	1269	A	C2-N3-C4	-10.38	105.41	110.60
1	1A	1862	G	C5-C6-N1	-10.37	106.31	111.50
1	1A	1800	G	O5'-P-OP2	-10.36	96.38	105.70
1	1A	1098	C	C6-N1-C2	-10.31	116.18	120.30
1	1A	1270	C	C2-N3-C4	-10.30	114.75	119.90
1	1A	2442	A	O5'-P-OP2	-10.30	96.42	105.70
1	1A	20	C	C2-N3-C4	-10.29	114.75	119.90
1	1A	2084	A	C8-N9-C4	10.28	109.91	105.80
1	1A	1382	A	N9-C4-C5	10.27	109.91	105.80
1	2A	2324	C	C6-N1-C2	10.25	124.40	120.30
1	1A	2331	G	O4'-C1'-N9	10.25	116.40	108.20
1	2A	249	C	C6-N1-C2	10.23	124.39	120.30
1	1A	2556	G	C5-C6-O6	-10.23	122.46	128.60
1	1A	1766	G	C4-C5-N7	10.22	114.89	110.80
1	1A	238	C	C6-N1-C2	10.22	124.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1386	U	C2-N3-C4	-10.21	120.87	127.00
1	1A	1695	C	O5'-P-OP2	10.21	122.95	110.70
1	2A	807	U	C5-C4-O4	-10.21	119.78	125.90
2	1B	75	G	C6-N1-C2	-10.20	118.98	125.10
1	2A	315	G	O5'-P-OP2	-10.19	96.53	105.70
32	2a	728	A	O5'-P-OP2	-10.19	96.53	105.70
1	1A	1199	C	N1-C2-O2	-10.19	112.79	118.90
1	2A	979	G	O5'-P-OP1	-10.19	96.53	105.70
1	2A	2069	G	O5'-P-OP2	-10.18	96.54	105.70
1	1A	2450	U	C5-C6-N1	-10.17	117.61	122.70
1	1A	441	C	O5'-P-OP2	-10.16	96.56	105.70
1	2A	363(C)	G	C8-N9-C4	10.15	110.46	106.40
1	1A	2610	A	C8-N9-C4	10.15	109.86	105.80
1	1A	125	A	C5-C6-N1	10.14	122.77	117.70
1	1A	2383	G	C5-C6-N1	10.13	116.57	111.50
32	2a	902	G	O5'-P-OP2	-10.13	96.58	105.70
1	1A	1150	C	C6-N1-C2	-10.12	116.25	120.30
1	1A	2579	G	N7-C8-N9	-10.12	108.04	113.10
1	1A	2238	C	N1-C2-O2	-10.11	112.83	118.90
1	1A	702	A	C8-N9-C4	-10.10	101.76	105.80
1	1A	2607	G	C5-C6-O6	10.10	134.66	128.60
1	2A	683	C	O5'-P-OP1	-10.10	96.61	105.70
1	1A	1320	A	N1-C6-N6	10.10	124.66	118.60
1	1A	1927	C	O5'-P-OP2	-10.10	96.61	105.70
1	1A	2331	G	C8-N9-C4	-10.09	102.36	106.40
1	2A	2177	C	C6-N1-C2	-10.09	116.26	120.30
1	2A	2427	C	O5'-P-OP1	-10.09	96.62	105.70
32	2a	1406	U	C2-N3-C4	-10.09	120.95	127.00
1	1A	474	U	O5'-P-OP2	-10.07	96.64	105.70
1	1A	2049	G	N1-C6-O6	-10.06	113.86	119.90
1	1A	760	G	C2-N3-C4	-10.05	106.88	111.90
1	1A	752	A	N1-C6-N6	10.05	124.63	118.60
1	1A	837	C	O5'-P-OP2	-10.04	96.66	105.70
1	1A	2379	G	C8-N9-C4	10.03	110.41	106.40
1	1A	2579	G	O5'-P-OP1	-10.02	96.68	105.70
1	1A	198	C	C2-N3-C4	-10.01	114.89	119.90
1	1A	1725	G	N3-C2-N2	-10.01	112.89	119.90
1	1A	2335	G	C5-N7-C8	-10.01	99.30	104.30
1	1A	1995	G	N1-C6-O6	-10.00	113.90	119.90
1	1A	735	U	C2-N3-C4	-10.00	121.00	127.00
32	1a	13	U	C5-C6-N1	-10.00	117.70	122.70
1	2A	2145	C	C5-C6-N1	10.00	126.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	554	A	C5-N7-C8	-10.00	98.90	103.90
1	2A	481	G	O5'-P-OP2	-9.99	96.71	105.70
1	1A	2106	C	C5-C6-N1	-9.98	116.01	121.00
1	1A	555	G	O5'-P-OP1	-9.97	96.73	105.70
1	2A	744	G	O5'-P-OP2	-9.97	96.72	105.70
1	1A	19	C	C6-N1-C2	9.97	124.29	120.30
1	1A	2724	U	C5-C4-O4	-9.96	119.92	125.90
2	1B	50	G	N1-C6-O6	-9.96	113.92	119.90
1	2A	205	G	O5'-P-OP2	-9.96	96.74	105.70
1	2A	2699	C	C2-N3-C4	-9.96	114.92	119.90
32	2a	1420	C	C6-N1-C2	-9.96	116.32	120.30
32	2a	898	G	C8-N9-C4	9.95	110.38	106.40
2	1B	98	G	O5'-P-OP2	-9.93	96.76	105.70
1	2A	1092	C	N1-C2-O2	9.92	124.85	118.90
1	1A	1462	G	O4'-C1'-N9	9.92	116.13	108.20
1	1A	1486	G	O5'-P-OP2	-9.91	96.78	105.70
1	1A	2003	A	C5-C6-N1	9.90	122.65	117.70
1	1A	828	A	C2-N3-C4	9.89	115.54	110.60
1	2A	2554	U	O5'-P-OP2	9.89	122.56	110.70
1	1A	1210	G	C5-C6-O6	9.88	134.53	128.60
1	2A	807	U	N1-C2-N3	9.86	120.82	114.90
1	1A	1664	A	N1-C6-N6	-9.85	112.69	118.60
1	2A	2682	U	O5'-P-OP2	-9.84	96.84	105.70
1	1A	720	C	C5-C4-N4	-9.84	113.31	120.20
1	2A	249	C	O5'-P-OP1	-9.83	96.85	105.70
1	1A	1174	A	O5'-P-OP1	-9.83	96.85	105.70
1	1A	1720	U	N3-C2-O2	9.83	129.08	122.20
1	1A	1571	G	O5'-P-OP2	-9.83	96.85	105.70
1	1A	725	C	N3-C4-C5	9.81	125.82	121.90
1	1A	1346	U	P-O3'-C3'	9.80	131.47	119.70
1	2A	1899	G	O5'-P-OP2	-9.80	96.88	105.70
1	1A	2030	C	C4-C5-C6	9.80	122.30	117.40
1	1A	1821	C	C5-C4-N4	-9.80	113.34	120.20
1	1A	556	C	C5-C6-N1	-9.78	116.11	121.00
32	2a	299	G	C5-C6-O6	-9.78	122.73	128.60
32	1a	404	U	N3-C2-O2	-9.78	115.36	122.20
1	1A	854	U	N1-C2-O2	-9.78	115.96	122.80
1	1A	1707	C	C2-N3-C4	-9.78	115.01	119.90
1	1A	2514	G	N3-C2-N2	9.78	126.74	119.90
1	1A	2375	C	C6-N1-C2	9.78	124.21	120.30
1	1A	1911	A	C8-N9-C4	9.77	109.71	105.80
1	1A	101	A	C4-C5-C6	9.76	121.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1003	G	C2-N3-C4	9.76	116.78	111.90
1	1A	781	A	C2-N3-C4	-9.76	105.72	110.60
1	1A	101	A	C5-C6-N1	-9.76	112.82	117.70
1	1A	2277	U	N3-C4-O4	9.75	126.22	119.40
32	1a	442	C	C6-N1-C2	-9.75	116.40	120.30
1	2A	1075	C	N1-C2-O2	9.75	124.75	118.90
1	1A	1216	G	N7-C8-N9	9.74	117.97	113.10
32	1a	33	A	O5'-P-OP2	-9.73	96.94	105.70
1	2A	2827	C	C6-N1-C2	9.73	124.19	120.30
1	1A	2406	C	C2-N3-C4	-9.72	115.04	119.90
1	1A	131	C	O5'-P-OP2	-9.72	96.95	105.70
1	1A	1690	G	N1-C6-O6	-9.71	114.08	119.90
1	1A	660	C	C6-N1-C2	-9.70	116.42	120.30
1	1A	2257	U	C5-C4-O4	-9.71	120.08	125.90
1	1A	952	G	N9-C4-C5	9.70	109.28	105.40
1	1A	752	A	C4-C5-N7	9.70	115.55	110.70
1	1A	2608	U	C2-N3-C4	-9.69	121.18	127.00
1	1A	2080	A	O5'-P-OP1	9.69	122.32	110.70
1	1A	2674	A	C8-N9-C4	-9.68	101.93	105.80
1	1A	354	A	N3-C4-N9	-9.67	119.66	127.40
23	2I	21	ARG	NE-CZ-NH1	9.66	125.13	120.30
15	1T	96	ARG	CG-CD-NE	-9.66	91.52	111.80
1	1A	19	C	C5-C6-N1	-9.65	116.17	121.00
1	1A	666	C	C6-N1-C2	-9.64	116.44	120.30
1	1A	1613	A	C8-N9-C4	9.64	109.66	105.80
1	1A	796	C	C6-N1-C2	9.62	124.15	120.30
32	2a	983	A	O5'-P-OP1	-9.62	97.04	105.70
32	2a	1034	G	C5-C6-N1	9.61	116.31	111.50
32	2a	1034	G	C2-N3-C4	9.61	116.70	111.90
1	1A	1985	U	C2-N1-C1'	9.61	129.23	117.70
1	2A	834	C	O5'-P-OP2	-9.61	97.05	105.70
1	1A	20	C	C5-C6-N1	-9.60	116.20	121.00
1	2A	476	G	O5'-P-OP2	-9.60	97.06	105.70
1	1A	578	U	O5'-P-OP1	-9.60	97.06	105.70
1	1A	952	G	C5-C6-O6	9.59	134.35	128.60
1	1A	2726	A	N1-C6-N6	-9.59	112.85	118.60
1	2A	1352	U	O5'-P-OP1	-9.59	97.07	105.70
32	2a	5	U	C5-C6-N1	9.58	127.49	122.70
1	2A	2621	A	C2-N3-C4	-9.58	105.81	110.60
32	1a	1417	G	C5-C6-N1	9.57	116.29	111.50
1	1A	1042	A	N7-C8-N9	-9.57	109.01	113.80
32	2a	299	G	C4-C5-N7	9.57	114.63	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	906	G	N9-C4-C5	9.56	109.22	105.40
1	1A	735	U	N1-C2-N3	9.56	120.64	114.90
1	1A	2059	G	N1-C2-N2	-9.56	107.60	116.20
32	2a	1024	G	C2-N3-C4	9.55	116.68	111.90
1	2A	2036	C	O5'-P-OP1	-9.55	97.11	105.70
1	1A	40	C	N1-C2-O2	-9.54	113.18	118.90
1	1A	918	U	N3-C2-O2	9.54	128.87	122.20
32	1a	343	U	C6-N1-C1'	9.53	134.54	121.20
1	1A	2828	G	N1-C6-O6	-9.53	114.18	119.90
1	1A	2081	A	N7-C8-N9	-9.51	109.05	113.80
1	1A	194	G	C8-N9-C4	9.51	110.20	106.40
1	1A	2401	G	O5'-P-OP1	-9.50	97.15	105.70
32	2a	506	G	O5'-P-OP1	-9.50	97.15	105.70
32	2a	574	A	N1-C6-N6	9.49	124.30	118.60
1	1A	1080	G	C5-C6-O6	-9.49	122.91	128.60
1	1A	786	G	OP2-P-O3'	-9.48	84.33	105.20
1	2A	512	G	O4'-C1'-N9	9.48	115.79	108.20
1	1A	1832	G	O5'-P-OP1	-9.48	97.17	105.70
2	1B	91	C	C6-N1-C2	9.48	124.09	120.30
1	1A	2024	G	C5-N7-C8	9.47	109.03	104.30
32	1a	750	G	O5'-P-OP1	-9.47	97.18	105.70
2	2B	115	G	C8-N9-C4	9.47	110.19	106.40
1	1A	1846	A	C6-N1-C2	-9.46	112.92	118.60
1	2A	2823	A	O5'-P-OP2	-9.45	97.19	105.70
1	2A	2248	C	O5'-P-OP2	-9.45	97.19	105.70
32	1a	912	C	C6-N1-C2	9.43	124.07	120.30
1	1A	1303	C	N3-C4-C5	-9.43	118.13	121.90
1	1A	859	C	N3-C4-C5	9.42	125.67	121.90
32	1a	732	C	O5'-P-OP1	-9.41	97.23	105.70
1	2A	1321	A	C8-N9-C4	9.41	109.56	105.80
1	1A	1747	A	O5'-P-OP1	-9.40	97.24	105.70
1	1A	2579	G	C8-N9-C4	9.39	110.16	106.40
1	1A	2587	C	N3-C2-O2	-9.39	115.33	121.90
1	1A	1093	G	O5'-P-OP2	-9.38	97.25	105.70
1	2A	1913	A	C8-N9-C4	-9.38	102.05	105.80
1	1A	295	C	O5'-P-OP2	-9.38	97.26	105.70
1	2A	2207	G	C6-C5-N7	-9.37	124.78	130.40
1	1A	594	A	N1-C2-N3	-9.36	124.62	129.30
1	1A	1130	A	N1-C6-N6	-9.36	112.98	118.60
1	1A	1848	G	C5-C6-O6	9.36	134.22	128.60
1	1A	1254	G	N3-C2-N2	-9.36	113.35	119.90
1	1A	1840	A	N1-C6-N6	-9.35	112.99	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1094	G	O5'-P-OP1	-9.34	97.29	105.70
32	1a	186	C	C6-N1-C2	-9.34	116.56	120.30
1	2A	906	G	N3-C4-N9	-9.34	120.40	126.00
32	2a	1530	G	N3-C4-C5	9.34	133.27	128.60
1	1A	1529	G	O5'-P-OP2	-9.33	97.30	105.70
2	1B	102	A	C6-N1-C2	-9.33	113.00	118.60
1	2A	1063	G	N7-C8-N9	9.33	117.77	113.10
1	2A	2443	C	C6-N1-C2	-9.33	116.57	120.30
1	1A	1921	G	C5-C6-O6	-9.32	123.01	128.60
1	1A	1294	G	C8-N9-C4	9.32	110.13	106.40
1	2A	123	G	O5'-P-OP2	-9.32	97.31	105.70
1	1A	2059	G	N1-C6-O6	-9.32	114.31	119.90
1	2A	2306	C	N1-C2-O2	9.32	124.49	118.90
1	2A	1662	C	C2-N3-C4	-9.31	115.24	119.90
1	1A	1811	A	O5'-P-OP2	-9.31	97.32	105.70
1	2A	2612	C	C6-N1-C2	9.31	124.02	120.30
1	1A	192	C	C6-N1-C2	9.31	124.02	120.30
1	1A	1336	C	C6-N1-C2	-9.31	116.58	120.30
32	2a	1396	A	O5'-P-OP2	-9.31	97.32	105.70
1	1A	652	A	O5'-P-OP2	-9.30	97.33	105.70
1	1A	1831	C	N3-C2-O2	-9.29	115.40	121.90
1	1A	1790	A	N1-C6-N6	9.28	124.17	118.60
1	1A	1986	G	N9-C4-C5	-9.28	101.69	105.40
1	1A	666	C	C5-C6-N1	9.27	125.64	121.00
1	2A	1269	A	C5-C6-N1	-9.27	113.07	117.70
1	2A	740	U	O5'-P-OP2	-9.26	97.37	105.70
1	1A	2883	A	O5'-P-OP2	-9.26	97.37	105.70
1	2A	2554	U	O5'-P-OP1	-9.26	97.37	105.70
1	1A	1051	C	N3-C4-N4	-9.25	111.53	118.00
1	1A	799	A	C8-N9-C4	9.24	109.50	105.80
1	1A	1747	A	C8-N9-C4	9.24	109.50	105.80
1	1A	2137	G	C8-N9-C4	-9.24	102.70	106.40
1	1A	2550	C	C2-N3-C4	-9.24	115.28	119.90
1	1A	2639	G	C5-C6-N1	9.24	116.12	111.50
1	1A	215	G	O4'-C1'-N9	9.24	115.59	108.20
1	1A	720	C	O5'-P-OP2	-9.24	97.39	105.70
1	2A	1602	U	O5'-P-OP2	9.24	121.79	110.70
32	1a	280	C	C6-N1-C2	9.23	123.99	120.30
32	1a	14	U	O5'-P-OP1	-9.23	97.40	105.70
1	1A	2738	A	C2-N3-C4	-9.21	105.99	110.60
1	1A	2784	C	O5'-P-OP2	9.21	121.75	110.70
1	1A	2835	C	C6-N1-C2	9.21	123.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	906	G	C4-C5-N7	-9.21	107.12	110.80
1	1A	1270	C	N3-C4-C5	9.21	125.58	121.90
1	2A	1776	G	O5'-P-OP2	-9.20	97.42	105.70
1	1A	519	G	C8-N9-C4	-9.20	102.72	106.40
1	2A	2643	G	O5'-P-OP1	-9.19	97.43	105.70
1	1A	2724	U	C2-N3-C4	-9.19	121.49	127.00
1	1A	2065	C	N1-C2-O2	-9.18	113.39	118.90
1	2A	2574	G	O5'-P-OP1	-9.17	97.45	105.70
32	2a	1093	A	N1-C6-N6	9.16	124.10	118.60
1	1A	101	A	N1-C2-N3	9.16	133.88	129.30
1	1A	1007	G	OP1-P-OP2	-9.16	105.87	119.60
1	2A	2576	G	O5'-P-OP1	-9.15	97.46	105.70
1	1A	702	A	C5-N7-C8	-9.15	99.32	103.90
1	1A	184	A	N7-C8-N9	9.15	118.37	113.80
1	1A	1249	A	C2-N3-C4	-9.13	106.03	110.60
1	1A	2525	G	C5-N7-C8	-9.13	99.73	104.30
1	1A	436	C	O5'-P-OP1	-9.13	97.49	105.70
1	1A	795	G	N3-C4-C5	-9.11	124.04	128.60
1	1A	415	G	C8-N9-C4	9.10	110.04	106.40
1	1A	1015	C	C6-N1-C2	9.10	123.94	120.30
1	1A	1450	C	O5'-P-OP2	-9.10	97.51	105.70
1	1A	2134	G	N3-C4-C5	-9.10	124.05	128.60
1	1A	2454	C	C6-N1-C2	9.09	123.94	120.30
1	2A	2505	G	C5-C6-O6	9.09	134.06	128.60
1	1A	479	C	O5'-P-OP1	-9.08	97.53	105.70
1	1A	834	U	O5'-P-OP1	-9.08	97.53	105.70
1	1A	932	C	C6-N1-C2	-9.08	116.67	120.30
1	1A	2578	A	O5'-P-OP2	-9.08	97.53	105.70
1	1A	1279	C	N3-C4-C5	9.07	125.53	121.90
1	1A	1300	A	C6-N1-C2	-9.07	113.16	118.60
1	1A	1472	G	C5-C6-O6	-9.07	123.16	128.60
1	1A	1772	C	C6-N1-C2	-9.07	116.67	120.30
1	1A	2627	U	N3-C4-O4	-9.07	113.05	119.40
1	1A	1843	A	O5'-P-OP1	-9.06	97.54	105.70
1	1A	859	C	N1-C2-O2	-9.06	113.47	118.90
1	1A	2158	C	C6-N1-C2	-9.06	116.68	120.30
1	2A	1008	C	N1-C2-O2	9.05	124.33	118.90
1	2A	673	C	C2-N3-C4	-9.05	115.37	119.90
1	1A	2454	C	C2-N3-C4	-9.05	115.38	119.90
1	1A	472	G	C4-C5-N7	9.05	114.42	110.80
1	2A	2356	C	N1-C2-O2	-9.04	113.47	118.90
1	1A	735	U	C5-C6-N1	-9.04	118.18	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1959	A	N1-C6-N6	-9.04	113.18	118.60
32	2a	1532	U	C5-C6-N1	9.04	127.22	122.70
1	1A	854	U	C2-N3-C4	-9.04	121.58	127.00
1	2A	1607	C	O5'-P-OP1	-9.04	97.57	105.70
1	1A	1175	A	OP1-P-OP2	9.04	133.15	119.60
1	1A	41	C	O5'-P-OP2	-9.03	97.58	105.70
1	1A	2271	G	C5-C6-O6	-9.03	123.18	128.60
1	1A	1091	A	O4'-C1'-N9	9.03	115.42	108.20
1	2A	659	C	C6-N1-C2	9.02	123.91	120.30
32	2a	30	U	OP1-P-OP2	9.02	133.13	119.60
32	1a	394	G	O5'-P-OP1	-9.02	97.58	105.70
1	1A	205	A	O5'-P-OP1	-9.02	97.59	105.70
1	2A	1253	A	C5-N7-C8	9.02	108.41	103.90
1	1A	419	C	O5'-P-OP1	-9.01	97.59	105.70
32	1a	1530	G	C4-C5-N7	9.01	114.41	110.80
1	1A	2372	A	O5'-P-OP2	-9.01	97.59	105.70
1	1A	1855	G	C8-N9-C4	9.01	110.00	106.40
1	1A	2585	C	C5-C4-N4	-9.00	113.90	120.20
2	1B	80	U	O5'-P-OP1	-9.00	97.60	105.70
1	2A	2318	G	C6-C5-N7	-9.00	125.00	130.40
32	1a	1492	A	C2-N3-C4	8.99	115.10	110.60
1	2A	2413	G	O5'-P-OP2	-8.99	97.61	105.70
1	2A	1992	G	N3-C4-C5	-8.98	124.11	128.60
1	1A	348	A	O5'-P-OP2	-8.98	97.61	105.70
1	1A	2610	A	N7-C8-N9	-8.98	109.31	113.80
1	2A	1372	U	C5-C4-O4	-8.98	120.51	125.90
1	1A	2639	G	C8-N9-C4	8.98	109.99	106.40
1	1A	1279	C	C6-N1-C2	8.98	123.89	120.30
1	1A	1690	G	C5-C6-O6	8.97	133.99	128.60
1	1A	2057	G	N7-C8-N9	8.97	117.59	113.10
1	1A	2639	G	C6-N1-C2	-8.97	119.72	125.10
1	1A	2818	U	N3-C2-O2	8.96	128.48	122.20
1	2A	956	G	N1-C6-O6	8.96	125.28	119.90
1	1A	2858	G	C4-C5-N7	-8.96	107.22	110.80
1	1A	618	C	N3-C4-C5	8.95	125.48	121.90
33	1b	178	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	2A	988	A	N1-C6-N6	8.95	123.97	118.60
1	1A	1255	A	P-O3'-C3'	8.95	130.44	119.70
1	2A	1769	G	C5-C6-O6	-8.95	123.23	128.60
32	1a	533	A	C4-C5-C6	8.95	121.47	117.00
1	1A	1181	G	C8-N9-C4	8.94	109.98	106.40
1	1A	1268	C	N1-C2-O2	-8.94	113.54	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2244	U	C5-C6-N1	-8.94	118.23	122.70
1	1A	791	G	C5-C6-O6	8.94	133.96	128.60
1	1A	2055	A	C2-N3-C4	8.94	115.07	110.60
32	2a	770	C	O5'-P-OP1	8.93	121.42	110.70
1	1A	2608	U	N3-C2-O2	8.92	128.45	122.20
1	2A	1082	U	C2-N1-C1'	8.92	128.41	117.70
1	1A	2439	C	O5'-P-OP1	-8.92	97.67	105.70
1	1A	1988	A	C8-N9-C4	8.92	109.37	105.80
1	1A	2902	G	P-O3'-C3'	8.91	130.40	119.70
1	1A	760	G	N9-C4-C5	-8.91	101.83	105.40
1	2A	1790	C	C6-N1-C2	8.91	123.86	120.30
1	1A	2879	G	C8-N9-C4	-8.91	102.84	106.40
32	1a	428	G	O5'-P-OP2	-8.90	97.69	105.70
32	1a	738	C	C6-N1-C2	-8.90	116.74	120.30
1	2A	2105	C	C5-C6-N1	8.90	125.45	121.00
1	1A	2331	G	N7-C8-N9	8.90	117.55	113.10
1	2A	1673	U	O5'-P-OP2	8.90	121.38	110.70
1	1A	1285	G	C5-C6-N1	-8.90	107.05	111.50
1	1A	2440	G	C8-N9-C4	-8.90	102.84	106.40
1	1A	790	G	C4-C5-N7	-8.89	107.24	110.80
1	1A	2718	G	C5-N7-C8	8.89	108.75	104.30
32	2a	5	U	C6-N1-C2	-8.89	115.66	121.00
32	2a	1495	U	N3-C2-O2	-8.89	115.97	122.20
1	1A	781	A	N1-C6-N6	8.89	123.93	118.60
1	1A	979	G	C5-N7-C8	8.89	108.75	104.30
1	1A	975	U	C5-C4-O4	-8.89	120.57	125.90
32	1a	148	G	N3-C4-C5	-8.89	124.16	128.60
1	2A	2318	G	C4-N9-C1'	8.88	138.04	126.50
1	2A	2268	A	O5'-P-OP1	-8.88	97.71	105.70
1	1A	283	G	C8-N9-C4	-8.88	102.85	106.40
1	2A	2817	G	C5-C6-O6	8.88	133.93	128.60
1	2A	2069	G	C8-N9-C4	8.88	109.95	106.40
1	1A	1031	C	O5'-P-OP2	-8.87	97.72	105.70
1	1A	856	G	C5-C6-N1	8.87	115.93	111.50
1	1A	1069	U	O5'-P-OP2	-8.86	97.72	105.70
1	1A	2331	G	N3-C2-N2	-8.86	113.70	119.90
1	2A	118	A	O5'-P-OP1	-8.86	97.72	105.70
1	1A	348	A	C8-N9-C4	8.86	109.34	105.80
1	1A	191	U	N3-C4-C5	8.86	119.92	114.60
1	1A	1033	G	N9-C4-C5	8.86	108.94	105.40
1	1A	1398	U	O5'-P-OP1	-8.85	97.73	105.70
1	1A	1630	A	O5'-P-OP2	-8.85	97.73	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1640	G	C8-N9-C4	-8.85	102.86	106.40
1	1A	31	C	O5'-P-OP1	-8.85	97.74	105.70
1	1A	1966	U	N3-C2-O2	-8.85	116.00	122.20
1	2A	528	A	C8-N9-C4	-8.85	102.26	105.80
1	1A	34	C	O4'-C1'-N1	8.85	115.28	108.20
32	2a	1026	G	N7-C8-N9	8.84	117.52	113.10
1	1A	1302	G	C8-N9-C4	8.84	109.94	106.40
1	2A	2566	A	O5'-P-OP2	-8.83	97.75	105.70
1	1A	1567	G	O5'-P-OP1	8.83	121.30	110.70
1	2A	2085	C	C6-N1-C2	8.83	123.83	120.30
1	1A	2100	C	C2-N3-C4	-8.82	115.49	119.90
1	2A	2855	C	C6-N1-C2	-8.82	116.77	120.30
1	1A	1007	G	O5'-P-OP2	8.82	121.28	110.70
32	1a	1077	G	O5'-P-OP2	-8.82	97.76	105.70
32	2a	834	C	O5'-P-OP2	-8.82	97.76	105.70
1	1A	918	U	N1-C2-O2	-8.82	116.63	122.80
32	1a	552	U	O5'-P-OP2	-8.82	97.76	105.70
32	1a	1530	G	N3-C4-C5	8.82	133.01	128.60
32	2a	266	G	N7-C8-N9	8.82	117.51	113.10
1	1A	2548	G	C2-N3-C4	-8.81	107.49	111.90
1	1A	979	G	N7-C8-N9	-8.80	108.70	113.10
1	1A	2402	U	O5'-P-OP1	-8.79	97.79	105.70
32	2a	912	C	C6-N1-C2	8.78	123.81	120.30
32	2a	60	A	P-O3'-C3'	8.78	130.24	119.70
32	2a	269	C	C6-N1-C2	8.78	123.81	120.30
1	1A	1414	G	N1-C6-O6	-8.77	114.64	119.90
1	2A	1187	G	N1-C6-O6	-8.77	114.64	119.90
1	1A	2092	G	C2-N3-C4	-8.77	107.52	111.90
2	1B	75	G	N3-C2-N2	-8.76	113.77	119.90
1	1A	1640	G	N3-C2-N2	-8.75	113.78	119.90
32	2a	340	U	O5'-P-OP2	-8.75	97.83	105.70
1	1A	2044	U	N3-C4-O4	8.74	125.52	119.40
1	1A	2587	C	N3-C4-C5	8.74	125.40	121.90
1	1A	2348	A	C8-N9-C4	8.74	109.30	105.80
1	1A	2439	C	C5-C6-N1	-8.74	116.63	121.00
32	1a	757	U	C5-C6-N1	-8.74	118.33	122.70
1	1A	2084	A	N9-C4-C5	-8.73	102.31	105.80
32	1a	299	G	C5-C6-N1	8.72	115.86	111.50
32	1a	233	C	C6-N1-C2	-8.71	116.81	120.30
1	2A	1071	G	C6-C5-N7	-8.71	125.17	130.40
1	2A	2699	C	N3-C4-N4	-8.71	111.90	118.00
1	1A	752	A	N9-C4-C5	-8.71	102.32	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1210	A	P-O3'-C3'	8.71	130.15	119.70
1	1A	472	G	N9-C4-C5	-8.70	101.92	105.40
1	1A	2383	G	C2-N3-C4	8.69	116.25	111.90
1	1A	725	C	C6-N1-C2	8.69	123.78	120.30
1	1A	2069	U	C5-C4-O4	-8.69	120.69	125.90
1	1A	1213	U	O5'-P-OP2	-8.69	97.88	105.70
1	1A	1104	G	N9-C4-C5	-8.69	101.92	105.40
1	1A	1907	A	O5'-P-OP2	-8.69	97.88	105.70
32	1a	770	C	OP1-P-OP2	-8.69	106.56	119.60
1	1A	569	G	C8-N9-C4	-8.69	102.92	106.40
1	1A	918	U	N3-C4-O4	8.69	125.48	119.40
1	1A	1043	G	N1-C6-O6	-8.69	114.69	119.90
1	2A	2177	C	C5-C6-N1	8.68	125.34	121.00
1	2A	463	G	O5'-P-OP2	-8.68	97.89	105.70
1	1A	2886	G	C5-N7-C8	-8.68	99.96	104.30
1	1A	2201	C	C6-N1-C2	-8.67	116.83	120.30
1	1A	2858	G	C6-C5-N7	8.67	135.60	130.40
2	1B	1	U	C5-C6-N1	8.67	127.03	122.70
1	1A	891	C	C6-N1-C2	8.67	123.77	120.30
1	1A	1299	A	C5-N7-C8	8.67	108.23	103.90
1	1A	1317	G	OP1-P-OP2	-8.67	106.60	119.60
1	1A	702	A	N7-C8-N9	8.66	118.13	113.80
1	1A	1739	U	C5-C6-N1	-8.66	118.37	122.70
1	1A	2881	C	O5'-P-OP2	-8.65	97.91	105.70
2	1B	108	U	C5-C4-O4	8.65	131.09	125.90
1	1A	106	U	N3-C4-C5	8.65	119.79	114.60
1	1A	494	G	C5-C6-N1	-8.65	107.18	111.50
1	1A	1702	A	C8-N9-C4	8.65	109.26	105.80
1	1A	1862	G	C8-N9-C4	-8.65	102.94	106.40
1	1A	1377	A	OP1-P-O3'	-8.65	86.18	105.20
32	1a	1158	C	C4-C5-C6	8.65	121.72	117.40
1	2A	752	A	P-O3'-C3'	8.65	130.08	119.70
1	1A	1395	A	N1-C6-N6	8.64	123.79	118.60
1	1A	1725	G	C6-C5-N7	-8.64	125.22	130.40
1	1A	803	C	N1-C2-O2	-8.64	113.72	118.90
1	2A	819	A	C8-N9-C4	-8.64	102.35	105.80
1	2A	570	G	N1-C6-O6	-8.63	114.72	119.90
32	2a	1335	C	N1-C2-O2	8.63	124.08	118.90
1	1A	2094	G	N1-C2-N3	-8.63	118.72	123.90
1	1A	1152	G	C8-N9-C4	8.62	109.85	106.40
32	1a	804	U	C5-C4-O4	8.62	131.07	125.90
1	1A	96	C	O5'-P-OP2	-8.61	97.95	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1766	G	C5-C6-O6	-8.61	123.44	128.60
1	1A	2453	C	N3-C4-C5	8.61	125.34	121.90
1	1A	1042	A	C5-N7-C8	8.61	108.20	103.90
1	1A	1702	A	N7-C8-N9	-8.61	109.50	113.80
32	1a	1417	G	N9-C4-C5	-8.60	101.96	105.40
1	1A	765	A	N1-C6-N6	8.60	123.76	118.60
1	1A	82	G	C6-C5-N7	-8.60	125.24	130.40
1	1A	2319	G	C5-C6-O6	-8.60	123.44	128.60
2	1B	91	C	N3-C4-C5	8.60	125.34	121.90
1	2A	1816	G	O5'-P-OP1	-8.60	97.96	105.70
1	2A	2385	C	O5'-P-OP1	-8.60	97.96	105.70
1	1A	893	C	N3-C4-C5	8.59	125.34	121.90
32	1a	117	G	O5'-P-OP1	8.58	121.00	110.70
1	2A	2867	G	N1-C6-O6	8.58	125.05	119.90
1	1A	1052	C	C5-C6-N1	-8.58	116.71	121.00
1	1A	1813	C	C5-C6-N1	-8.58	116.71	121.00
1	1A	2718	G	N7-C8-N9	-8.58	108.81	113.10
1	1A	748	G	O5'-P-OP2	-8.57	97.98	105.70
1	1A	2621	U	C5-C6-N1	-8.57	118.41	122.70
32	2a	1127	G	C8-N9-C4	8.57	109.83	106.40
1	1A	1092	A	O4'-C1'-N9	8.57	115.06	108.20
32	1a	254	G	O5'-P-OP1	-8.56	98.00	105.70
32	2a	893	C	C6-N1-C2	8.56	123.72	120.30
1	1A	2538	G	C8-N9-C4	8.56	109.82	106.40
1	1A	2497	G	C8-N9-C4	8.55	109.82	106.40
1	1A	1832	G	C5-C6-O6	-8.55	123.47	128.60
32	1a	533	A	N9-C4-C5	-8.55	102.38	105.80
1	1A	385	G	N1-C6-O6	8.54	125.03	119.90
1	2A	2180	U	C5-C6-N1	8.54	126.97	122.70
2	1B	38	C	N3-C4-N4	-8.54	112.02	118.00
32	1a	438	G	O5'-P-OP2	-8.54	98.01	105.70
1	1A	246	A	O5'-P-OP2	-8.54	98.02	105.70
1	1A	1320	A	C6-C5-N7	-8.54	126.33	132.30
1	2A	1647	G	C8-N9-C4	8.53	109.81	106.40
32	1a	802	A	N9-C4-C5	-8.53	102.39	105.80
32	2a	758	G	O5'-P-OP2	-8.53	98.02	105.70
1	1A	98	U	C2-N1-C1'	8.53	127.93	117.70
1	1A	594	A	C2-N3-C4	8.52	114.86	110.60
1	1A	2134	G	N3-C4-N9	8.52	131.11	126.00
1	2A	752	A	N7-C8-N9	8.52	118.06	113.80
1	1A	1043	G	C5-C6-O6	8.51	133.71	128.60
1	1A	1364	C	O5'-P-OP2	8.51	120.91	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1696	G	O5'-P-OP2	-8.51	98.04	105.70
32	2a	1465	C	C2-N3-C4	-8.51	115.64	119.90
1	1A	1472	G	N9-C4-C5	-8.51	102.00	105.40
1	1A	1803	G	C8-N9-C4	8.51	109.80	106.40
1	2A	789	A	N1-C6-N6	8.51	123.70	118.60
1	2A	2207	G	N7-C8-N9	8.51	117.35	113.10
1	1A	2496	G	C6-C5-N7	-8.50	125.30	130.40
1	1A	2620	G	C5-C6-O6	-8.50	123.50	128.60
1	1A	2579	G	N1-C6-O6	-8.50	114.80	119.90
1	1A	2657	G	C5-N7-C8	-8.50	100.05	104.30
1	1A	1148	C	N1-C2-O2	8.49	124.00	118.90
1	1A	2034	G	N1-C6-O6	-8.49	114.81	119.90
1	1A	2048	C	N1-C2-O2	-8.49	113.81	118.90
1	1A	2606	C	C5-C6-N1	-8.49	116.75	121.00
32	1a	1406	U	C2-N3-C4	-8.49	121.91	127.00
1	2A	2430	A	OP1-P-OP2	8.49	132.33	119.60
32	2a	493	G	O5'-P-OP1	-8.49	98.06	105.70
1	1A	101	A	C2-N3-C4	-8.48	106.36	110.60
1	1A	447	C	C5-C6-N1	-8.48	116.76	121.00
1	1A	830	A	C8-N9-C4	-8.48	102.41	105.80
1	2A	2319	G	N3-C4-C5	8.48	132.84	128.60
1	1A	2556	G	N1-C6-O6	8.48	124.99	119.90
32	1a	1532	U	C6-N1-C2	-8.47	115.92	121.00
1	1A	1301	U	C5-C4-O4	-8.47	120.82	125.90
1	1A	1447	G	O5'-P-OP2	-8.47	98.08	105.70
1	1A	82	G	N1-C6-O6	8.46	124.98	119.90
1	1A	549	U	O5'-P-OP1	-8.46	98.08	105.70
1	1A	950	C	C6-N1-C2	8.46	123.69	120.30
1	2A	2679	A	O5'-P-OP2	-8.46	98.08	105.70
32	1a	758	G	O5'-P-OP1	8.46	120.85	110.70
1	2A	990	A	O5'-P-OP2	-8.46	98.09	105.70
1	1A	1965	U	C5-C6-N1	-8.46	118.47	122.70
1	2A	2073	C	N1-C2-O2	-8.46	113.83	118.90
1	1A	191	U	C2-N3-C4	-8.45	121.93	127.00
1	1A	1785	C	O5'-P-OP2	-8.45	98.09	105.70
1	1A	1874	C	C6-N1-C2	8.45	123.68	120.30
1	1A	2484	G	C6-N1-C2	-8.45	120.03	125.10
1	1A	1300	A	C5-C6-N1	8.44	121.92	117.70
1	2A	214	G	O4'-C1'-N9	8.44	114.95	108.20
1	2A	2463	C	C6-N1-C2	8.44	123.67	120.30
32	1a	1228	C	C6-N1-C2	-8.43	116.93	120.30
1	2A	2041	U	C5-C4-O4	-8.43	120.84	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2001	C	C2-N3-C4	-8.43	115.69	119.90
1	1A	1474	C	C2-N1-C1'	-8.42	109.53	118.80
1	1A	731	G	C5-C6-N1	8.42	115.71	111.50
1	2A	9	U	C2-N3-C4	8.42	132.05	127.00
1	2A	2010	G	O5'-P-OP2	8.42	120.80	110.70
1	1A	2261	U	N3-C4-O4	-8.41	113.51	119.40
1	1A	1453	C	C5-C6-N1	-8.41	116.79	121.00
1	1A	472	G	N1-C6-O6	8.41	124.95	119.90
1	1A	849	A	O5'-P-OP1	-8.41	98.13	105.70
1	2A	1681	G	C5-N7-C8	-8.41	100.09	104.30
32	2a	1034	G	C5-C6-O6	-8.41	123.55	128.60
1	1A	2476	C	C5-C4-N4	-8.41	114.31	120.20
1	1A	2377	G	O5'-P-OP2	-8.40	98.14	105.70
1	1A	197	C	C5-C6-N1	-8.40	116.80	121.00
32	1a	1415	G	OP1-P-O3'	8.40	123.67	105.20
1	1A	1854	G	C8-N9-C4	8.40	109.76	106.40
32	1a	1442	G	N3-C4-C5	-8.40	124.40	128.60
1	2A	1721	G	N3-C2-N2	8.40	125.78	119.90
1	1A	127	C	N1-C2-O2	-8.39	113.86	118.90
1	1A	907	U	O5'-P-OP2	-8.39	98.15	105.70
1	1A	1379	C	O5'-P-OP1	-8.39	98.15	105.70
1	1A	1995	G	C5-N7-C8	8.39	108.49	104.30
1	1A	1395	A	N9-C4-C5	-8.39	102.44	105.80
1	2A	213	A	N1-C6-N6	-8.39	113.57	118.60
1	1A	1003	U	C6-N1-C2	-8.38	115.97	121.00
1	1A	1026	A	C5-C6-N6	-8.38	116.99	123.70
1	1A	2016	C	N1-C2-O2	-8.38	113.87	118.90
1	1A	2590	G	N1-C6-O6	-8.38	114.87	119.90
1	1A	995	G	C5-C6-O6	8.38	133.63	128.60
1	1A	1009	C	O5'-P-OP2	-8.38	98.16	105.70
1	2A	1775	U	N1-C2-O2	-8.37	116.94	122.80
32	2a	1030(D)	A	C8-N9-C4	-8.36	102.46	105.80
1	1A	191	U	C6-N1-C2	8.36	126.01	121.00
1	2A	1097	U	C5-C6-N1	8.36	126.88	122.70
32	1a	343	U	C5-C6-N1	-8.36	118.52	122.70
1	2A	341	G	O5'-P-OP2	-8.36	98.18	105.70
1	1A	2503	U	C5-C4-O4	-8.35	120.89	125.90
32	2a	913	A	P-O3'-C3'	8.35	129.72	119.70
1	1A	1296	G	N1-C6-O6	-8.35	114.89	119.90
1	1A	1831	C	C6-N1-C2	-8.35	116.96	120.30
1	1A	121	G	OP1-P-OP2	8.34	132.12	119.60
1	2A	1340	U	C5-C4-O4	-8.34	120.89	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1075	A	N1-C6-N6	8.34	123.60	118.60
32	1a	814	A	C2-N3-C4	-8.34	106.43	110.60
1	2A	793	A	O5'-P-OP2	-8.34	98.19	105.70
1	2A	2202	C	O5'-P-OP2	-8.34	98.20	105.70
1	2A	247	G	O5'-P-OP2	-8.34	98.20	105.70
1	1A	2496	G	N9-C4-C5	-8.33	102.07	105.40
1	1A	705	C	N3-C2-O2	-8.32	116.07	121.90
1	1A	817	G	O5'-P-OP2	-8.32	98.21	105.70
1	2A	203	C	C6-N1-C2	8.32	123.63	120.30
1	1A	512	C	C4-C5-C6	8.32	121.56	117.40
1	1A	1028	C	N1-C2-O2	-8.32	113.91	118.90
1	2A	2441	C	O5'-P-OP1	-8.32	98.22	105.70
1	1A	2092	G	N3-C2-N2	8.31	125.72	119.90
1	1A	575	G	N1-C6-O6	-8.31	114.91	119.90
1	1A	2006	G	C5-C6-O6	8.31	133.59	128.60
2	1B	38	C	N1-C2-O2	8.31	123.89	118.90
32	2a	346	G	C6-N1-C2	-8.31	120.11	125.10
1	1A	1296	G	C8-N9-C4	-8.31	103.08	106.40
1	1A	1734	G	C8-N9-C4	-8.31	103.08	106.40
1	2A	507	A	C8-N9-C4	8.31	109.12	105.80
1	1A	2858	G	N3-C2-N2	-8.30	114.09	119.90
1	1A	1620	G	C5-C6-O6	-8.30	123.62	128.60
32	2a	574	A	N9-C4-C5	-8.30	102.48	105.80
1	2A	1802	A	C8-N9-C4	8.29	109.12	105.80
1	1A	36	G	O5'-P-OP2	-8.29	98.24	105.70
1	1A	1011	G	C5-C6-O6	8.29	133.57	128.60
1	1A	870	G	O5'-P-OP2	-8.28	98.24	105.70
1	1A	2719	G	C8-N9-C4	8.28	109.71	106.40
1	1A	2452	C	C6-N1-C2	8.27	123.61	120.30
1	1A	2460	A	C6-N1-C2	-8.27	113.64	118.60
1	1A	2611	G	C5-C6-O6	8.27	133.56	128.60
1	2A	2179	C	C6-N1-C2	-8.27	116.99	120.30
32	1a	1442	G	C2-N3-C4	8.27	116.04	111.90
1	1A	2262	G	OP1-P-OP2	8.27	132.00	119.60
1	1A	214	A	O5'-P-OP2	-8.27	98.26	105.70
1	1A	2639	G	N9-C4-C5	-8.27	102.09	105.40
1	2A	2041	U	N1-C2-O2	-8.27	117.01	122.80
1	1A	271	U	O4'-C1'-N1	8.27	114.81	108.20
1	1A	2835	C	C2-N3-C4	-8.27	115.77	119.90
1	1A	1031	C	C4-C5-C6	-8.26	113.27	117.40
1	1A	2346	G	C5-C6-O6	-8.26	123.64	128.60
1	1A	494	G	C5-C6-O6	8.26	133.56	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1921	G	C4-C5-N7	8.26	114.10	110.80
1	1A	36	G	C5-N7-C8	8.26	108.43	104.30
32	2a	173	U	O5'-P-OP1	-8.25	98.27	105.70
1	1A	952	G	N3-C4-N9	-8.25	121.05	126.00
1	2A	1008	C	N3-C2-O2	-8.25	116.12	121.90
1	1A	1988	A	N7-C8-N9	-8.25	109.68	113.80
1	2A	12	U	N3-C2-O2	-8.25	116.43	122.20
1	1A	137	G	C5-N7-C8	8.24	108.42	104.30
1	1A	108	G	O5'-P-OP2	-8.24	98.28	105.70
32	1a	1465	C	C2-N3-C4	-8.24	115.78	119.90
1	2A	1082	U	N1-C1'-C2'	-8.24	102.93	112.00
1	2A	510	C	O5'-P-OP2	-8.24	98.28	105.70
1	1A	2703	C	C6-N1-C2	8.24	123.60	120.30
1	1A	2066	C	C2-N3-C4	-8.24	115.78	119.90
32	1a	1524	C	O5'-P-OP2	-8.24	98.29	105.70
1	2A	598	G	N1-C6-O6	-8.24	114.96	119.90
1	1A	2459	G	OP2-P-O3'	8.23	123.32	105.20
2	1B	59	A	C6-N1-C2	-8.23	113.66	118.60
1	1A	1663	C	C2-N3-C4	-8.23	115.78	119.90
1	1A	1307	C	C6-N1-C2	8.22	123.59	120.30
1	1A	2091	G	C4-C5-N7	-8.22	107.51	110.80
1	2A	188	G	C2-N3-C4	-8.22	107.79	111.90
1	1A	191	U	C5-C6-N1	-8.22	118.59	122.70
32	2a	1436	U	C2-N3-C4	-8.22	122.07	127.00
32	2a	1003	G	N7-C8-N9	8.22	117.21	113.10
1	2A	154	G	C8-N9-C4	8.21	109.69	106.40
1	2A	1363	C	O5'-P-OP2	-8.21	98.31	105.70
1	1A	2018	C	N3-C4-C5	8.21	125.18	121.90
1	1A	2272	C	C4-C5-C6	8.21	121.50	117.40
1	2A	630	G	O5'-P-OP2	-8.21	98.32	105.70
32	1a	483	C	C6-N1-C2	8.19	123.58	120.30
1	1A	1856	A	N1-C6-N6	-8.19	113.69	118.60
1	1A	720	C	N3-C4-C5	8.19	125.17	121.90
1	1A	2048	C	C2-N3-C4	-8.19	115.81	119.90
1	1A	2044	U	C5-C4-O4	-8.19	120.99	125.90
32	1a	297	G	C2-N3-C4	-8.19	107.81	111.90
1	2A	2207	G	C4-N9-C1'	8.19	137.14	126.50
32	2a	266	G	N3-C4-C5	-8.18	124.51	128.60
2	1B	102	A	N1-C2-N3	8.18	133.39	129.30
1	1A	1046	A	O5'-P-OP1	-8.18	98.34	105.70
1	1A	1726	U	C5-C4-O4	-8.18	120.99	125.90
1	2A	1694	C	C6-N1-C2	8.18	123.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1237	G	C5-N7-C8	8.18	108.39	104.30
1	1A	2403	G	O5'-P-OP2	-8.18	98.34	105.70
1	1A	830	A	O5'-P-OP2	-8.17	98.34	105.70
1	1A	752	A	C5-C6-N6	-8.17	117.16	123.70
2	1B	50	G	C5-C6-O6	8.17	133.50	128.60
1	1A	183	G	O5'-P-OP2	-8.17	98.35	105.70
1	1A	854	U	N1-C2-N3	8.17	119.80	114.90
1	1A	2545	A	O5'-P-OP2	-8.16	98.36	105.70
1	1A	1184	G	N9-C4-C5	8.16	108.66	105.40
32	2a	245	C	O5'-P-OP1	-8.16	98.36	105.70
2	1B	55	U	O5'-P-OP1	-8.15	98.36	105.70
1	1A	841	G	N1-C6-O6	-8.15	115.01	119.90
1	1A	554	A	O4'-C1'-N9	8.15	114.72	108.20
1	1A	1210	G	O5'-P-OP2	-8.15	98.37	105.70
32	1a	266	G	C6-C5-N7	-8.15	125.51	130.40
1	1A	952	G	N1-C6-O6	-8.15	115.01	119.90
1	1A	1861	C	N3-C4-C5	8.14	125.16	121.90
1	1A	2447	A	O5'-P-OP1	-8.14	98.37	105.70
32	1a	438	G	N1-C6-O6	-8.14	115.02	119.90
32	1a	250	A	C8-N9-C4	-8.14	102.55	105.80
1	1A	1210	G	N1-C6-O6	-8.13	115.02	119.90
1	1A	2597	U	O5'-P-OP1	8.13	120.46	110.70
1	1A	673	G	O5'-P-OP2	-8.13	98.38	105.70
1	2A	2013	A	C2-N3-C4	-8.12	106.54	110.60
1	1A	2671	G	C2-N3-C4	-8.12	107.84	111.90
1	2A	1471	A	C8-N9-C4	-8.12	102.55	105.80
32	1a	1505	G	N9-C4-C5	8.12	108.65	105.40
32	2a	1027	C	N1-C2-O2	8.11	123.77	118.90
1	1A	294	C	O5'-P-OP2	-8.11	98.40	105.70
1	1A	1154	U	N3-C4-O4	8.11	125.08	119.40
1	1A	1655	A	N1-C6-N6	8.11	123.47	118.60
1	1A	1785	C	N1-C2-O2	8.11	123.76	118.90
1	1A	1811	A	N7-C8-N9	8.11	117.85	113.80
1	1A	1847	G	O5'-P-OP1	-8.11	98.41	105.70
2	2B	54	G	N3-C2-N2	-8.11	114.23	119.90
32	2a	266	G	C4-N9-C1'	8.11	137.04	126.50
1	2A	1073	A	N9-C1'-C2'	-8.10	103.08	112.00
1	1A	2877	G	N1-C6-O6	8.09	124.76	119.90
1	1A	1434	G	O5'-P-OP2	-8.09	98.42	105.70
1	1A	562	C	C5-C6-N1	-8.09	116.96	121.00
2	1B	41	U	N1-C2-N3	8.09	119.75	114.90
1	2A	1778	U	C5-C6-N1	-8.09	118.66	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	132	G	O5'-P-OP2	-8.09	98.42	105.70
32	2a	1378	C	C6-N1-C2	-8.09	117.07	120.30
1	2A	1966	A	N1-C6-N6	-8.08	113.75	118.60
1	1A	2623	U	O5'-P-OP1	-8.08	98.43	105.70
1	1A	37	C	O5'-P-OP2	-8.07	98.43	105.70
1	1A	1151	U	N1-C2-N3	-8.07	110.06	114.90
1	2A	1045	A	N7-C8-N9	8.07	117.84	113.80
1	1A	594	A	O5'-P-OP1	-8.07	98.44	105.70
1	1A	1065	U	O5'-P-OP2	-8.07	98.44	105.70
1	1A	1640	G	N9-C4-C5	8.07	108.63	105.40
1	1A	1611	C	C5-C4-N4	8.07	125.85	120.20
1	2A	1926	U	C5-C4-O4	8.07	130.74	125.90
32	2a	1499	A	C8-N9-C4	8.07	109.03	105.80
1	1A	718	C	C5-C4-N4	8.07	125.85	120.20
1	1A	2454	C	C5-C6-N1	-8.07	116.97	121.00
32	1a	1492	A	C8-N9-C4	-8.07	102.57	105.80
1	2A	1394	U	O5'-P-OP2	8.07	120.38	110.70
1	2A	1663	C	N3-C4-C5	8.07	125.13	121.90
1	2A	1904	G	C5-C6-O6	8.07	133.44	128.60
1	1A	892	G	O4'-C1'-N9	8.06	114.65	108.20
32	1a	896	C	C6-N1-C2	8.06	123.53	120.30
1	2A	97	C	C6-N1-C2	8.06	123.53	120.30
1	2A	2105	C	C6-N1-C2	-8.06	117.07	120.30
1	2A	1906	G	O5'-P-OP1	-8.06	98.45	105.70
1	1A	2780	C	C6-N1-C2	-8.06	117.08	120.30
32	1a	217	C	C6-N1-C2	8.06	123.52	120.30
1	1A	876	A	OP1-P-OP2	8.05	131.68	119.60
1	1A	1612	C	C6-N1-C2	8.06	123.52	120.30
1	1A	2081	A	C5-N7-C8	8.06	107.93	103.90
1	1A	2106	C	N3-C4-C5	8.05	125.12	121.90
1	1A	2638	C	N1-C2-O2	-8.05	114.07	118.90
6	1G	126	ASP	CB-CG-OD1	-8.05	111.06	118.30
13	1R	17	ARG	NE-CZ-NH1	-8.05	116.27	120.30
1	1A	808	A	O5'-P-OP1	8.04	120.35	110.70
1	1A	1420	G	OP1-P-OP2	-8.04	107.54	119.60
1	1A	2436	C	N1-C2-O2	-8.04	114.08	118.90
1	1A	2579	G	C5-N7-C8	8.04	108.32	104.30
1	1A	790	G	C5-N7-C8	8.04	108.32	104.30
32	1a	1495	U	C2-N1-C1'	8.03	127.34	117.70
1	1A	436	C	C6-N1-C2	8.03	123.51	120.30
1	2A	807	U	C4-C5-C6	8.03	124.52	119.70
1	1A	792	G	C5-C6-O6	-8.02	123.79	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	836	A	C2-N3-C4	-8.02	106.59	110.60
32	1a	115	G	O5'-P-OP2	-8.02	98.48	105.70
1	2A	652(T)	C	C5-C6-N1	8.02	125.01	121.00
1	2A	741	G	O5'-P-OP1	-8.02	98.48	105.70
1	1A	1092	A	C8-N9-C4	-8.02	102.59	105.80
1	1A	2387	G	N9-C4-C5	-8.02	102.19	105.40
1	1A	2551	C	C5-C6-N1	-8.02	116.99	121.00
1	2A	2501	C	C2-N1-C1'	-8.02	109.98	118.80
1	2A	2540	C	O5'-P-OP2	-8.02	98.48	105.70
1	1A	106	U	C2-N3-C4	-8.01	122.19	127.00
1	2A	1075	C	N3-C2-O2	-8.01	116.29	121.90
1	1A	121	G	C5-C6-O6	-8.01	123.80	128.60
1	1A	418	G	C8-N9-C4	8.01	109.60	106.40
1	1A	1050	C	C2-N3-C4	-8.01	115.90	119.90
1	2A	1097	U	C6-N1-C1'	-8.01	109.99	121.20
1	2A	2010	G	OP1-P-OP2	-8.00	107.59	119.60
1	2A	2046	G	C8-N9-C4	8.00	109.60	106.40
32	2a	768	A	N1-C2-N3	8.00	133.30	129.30
1	1A	2432	C	N1-C2-O2	-8.00	114.10	118.90
1	2A	669	G	N3-C2-N2	-8.00	114.30	119.90
1	1A	1325	G	N1-C6-O6	-7.99	115.10	119.90
1	1A	369	A	C5-C6-N6	-7.99	117.31	123.70
1	1A	777	C	O5'-P-OP1	-7.99	98.51	105.70
1	2A	1678	G	C8-N9-C4	-7.99	103.20	106.40
1	1A	101	A	N1-C6-N6	7.99	123.39	118.60
1	1A	1838	G	N1-C6-O6	7.99	124.69	119.90
1	1A	2181	G	N3-C4-N9	7.99	130.79	126.00
1	1A	1472	G	C4-C5-N7	7.98	113.99	110.80
1	1A	1828	C	C6-N1-C2	7.98	123.49	120.30
1	2A	113	G	N3-C4-C5	7.98	132.59	128.60
1	1A	2003	A	C5-C6-N6	-7.98	117.32	123.70
1	1A	2188	G	N3-C4-N9	-7.98	121.21	126.00
1	2A	2875	C	C6-N1-C2	7.98	123.49	120.30
1	1A	61	C	C6-N1-C2	7.97	123.49	120.30
1	1A	2264	G	C5-C6-O6	-7.97	123.81	128.60
32	1a	802	A	C5-C6-N6	-7.97	117.32	123.70
1	1A	1766	G	C5-N7-C8	-7.97	100.31	104.30
32	1a	366	C	O5'-P-OP2	-7.97	98.53	105.70
1	1A	2503	U	N3-C2-O2	7.96	127.77	122.20
1	1A	2158	C	N3-C2-O2	-7.96	116.33	121.90
1	1A	1282	G	N7-C8-N9	-7.96	109.12	113.10
1	1A	1742	G	C2-N3-C4	-7.96	107.92	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2525	G	O5'-P-OP2	-7.96	98.54	105.70
1	2A	2319	G	C2-N3-C4	-7.96	107.92	111.90
1	1A	476	G	C5-C6-N1	7.96	115.48	111.50
32	1a	1422	G	O5'-P-OP2	-7.96	98.54	105.70
1	1A	417	A	C8-N9-C4	7.95	108.98	105.80
1	1A	1135	G	N3-C4-C5	-7.95	124.62	128.60
1	1A	1700	G	P-O3'-C3'	7.95	129.24	119.70
1	2A	2318	G	N7-C8-N9	7.95	117.08	113.10
1	2A	2324	C	C5-C4-N4	-7.95	114.63	120.20
1	2A	2585	U	C2-N1-C1'	-7.95	108.16	117.70
1	1A	2227	G	C4-N9-C1'	-7.95	116.17	126.50
32	1a	156	G	C8-N9-C4	-7.95	103.22	106.40
1	1A	786	G	C5-C6-O6	-7.94	123.83	128.60
32	1a	172	A	C8-N9-C4	-7.93	102.63	105.80
32	1a	718	G	O5'-P-OP2	7.93	120.21	110.70
32	1a	487	A	C8-N9-C4	7.93	108.97	105.80
1	2A	1349	A	O5'-P-OP1	-7.92	98.57	105.70
32	2a	901	A	N1-C2-N3	7.92	133.26	129.30
1	1A	1853	G	N3-C2-N2	7.92	125.44	119.90
1	1A	2496	G	N1-C6-O6	7.92	124.65	119.90
1	2A	2282	G	O5'-P-OP2	7.92	120.21	110.70
1	2A	391	G	C5-C6-O6	-7.92	123.85	128.60
1	1A	1279	C	C5-C6-N1	-7.92	117.04	121.00
1	1A	793	A	O4'-C1'-N9	7.92	114.53	108.20
1	2A	1670	C	N3-C4-C5	-7.91	118.73	121.90
32	2a	1495	U	C2-N1-C1'	7.91	127.20	117.70
1	1A	2134	G	C4-N9-C1'	7.91	136.78	126.50
1	1A	545	G	N1-C6-O6	-7.91	115.16	119.90
1	1A	801	C	N3-C4-C5	7.91	125.06	121.90
1	1A	1662	A	O5'-P-OP1	-7.91	98.58	105.70
1	1A	2475	C	C6-N1-C2	7.91	123.46	120.30
1	2A	2207	G	N1-C6-O6	7.91	124.64	119.90
1	1A	12	U	N3-C2-O2	-7.90	116.67	122.20
1	2A	383	U	N1-C2-O2	7.90	128.33	122.80
1	1A	1033	G	N3-C2-N2	-7.90	114.37	119.90
1	1A	1242	G	N1-C6-O6	-7.90	115.16	119.90
1	1A	2273	C	O5'-P-OP2	-7.90	98.59	105.70
32	2a	115	G	O5'-P-OP2	-7.90	98.59	105.70
1	1A	1857	G	N9-C4-C5	7.90	108.56	105.40
1	2A	2744	G	O5'-P-OP2	-7.89	98.59	105.70
32	1a	821	G	N1-C6-O6	7.89	124.64	119.90
32	2a	834	C	C6-N1-C2	7.89	123.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	779	C	C6-N1-C2	-7.89	117.14	120.30
1	1A	2187	G	N1-C6-O6	-7.89	115.17	119.90
1	1A	874	U	C5-C6-N1	-7.89	118.76	122.70
1	1A	1001	G	C2-N3-C4	-7.88	107.96	111.90
1	1A	1707	C	N3-C4-C5	7.88	125.05	121.90
1	2A	391	G	C6-N1-C2	-7.88	120.37	125.10
32	2a	574	A	C5-C6-N6	-7.88	117.40	123.70
1	1A	2460	A	N1-C6-N6	7.88	123.33	118.60
32	2a	299	G	N9-C4-C5	-7.87	102.25	105.40
1	1A	198	C	C5-C6-N1	-7.87	117.06	121.00
32	1a	900	A	OP1-P-OP2	-7.87	107.80	119.60
1	1A	2023	A	C2-N3-C4	7.87	114.53	110.60
1	1A	1001	G	N1-C6-O6	7.87	124.62	119.90
1	1A	1567	G	C8-N9-C4	-7.87	103.25	106.40
1	1A	2277	U	C4-C5-C6	7.87	124.42	119.70
32	2a	404	U	C2-N1-C1'	7.87	127.14	117.70
1	1A	859	C	N3-C2-O2	7.86	127.40	121.90
1	1A	2107	C	C6-N1-C2	7.86	123.44	120.30
1	1A	1395	A	C5-C6-N6	-7.86	117.41	123.70
1	1A	957	A	OP1-P-OP2	7.86	131.39	119.60
1	2A	1308	A	O5'-P-OP2	-7.86	98.62	105.70
1	1A	27	G	O5'-P-OP2	-7.86	98.63	105.70
1	1A	1312	G	C5-C6-N1	7.86	115.43	111.50
1	1A	2259	A	N9-C4-C5	-7.86	102.66	105.80
1	1A	2440	G	N9-C4-C5	7.86	108.54	105.40
32	1a	299	G	C5-C6-O6	-7.86	123.89	128.60
1	2A	1236	G	O5'-P-OP1	-7.86	98.63	105.70
1	2A	1881	C	O5'-P-OP1	-7.86	98.63	105.70
1	1A	2034	G	O5'-P-OP2	-7.85	98.63	105.70
1	1A	2880	C	N1-C2-O2	-7.85	114.19	118.90
1	1A	1170	C	C2-N3-C4	-7.85	115.97	119.90
1	2A	2275	C	O4'-C1'-N1	-7.85	101.92	108.20
1	1A	10	G	N1-C6-O6	-7.85	115.19	119.90
1	1A	174	U	C5-C6-N1	-7.85	118.78	122.70
1	1A	1281	G	C5-C6-N1	-7.84	107.58	111.50
1	1A	1827	U	C5-C6-N1	-7.84	118.78	122.70
1	2A	1664	A	O5'-P-OP2	-7.84	98.64	105.70
1	1A	1965	U	N1-C2-N3	7.84	119.60	114.90
1	1A	1977	U	N1-C2-O2	-7.84	117.31	122.80
1	1A	2611	G	N1-C6-O6	-7.84	115.20	119.90
1	2A	2166	G	N3-C2-N2	-7.84	114.41	119.90
1	1A	583	C	C6-N1-C2	7.84	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1067	A	P-O3'-C3'	7.84	129.10	119.70
1	2A	1284	A	O5'-P-OP2	-7.84	98.65	105.70
1	1A	2108	U	N3-C2-O2	-7.83	116.72	122.20
1	1A	2839	C	C6-N1-C2	-7.83	117.17	120.30
32	1a	322	C	C6-N1-C2	7.83	123.43	120.30
32	2a	655	A	O5'-P-OP2	-7.83	98.65	105.70
32	2a	1054	C	C2-N1-C1'	7.83	127.42	118.80
1	1A	640	A	OP1-P-OP2	7.83	131.35	119.60
1	1A	1614	A	N1-C6-N6	-7.83	113.90	118.60
1	1A	592	U	C5-C4-O4	-7.83	121.20	125.90
1	1A	2397	C	O5'-P-OP1	-7.83	98.65	105.70
1	2A	1769	G	N1-C6-O6	7.83	124.60	119.90
1	2A	912	C	C6-N1-C2	-7.83	117.17	120.30
1	1A	733	G	C5-C6-O6	-7.82	123.91	128.60
1	1A	649	C	C6-N1-C2	7.82	123.43	120.30
1	1A	2835	C	C5-C6-N1	-7.82	117.09	121.00
1	1A	189	U	N1-C2-O2	-7.82	117.33	122.80
32	1a	533	A	N3-C4-N9	7.82	133.66	127.40
1	1A	2346	G	C5-N7-C8	-7.82	100.39	104.30
1	1A	2537	G	O5'-P-OP2	-7.82	98.67	105.70
32	2a	896	C	C6-N1-C2	7.82	123.43	120.30
1	1A	1518	A	C8-N9-C4	-7.82	102.67	105.80
1	1A	13	A	C8-N9-C4	-7.81	102.67	105.80
2	1B	13	A	N7-C8-N9	-7.81	109.89	113.80
32	1a	1495	U	N1-C2-O2	7.81	128.27	122.80
1	1A	194	G	O5'-P-OP2	-7.81	98.67	105.70
32	1a	58	C	O5'-P-OP1	-7.80	98.68	105.70
1	2A	2896	C	C5-C6-N1	7.80	124.90	121.00
1	2A	2523	G	O5'-P-OP1	7.80	120.06	110.70
1	1A	826	U	N3-C4-O4	7.80	124.86	119.40
1	2A	2062	A	C8-N9-C4	7.80	108.92	105.80
2	1B	98	G	C5-C6-O6	-7.80	123.92	128.60
1	2A	958	U	C6-N1-C2	-7.80	116.32	121.00
1	1A	2111	U	C5-C4-O4	-7.79	121.22	125.90
1	1A	2691	A	C5-C6-N1	7.79	121.60	117.70
32	2a	487	A	C8-N9-C4	7.79	108.92	105.80
1	1A	2348	A	N9-C4-C5	-7.79	102.69	105.80
1	2A	2505	G	C5-C6-N1	-7.79	107.61	111.50
32	2a	1432	G	N1-C6-O6	-7.79	115.23	119.90
1	1A	2858	G	N9-C4-C5	7.79	108.51	105.40
1	1A	1279	C	C2-N3-C4	-7.78	116.01	119.90
32	1a	221	C	C6-N1-C2	-7.78	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1933	G	OP1-P-OP2	7.78	131.28	119.60
1	1A	2630	G	C5-C6-O6	7.78	133.27	128.60
1	1A	762	G	C5-C6-O6	-7.78	123.93	128.60
1	1A	1474	C	C6-N1-C2	7.77	123.41	120.30
2	1B	52	A	N9-C4-C5	-7.77	102.69	105.80
32	2a	1391	U	C5-C4-O4	7.77	130.56	125.90
1	1A	1991	A	O5'-P-OP2	7.77	120.03	110.70
1	2A	2511	U	N1-C2-N3	7.77	119.56	114.90
32	2a	1530	G	C5-C6-O6	-7.77	123.94	128.60
1	1A	952	G	C8-N9-C4	-7.77	103.29	106.40
1	1A	2390	A	O5'-P-OP1	-7.77	98.71	105.70
2	1B	51	G	O5'-P-OP1	7.77	120.02	110.70
32	1a	863	U	O5'-P-OP2	-7.77	98.71	105.70
1	1A	2067	C	C5-C6-N1	-7.76	117.12	121.00
1	2A	469	G	C5-C6-O6	-7.76	123.94	128.60
1	1A	724	A	C4-C5-C6	7.76	120.88	117.00
1	1A	1142	A	O4'-C1'-N9	7.76	114.41	108.20
1	1A	1303	C	C4-C5-C6	7.76	121.28	117.40
1	1A	705	C	C2-N1-C1'	7.76	127.33	118.80
1	2A	123	G	N1-C6-O6	7.76	124.55	119.90
1	2A	2451	A	C5-N7-C8	-7.75	100.02	103.90
32	2a	346	G	C2-N3-C4	7.75	115.78	111.90
1	1A	795	G	C5-C6-N1	7.75	115.38	111.50
1	1A	184	A	P-O3'-C3'	7.75	129.00	119.70
1	1A	1056	A	C8-N9-C4	7.75	108.90	105.80
1	1A	2511	C	N3-C4-N4	7.75	123.42	118.00
32	1a	615	C	C6-N1-C2	-7.75	117.20	120.30
32	2a	1030(B)	C	C6-N1-C2	-7.75	117.20	120.30
1	1A	271	U	C5-C4-O4	7.74	130.55	125.90
1	1A	1066	A	O5'-P-OP2	-7.74	98.73	105.70
32	2a	993	G	N3-C4-N9	7.74	130.65	126.00
1	1A	2551	C	C6-N1-C2	7.74	123.40	120.30
32	1a	1181	G	N3-C4-C5	7.74	132.47	128.60
1	1A	127	C	N3-C2-O2	7.74	127.32	121.90
1	1A	2499	G	N9-C4-C5	-7.74	102.31	105.40
1	1A	1026	A	N9-C4-C5	-7.74	102.71	105.80
1	1A	1028	C	N3-C2-O2	7.74	127.31	121.90
1	1A	1121	C	N1-C2-O2	7.74	123.54	118.90
32	2a	555	C	N3-C4-N4	7.73	123.41	118.00
1	1A	1993	A	C8-N9-C4	7.73	108.89	105.80
2	1B	113	G	N9-C4-C5	-7.73	102.31	105.40
32	1a	1233	G	N1-C6-O6	-7.73	115.26	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2308	U	N3-C4-O4	7.73	124.81	119.40
1	1A	2802	C	N3-C4-N4	-7.73	112.59	118.00
1	1A	88	G	C8-N9-C4	-7.73	103.31	106.40
1	1A	1168	G	C5-C6-N1	7.73	115.36	111.50
32	1a	1532	U	C5-C6-N1	7.73	126.56	122.70
32	2a	898	G	N9-C4-C5	-7.73	102.31	105.40
1	1A	934	A	O4'-C1'-N9	7.72	114.38	108.20
1	1A	873	U	C5-C6-N1	-7.72	118.84	122.70
1	2A	1639	U	C5-C6-N1	-7.72	118.84	122.70
1	2A	1497	U	C5-C6-N1	-7.72	118.84	122.70
1	2A	2629	A	O4'-C1'-N9	7.72	114.38	108.20
1	1A	514	G	C4-C5-N7	-7.72	107.71	110.80
32	2a	615	C	C6-N1-C2	-7.72	117.21	120.30
1	1A	1040	C	C5-C6-N1	-7.72	117.14	121.00
1	1A	1494	G	N9-C4-C5	7.72	108.49	105.40
1	1A	2366	G	C5-C6-O6	7.72	133.23	128.60
1	1A	2409	G	N3-C2-N2	-7.72	114.50	119.90
1	1A	2523	U	N1-C2-O2	-7.72	117.40	122.80
32	2a	1445	C	C6-N1-C2	7.72	123.39	120.30
1	2A	1405	U	O5'-P-OP2	-7.71	98.76	105.70
1	1A	725	C	C2-N3-C4	-7.71	116.04	119.90
1	1A	2075	G	N9-C4-C5	7.71	108.48	105.40
1	1A	2238	C	C6-N1-C2	7.71	123.39	120.30
2	1B	50	G	O5'-P-OP2	-7.71	98.76	105.70
1	1A	2835	C	C5-C4-N4	-7.71	114.80	120.20
32	2a	1406	U	N1-C2-N3	7.71	119.53	114.90
1	2A	1837	C	O5'-P-OP1	-7.71	98.76	105.70
32	1a	175	C	C6-N1-C2	-7.71	117.22	120.30
1	1A	1102	G	N9-C4-C5	-7.70	102.32	105.40
1	1A	1247	C	C4-C5-C6	7.70	121.25	117.40
32	2a	816	A	O5'-P-OP1	7.70	119.94	110.70
1	1A	2094	G	C2-N3-C4	7.70	115.75	111.90
1	1A	2087	C	C6-N1-C2	7.69	123.38	120.30
32	1a	653	A	N1-C6-N6	7.69	123.22	118.60
1	1A	976	G	N3-C4-C5	-7.69	124.75	128.60
1	1A	1243	U	N1-C2-N3	7.69	119.51	114.90
1	2A	1271	G	N9-C4-C5	-7.69	102.32	105.40
1	1A	2024	G	N7-C8-N9	-7.69	109.26	113.10
1	1A	276	C	O5'-P-OP2	-7.68	98.79	105.70
32	1a	181	G	C8-N9-C4	-7.68	103.33	106.40
32	1a	266	G	N7-C8-N9	7.68	116.94	113.10
32	1a	1021	G	N1-C6-O6	-7.68	115.29	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	52	A	N1-C6-N6	7.68	123.21	118.60
1	1A	2774	G	C8-N9-C4	7.68	109.47	106.40
1	2A	679	C	N3-C2-O2	7.68	127.28	121.90
1	1A	709	G	C5-C6-O6	7.68	133.21	128.60
1	1A	790	G	N3-C4-C5	-7.68	124.76	128.60
1	1A	857	U	N3-C4-O4	7.68	124.77	119.40
1	1A	1985	U	C5-C6-N1	7.68	126.54	122.70
32	2a	830	G	N1-C6-O6	7.68	124.51	119.90
2	1B	63	G	O5'-P-OP2	-7.67	98.80	105.70
2	1B	115	G	C8-N9-C4	7.67	109.47	106.40
1	1A	2475	C	N3-C4-N4	-7.67	112.63	118.00
1	1A	1994	A	O5'-P-OP2	-7.67	98.80	105.70
1	1A	612	C	O5'-P-OP2	-7.67	98.80	105.70
1	1A	2063	U	C2-N3-C4	-7.66	122.40	127.00
1	1A	2538	G	N7-C8-N9	-7.66	109.27	113.10
2	1B	52	A	C8-N9-C4	7.66	108.86	105.80
2	2B	41	U	N3-C2-O2	-7.66	116.84	122.20
1	1A	2525	G	C4-C5-N7	7.66	113.86	110.80
1	2A	1075	C	C6-N1-C2	-7.66	117.24	120.30
1	2A	1984	G	C8-N9-C4	-7.66	103.34	106.40
1	1A	218	A	C8-N9-C4	-7.66	102.74	105.80
1	1A	1314	A	C5-C6-N1	-7.66	113.87	117.70
1	1A	1026	A	C5-C6-N1	7.65	121.53	117.70
1	1A	2106	C	C2-N3-C4	-7.65	116.07	119.90
1	1A	2335	G	N7-C8-N9	7.65	116.93	113.10
32	2a	144	G	C8-N9-C4	-7.65	103.34	106.40
1	1A	197	C	C6-N1-C2	7.65	123.36	120.30
1	1A	905	U	O5'-P-OP2	-7.65	98.82	105.70
1	1A	1986	G	C4-C5-N7	7.65	113.86	110.80
1	1A	1666	G	C5-C6-O6	7.65	133.19	128.60
1	1A	41	C	O5'-P-OP1	7.64	119.87	110.70
1	1A	194	G	N9-C4-C5	-7.64	102.34	105.40
1	1A	2251	G	N1-C6-O6	-7.64	115.31	119.90
1	2A	2137	C	C6-N1-C2	-7.64	117.24	120.30
1	1A	2593	G	C4-C5-N7	7.64	113.86	110.80
32	2a	1531	A	N1-C6-N6	7.64	123.19	118.60
32	1a	1331	G	O4'-C1'-N9	7.64	114.31	108.20
1	2A	2577	A	C5-C6-N1	-7.64	113.88	117.70
1	1A	1952	G	O5'-P-OP2	-7.64	98.83	105.70
1	2A	2560	C	C6-N1-C2	7.63	123.35	120.30
1	2A	2699	C	N3-C4-C5	7.63	124.95	121.90
32	2a	115	G	C8-N9-C4	-7.63	103.35	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	950	C	N3-C4-C5	7.63	124.95	121.90
1	1A	138	G	C5-N7-C8	7.63	108.12	104.30
1	1A	1475	G	C5-C6-O6	7.63	133.18	128.60
1	1A	2079	A	OP2-P-O3'	7.63	121.99	105.20
1	1A	591	U	C6-N1-C2	7.63	125.58	121.00
1	1A	567	C	N3-C4-C5	7.63	124.95	121.90
1	2A	417	C	C6-N1-C2	-7.63	117.25	120.30
1	2A	2378	A	C6-C5-N7	-7.63	126.96	132.30
1	1A	107	G	C4-C5-N7	-7.63	107.75	110.80
1	1A	415	G	N9-C4-C5	-7.62	102.35	105.40
2	2B	59	A	C6-N1-C2	-7.62	114.03	118.60
1	1A	2344	U	C6-N1-C2	7.62	125.57	121.00
1	1A	830	A	N9-C4-C5	7.62	108.85	105.80
1	1A	902	G	N3-C2-N2	7.62	125.23	119.90
1	1A	2252	C	O5'-P-OP1	7.62	119.84	110.70
1	1A	2416	C	N1-C2-O2	-7.62	114.33	118.90
1	2A	97	C	C5-C6-N1	-7.62	117.19	121.00
1	1A	2724	U	C5-C6-N1	-7.62	118.89	122.70
32	1a	339	C	C6-N1-C2	7.62	123.35	120.30
32	1a	563	A	C8-N9-C4	-7.62	102.75	105.80
2	1B	41	U	C5-C4-O4	7.61	130.47	125.90
1	2A	1936	A	O4'-C1'-N9	7.61	114.29	108.20
32	2a	1370	G	N9-C4-C5	-7.61	102.36	105.40
1	2A	718	A	C6-C5-N7	-7.61	126.97	132.30
1	1A	799	A	N3-C4-C5	7.61	132.13	126.80
1	1A	2632	C	C6-N1-C2	7.61	123.34	120.30
32	1a	1278	U	C5-C6-N1	7.61	126.50	122.70
1	2A	572	A	C8-N9-C4	-7.61	102.76	105.80
1	1A	1190	G	N1-C6-O6	-7.61	115.34	119.90
1	1A	1539	C	N3-C2-O2	-7.61	116.58	121.90
1	2A	1518	U	C5-C4-O4	7.61	130.46	125.90
1	1A	918	U	O5'-P-OP2	7.60	119.83	110.70
2	1B	24	G	N3-C4-N9	7.60	130.56	126.00
32	1a	913	A	P-O3'-C3'	7.60	128.82	119.70
32	1a	1176	A	C8-N9-C4	-7.60	102.76	105.80
32	1a	1276	G	C8-N9-C4	-7.60	103.36	106.40
1	1A	2093	A	C4-C5-C6	7.60	120.80	117.00
32	1a	1515	C	N1-C2-O2	-7.60	114.34	118.90
1	1A	733	G	C6-C5-N7	-7.60	125.84	130.40
1	1A	2590	G	C5-C6-O6	7.60	133.16	128.60
32	1a	1287	A	C5-C6-N6	7.60	129.78	123.70
32	1a	1331	G	O5'-P-OP2	-7.60	98.86	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	771	G	N1-C6-O6	7.60	124.46	119.90
32	2a	993	G	N3-C4-C5	-7.60	124.80	128.60
1	1A	1453	C	C6-N1-C2	7.60	123.34	120.30
1	1A	889	G	O5'-P-OP1	7.59	119.81	110.70
1	1A	990	A	O5'-P-OP1	7.59	119.81	110.70
32	1a	1021	G	C2-N3-C4	7.59	115.70	111.90
1	2A	1399	C	OP2-P-O3'	7.59	121.91	105.20
1	1A	102	U	C5-C4-O4	-7.59	121.34	125.90
2	1B	74	U	N1-C2-O2	-7.59	117.48	122.80
1	1A	1562	U	O5'-P-OP2	-7.59	98.87	105.70
1	1A	2106	C	C6-N1-C2	7.59	123.34	120.30
1	1A	2902	G	N1-C2-N3	-7.59	119.34	123.90
1	2A	2399	G	C5-C6-O6	7.59	133.15	128.60
1	1A	655	G	C5-C6-O6	-7.59	124.05	128.60
1	1A	672	G	C4-C5-N7	-7.59	107.76	110.80
1	1A	809	U	O5'-P-OP1	-7.59	98.87	105.70
1	1A	2251	G	N7-C8-N9	-7.59	109.31	113.10
1	2A	576	U	O5'-P-OP1	-7.59	98.87	105.70
1	2A	1430	C	C6-N1-C2	-7.59	117.26	120.30
32	1a	399	G	N1-C6-O6	7.59	124.45	119.90
1	1A	1403	U	N3-C2-O2	-7.58	116.89	122.20
1	1A	2384	G	C5-C6-O6	-7.58	124.05	128.60
1	2A	271(Y)	U	N3-C2-O2	-7.58	116.89	122.20
1	2A	1678	G	N3-C4-C5	-7.58	124.81	128.60
1	2A	1187	G	C5-C6-O6	7.58	133.15	128.60
1	1A	2082	A	N1-C6-N6	-7.58	114.05	118.60
32	1a	1515	C	N3-C4-N4	7.58	123.31	118.00
1	1A	1255	A	C8-N9-C4	-7.58	102.77	105.80
1	1A	2576	A	N1-C6-N6	7.58	123.15	118.60
1	1A	2703	C	N3-C4-C5	7.58	124.93	121.90
1	1A	1816	A	C8-N9-C4	-7.58	102.77	105.80
1	1A	2591	C	N1-C2-O2	7.58	123.44	118.90
1	1A	2059	G	C5-C6-O6	7.57	133.14	128.60
1	2A	858	U	N3-C2-O2	-7.57	116.90	122.20
1	2A	2093	G	C5-C6-O6	-7.57	124.06	128.60
1	2A	1368	G	O5'-P-OP2	-7.57	98.89	105.70
1	1A	1855	G	O5'-P-OP2	-7.57	98.89	105.70
1	1A	990	A	C8-N9-C4	7.56	108.83	105.80
1	2A	614	U	C6-N1-C2	-7.56	116.46	121.00
1	1A	1245	C	N3-C4-N4	-7.56	112.71	118.00
1	1A	799	A	N9-C4-C5	-7.56	102.78	105.80
1	1A	2281	A	O5'-P-OP1	-7.56	98.90	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	645	C	C5-C6-N1	7.56	124.78	121.00
1	1A	2780	C	N3-C2-O2	-7.56	116.61	121.90
1	2A	2508	G	C8-N9-C4	7.56	109.42	106.40
1	2A	2817	G	N1-C6-O6	-7.56	115.37	119.90
1	2A	2893	G	C5-C6-O6	-7.56	124.07	128.60
1	1A	760	G	C8-N9-C4	7.55	109.42	106.40
1	1A	2336	C	C5-C4-N4	-7.55	114.91	120.20
1	1A	2590	G	C4-C5-N7	-7.55	107.78	110.80
1	1A	2044	U	N3-C2-O2	7.55	127.49	122.20
1	2A	739	G	O5'-P-OP1	-7.55	98.91	105.70
1	2A	2805	G	N3-C4-C5	-7.55	124.82	128.60
32	2a	1034	G	C6-N1-C2	-7.55	120.57	125.10
32	2a	1081	G	O5'-P-OP2	-7.55	98.91	105.70
1	1A	533	G	O5'-P-OP1	-7.55	98.91	105.70
1	2A	759	G	O5'-P-OP1	-7.55	98.91	105.70
1	1A	791	G	N1-C6-O6	-7.54	115.37	119.90
1	1A	1440	U	O5'-P-OP2	7.54	119.75	110.70
1	1A	2342	G	C5-C6-O6	-7.54	124.08	128.60
1	2A	718	A	C4-C5-C6	7.54	120.77	117.00
32	2a	1530	G	N1-C6-O6	7.54	124.42	119.90
32	1a	1436	U	N1-C2-N3	7.54	119.42	114.90
1	2A	2022	U	O5'-P-OP1	-7.54	98.92	105.70
1	1A	1613	A	N9-C4-C5	-7.53	102.79	105.80
1	1A	271	U	C6-N1-C1'	7.53	131.74	121.20
1	2A	1694	C	N3-C4-C5	7.53	124.91	121.90
1	1A	580	U	C5-C4-O4	-7.53	121.38	125.90
1	2A	1637	A	C2-N3-C4	-7.53	106.84	110.60
32	2a	1405	G	O5'-P-OP2	-7.53	98.92	105.70
1	1A	886	U	N3-C4-O4	-7.53	114.13	119.40
1	1A	1991	A	O5'-P-OP1	-7.53	98.93	105.70
1	2A	702	G	O5'-P-OP2	-7.53	98.93	105.70
32	1a	23	C	C6-N1-C2	-7.52	117.29	120.30
1	2A	2685	G	N1-C6-O6	-7.52	115.39	119.90
1	2A	2811	G	O5'-P-OP2	-7.52	98.93	105.70
1	1A	1132	A	C8-N9-C4	-7.52	102.79	105.80
1	1A	1457	C	N3-C4-C5	7.52	124.91	121.90
32	2a	898	G	N3-C4-C5	7.52	132.36	128.60
1	1A	621	G	N9-C4-C5	7.52	108.41	105.40
1	1A	1268	C	C2-N3-C4	-7.51	116.14	119.90
1	1A	2110	G	C8-N9-C4	7.51	109.41	106.40
1	1A	102	U	N1-C2-O2	-7.51	117.54	122.80
1	1A	493	G	O5'-P-OP2	-7.51	98.94	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	792	G	C4-C5-N7	7.51	113.80	110.80
1	1A	1758	C	OP1-P-OP2	-7.51	108.34	119.60
1	2A	421	U	OP2-P-O3'	-7.51	88.68	105.20
1	2A	1085	A	O5'-P-OP1	-7.51	98.94	105.70
1	2A	1699	G	C8-N9-C4	-7.50	103.40	106.40
32	1a	300	A	N1-C6-N6	7.50	123.10	118.60
1	2A	713	G	C2-N3-C4	-7.50	108.15	111.90
32	2a	578	C	O5'-P-OP1	-7.49	98.96	105.70
1	1A	2418	U	O5'-P-OP2	7.49	119.69	110.70
1	1A	2712	C	O5'-P-OP2	-7.49	98.96	105.70
2	2B	8	U	N3-C2-O2	7.49	127.44	122.20
32	2a	5	U	C2-N1-C1'	7.49	126.69	117.70
1	1A	2364	A	O5'-P-OP1	-7.49	98.96	105.70
32	2a	398	C	N3-C4-N4	-7.48	112.76	118.00
1	1A	505	A	C5-C6-N6	7.48	129.69	123.70
1	1A	2158	C	N1-C2-O2	7.48	123.39	118.90
1	2A	906	G	C5-C6-N1	-7.48	107.76	111.50
32	2a	1028	C	C6-N1-C2	-7.48	117.31	120.30
32	2a	1084	G	O5'-P-OP2	-7.48	98.97	105.70
1	2A	1798	U	O5'-P-OP2	-7.48	98.97	105.70
1	1A	1093	G	N3-C4-C5	-7.48	124.86	128.60
32	2a	1279	A	C8-N9-C4	-7.48	102.81	105.80
32	2a	1465	C	C5-C4-N4	-7.48	114.97	120.20
1	1A	2064	A	C8-N9-C4	7.48	108.79	105.80
1	1A	2354	C	O5'-P-OP2	7.47	119.67	110.70
1	1A	1262	C	N1-C2-O2	-7.47	114.42	118.90
1	2A	2848	G	C4-C5-N7	-7.46	107.81	110.80
32	2a	1030	C	N1-C2-O2	7.46	123.38	118.90
1	2A	2467	C	N3-C4-C5	-7.46	118.92	121.90
1	1A	762	G	C6-C5-N7	-7.46	125.92	130.40
1	1A	2561	G	OP2-P-O3'	7.46	121.61	105.20
1	2A	1998	G	N1-C6-O6	-7.46	115.42	119.90
1	1A	1862	G	N9-C4-C5	7.46	108.38	105.40
1	2A	13	A	N1-C6-N6	-7.46	114.12	118.60
1	1A	1418	U	C5-C4-O4	-7.46	121.42	125.90
1	1A	617	U	C5-C6-N1	-7.45	118.97	122.70
1	1A	641	G	O5'-P-OP2	-7.45	98.99	105.70
1	2A	2378	A	C4-C5-C6	7.45	120.73	117.00
1	2A	271(P)	C	O5'-P-OP2	-7.45	98.99	105.70
1	1A	280	C	C6-N1-C2	7.45	123.28	120.30
1	1A	2460	A	C5-C6-N1	7.45	121.42	117.70
32	1a	1513	A	C5-C6-N1	7.45	121.42	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1204	A	C8-N9-C4	7.45	108.78	105.80
1	1A	1861	C	C5-C4-N4	-7.45	114.99	120.20
1	1A	1875	C	C6-N1-C2	7.45	123.28	120.30
1	1A	2273	C	C4-C5-C6	7.45	121.12	117.40
1	2A	1318	C	C6-N1-C2	-7.45	117.32	120.30
1	1A	1707	C	C5-C6-N1	-7.45	117.28	121.00
2	1B	38	C	N3-C2-O2	-7.45	116.69	121.90
1	2A	832	G	O5'-P-OP2	7.45	119.64	110.70
1	1A	2802	C	C6-N1-C1'	7.45	129.73	120.80
1	2A	1605	C	C4-C5-C6	7.45	121.12	117.40
32	2a	1183	A	P-O3'-C3'	7.44	128.63	119.70
32	1a	57	G	N3-C4-C5	-7.44	124.88	128.60
1	1A	2653	G	O5'-P-OP2	-7.44	99.00	105.70
1	2A	1271	G	C8-N9-C4	7.44	109.38	106.40
1	1A	2692	C	N3-C4-C5	-7.44	118.92	121.90
1	1A	2525	G	N7-C8-N9	7.43	116.82	113.10
1	1A	2885	C	O5'-P-OP2	-7.43	99.01	105.70
1	1A	823	G	N1-C2-N3	7.43	128.36	123.90
1	1A	354	A	N1-C6-N6	7.43	123.06	118.60
1	1A	800	C	C5-C4-N4	7.43	125.40	120.20
1	1A	1092	A	OP2-P-O3'	7.43	121.54	105.20
1	1A	2463	A	C8-N9-C4	-7.43	102.83	105.80
10	1O	8	LEU	CA-CB-CG	7.43	132.38	115.30
1	1A	2107	C	C5-C6-N1	-7.43	117.29	121.00
1	1A	590	A	OP1-P-OP2	-7.42	108.46	119.60
1	1A	2704	C	N3-C4-C5	7.42	124.87	121.90
32	2a	266	G	P-O3'-C3'	7.42	128.61	119.70
1	1A	2628	C	C6-N1-C2	-7.42	117.33	120.30
1	1A	1235	G	C5-N7-C8	7.42	108.01	104.30
1	1A	2348	A	O4'-C1'-N9	-7.42	102.26	108.20
1	1A	204	G	O5'-P-OP2	7.42	119.60	110.70
32	1a	874	G	C8-N9-C4	7.42	109.37	106.40
1	2A	588	U	O5'-P-OP2	-7.42	99.02	105.70
1	1A	237	G	C5-C6-O6	7.42	133.05	128.60
1	1A	1069	U	C5-C4-O4	-7.42	121.45	125.90
1	1A	2569	G	C5-C6-O6	7.42	133.05	128.60
32	2a	1495	U	C2-N3-C4	7.42	131.45	127.00
32	1a	550	G	O5'-P-OP1	-7.42	99.03	105.70
1	1A	98	U	C6-N1-C1'	-7.41	110.82	121.20
1	1A	1168	G	N1-C6-O6	-7.41	115.45	119.90
1	1A	2069	U	C2-N3-C4	-7.41	122.55	127.00
1	2A	1082	U	C6-N1-C1'	-7.41	110.82	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	65	U	P-O3'-C3'	7.41	128.59	119.70
1	1A	1425	A	C8-N9-C4	7.41	108.76	105.80
1	1A	2368	C	N3-C4-C5	7.41	124.86	121.90
1	1A	2681	G	O5'-P-OP2	-7.41	99.03	105.70
1	2A	307	G	O5'-P-OP2	-7.41	99.03	105.70
1	2A	1616	A	N7-C8-N9	7.41	117.50	113.80
1	1A	2241	C	N3-C4-C5	-7.41	118.94	121.90
2	2B	5	C	C6-N1-C2	7.41	123.26	120.30
1	1A	2296	C	N3-C4-C5	-7.40	118.94	121.90
1	2A	250	G	N9-C4-C5	7.40	108.36	105.40
1	1A	184	A	C4-C5-N7	7.40	114.40	110.70
1	2A	568	U	N3-C4-C5	7.40	119.04	114.60
1	2A	1690	A	N1-C6-N6	7.40	123.04	118.60
1	2A	2689	U	P-O3'-C3'	7.40	128.58	119.70
32	1a	187	C	C5-C6-N1	7.40	124.70	121.00
1	1A	1027	A	C8-N9-C4	7.39	108.76	105.80
32	1a	328	C	C6-N1-C2	7.39	123.26	120.30
1	1A	554	A	C4-C5-N7	7.39	114.40	110.70
32	1a	1370	G	N9-C4-C5	-7.39	102.44	105.40
1	2A	149	A	C8-N9-C4	7.39	108.76	105.80
32	2a	1387	G	O5'-P-OP2	-7.39	99.05	105.70
1	1A	795	G	N3-C4-N9	7.39	130.43	126.00
1	1A	2046	G	C8-N9-C4	7.39	109.36	106.40
1	1A	2790	G	O5'-P-OP2	-7.39	99.05	105.70
1	2A	409	C	O5'-P-OP1	-7.39	99.05	105.70
1	1A	1093	G	N3-C4-N9	7.39	130.43	126.00
32	2a	458	C	N3-C2-O2	-7.39	116.73	121.90
1	1A	418	G	C5-C6-N1	7.39	115.19	111.50
2	1B	13	A	C8-N9-C4	7.39	108.75	105.80
1	1A	801	C	C5-C4-N4	-7.38	115.03	120.20
1	2A	1330	C	O5'-P-OP1	-7.38	99.06	105.70
32	2a	1412	C	O5'-P-OP1	-7.38	99.05	105.70
1	1A	212	A	O5'-P-OP1	-7.38	99.06	105.70
1	1A	1786	A	C8-N9-C4	-7.38	102.85	105.80
1	1A	1861	C	C2-N3-C4	-7.38	116.21	119.90
1	1A	2552	C	N3-C4-C5	7.38	124.85	121.90
32	1a	421	U	N3-C2-O2	-7.38	117.04	122.20
1	1A	835	A	C4-C5-C6	7.38	120.69	117.00
1	1A	741	U	N3-C2-O2	-7.37	117.04	122.20
1	1A	1068	G	C8-N9-C4	7.37	109.35	106.40
4	2E	136	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	1A	1196	C	C6-N1-C2	7.37	123.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	745	C	C4-C5-C6	7.37	121.08	117.40
1	1A	1831	C	N1-C2-N3	7.37	124.36	119.20
1	1A	1474	C	N1-C2-O2	-7.37	114.48	118.90
1	2A	1063	G	O5'-P-OP2	-7.37	99.07	105.70
1	1A	1031	C	N3-C4-C5	7.36	124.85	121.90
1	1A	954	C	OP2-P-O3'	7.36	121.40	105.20
1	1A	2450	U	OP2-P-O3'	7.36	121.40	105.20
1	1A	138	G	C4-C5-N7	-7.36	107.86	110.80
2	2B	113	G	N1-C6-O6	7.36	124.31	119.90
1	1A	1176	U	O5'-P-OP1	-7.36	99.08	105.70
1	1A	1398	U	O5'-P-OP2	7.36	119.53	110.70
32	1a	460	G	C8-N9-C4	-7.36	103.46	106.40
1	2A	1128	A	C8-N9-C4	7.36	108.74	105.80
1	2A	1300	U	O5'-P-OP2	-7.36	99.08	105.70
1	1A	35	G	C8-N9-C4	7.36	109.34	106.40
1	1A	2269	U	N1-C2-N3	7.36	119.31	114.90
1	1A	840	A	O5'-P-OP2	-7.35	99.08	105.70
1	1A	192	C	O5'-P-OP2	-7.35	99.08	105.70
1	1A	1965	U	C2-N3-C4	-7.35	122.59	127.00
1	1A	196	A	N9-C4-C5	-7.35	102.86	105.80
1	2A	1764	G	N1-C6-O6	-7.35	115.49	119.90
1	1A	555	G	C5-C6-N1	7.34	115.17	111.50
1	1A	1082	G	C8-N9-C4	7.34	109.34	106.40
1	1A	2265	G	O5'-P-OP1	7.34	119.51	110.70
1	1A	2758	C	N3-C4-C5	7.34	124.84	121.90
1	2A	2505	G	C6-N1-C2	7.34	129.51	125.10
27	15	58	LEU	CA-CB-CG	7.34	132.18	115.30
32	2a	902	G	N3-C4-C5	-7.34	124.93	128.60
1	1A	244	A	C2-N3-C4	-7.34	106.93	110.60
1	1A	2890	C	OP1-P-OP2	7.34	130.60	119.60
1	2A	807	U	N3-C4-O4	7.34	124.53	119.40
32	2a	1003	G	C4-N9-C1'	7.34	136.04	126.50
1	2A	221	A	O5'-P-OP1	-7.33	99.10	105.70
1	1A	1848	G	O5'-P-OP2	-7.33	99.10	105.70
32	2a	408	A	O5'-P-OP2	-7.33	99.10	105.70
1	1A	1573	G	N3-C2-N2	-7.33	114.77	119.90
1	2A	1497	U	C2-N3-C4	-7.33	122.60	127.00
1	1A	1080	G	N7-C8-N9	-7.33	109.44	113.10
1	2A	113	G	N3-C4-N9	-7.33	121.60	126.00
32	2a	625	G	C8-N9-C4	-7.33	103.47	106.40
1	1A	2254	G	N7-C8-N9	-7.33	109.44	113.10
1	2A	1662	C	N3-C4-C5	7.33	124.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2116	G	N1-C6-O6	-7.32	115.51	119.90
32	1a	117	G	O5'-P-OP2	-7.32	99.11	105.70
1	1A	989	G	O5'-P-OP2	-7.32	99.11	105.70
32	1a	219	C	C6-N1-C2	-7.32	117.37	120.30
1	1A	1170	C	C5-C6-N1	-7.32	117.34	121.00
1	1A	2405	A	N1-C6-N6	7.32	122.99	118.60
1	2A	614	U	N1-C2-N3	7.32	119.29	114.90
1	1A	27	G	O4'-C1'-N9	7.32	114.05	108.20
1	1A	1312	G	C4-C5-N7	7.32	113.73	110.80
32	1a	1370	G	C6-C5-N7	-7.32	126.01	130.40
1	2A	1046	A	C8-N9-C4	-7.32	102.87	105.80
1	1A	554	A	C5-C6-N6	-7.32	117.85	123.70
32	1a	1406	U	C5-C6-N1	-7.31	119.04	122.70
1	2A	1992	G	C2'-C3'-O3'	7.31	125.59	109.50
1	2A	2360	A	C8-N9-C4	7.31	108.72	105.80
1	1A	1909	C	O5'-P-OP2	7.31	119.47	110.70
1	2A	2042	A	C2-N3-C4	-7.31	106.95	110.60
1	1A	1154	U	C5-C4-O4	-7.31	121.52	125.90
32	1a	1019	C	C6-N1-C2	-7.31	117.38	120.30
1	2A	1956	U	C2-N3-C4	-7.31	122.62	127.00
32	2a	530	G	N3-C4-C5	-7.31	124.95	128.60
1	1A	146	G	N3-C2-N2	7.31	125.01	119.90
1	1A	206	G	N3-C2-N2	-7.30	114.79	119.90
1	1A	2312	G	O5'-P-OP1	-7.30	99.13	105.70
1	1A	2499	G	C5-C6-O6	-7.30	124.22	128.60
1	2A	61	G	N1-C6-O6	7.30	124.28	119.90
1	2A	1079	C	N3-C4-C5	-7.30	118.98	121.90
1	1A	2099	A	O5'-P-OP1	-7.30	99.13	105.70
1	1A	2828	G	C5-C6-O6	7.30	132.98	128.60
1	1A	2879	G	N3-C2-N2	-7.30	114.79	119.90
32	1a	435	C	C6-N1-C2	-7.30	117.38	120.30
1	2A	572	A	N9-C4-C5	7.30	108.72	105.80
32	2a	200	G	C8-N9-C4	7.30	109.32	106.40
1	1A	591	U	N3-C4-C5	7.30	118.98	114.60
1	1A	854	U	C4-C5-C6	7.30	124.08	119.70
1	1A	2455	C	C5-C4-N4	-7.30	115.09	120.20
1	2A	2131	G	C8-N9-C4	-7.30	103.48	106.40
1	2A	2319	G	C5-N7-C8	-7.30	100.65	104.30
1	1A	452	G	C5-C6-N1	7.29	115.15	111.50
1	1A	1816	A	C6-C5-N7	-7.29	127.19	132.30
2	1B	106	G	N3-C2-N2	-7.29	114.80	119.90
1	1A	452	G	C6-N1-C2	-7.29	120.72	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1247	C	C5-C6-N1	-7.29	117.35	121.00
1	1A	2623	U	N1-C2-O2	-7.29	117.69	122.80
1	2A	779	U	N3-C4-O4	7.29	124.50	119.40
1	1A	1112	U	C5-C6-N1	7.29	126.34	122.70
1	2A	529	A	N1-C6-N6	7.29	122.97	118.60
1	1A	1390	G	N3-C2-N2	-7.29	114.80	119.90
1	1A	2102	G	O5'-P-OP1	7.29	119.44	110.70
1	1A	2674	A	N7-C8-N9	7.29	117.44	113.80
1	2A	2645	G	N3-C4-N9	-7.29	121.63	126.00
1	2A	702	G	OP2-P-O3'	7.28	121.22	105.20
1	1A	556	C	C6-N1-C2	7.28	123.21	120.30
1	1A	89	U	C5-C4-O4	7.28	130.27	125.90
1	1A	2550	C	C6-N1-C2	7.28	123.21	120.30
32	1a	795	C	N1-C2-O2	-7.28	114.53	118.90
1	2A	1341	U	O5'-P-OP1	-7.28	99.15	105.70
32	2a	1026	G	C5-N7-C8	-7.28	100.66	104.30
1	2A	247	G	C2-N3-C4	-7.27	108.26	111.90
1	1A	1785	C	N3-C2-O2	-7.27	116.81	121.90
1	1A	2044	U	N1-C2-O2	-7.27	117.71	122.80
1	1A	815	G	N3-C2-N2	-7.27	114.81	119.90
1	1A	2568	C	N3-C4-C5	7.27	124.81	121.90
32	1a	848	C	C6-N1-C2	-7.27	117.39	120.30
1	1A	1672	G	N3-C2-N2	-7.27	114.81	119.90
1	1A	1723	A	N7-C8-N9	-7.27	110.17	113.80
2	1B	87	G	C8-N9-C4	7.27	109.31	106.40
1	2A	2394	C	N3-C4-C5	7.27	124.81	121.90
1	2A	2848	G	O4'-C1'-N9	7.27	114.01	108.20
32	2a	368	U	O5'-P-OP1	-7.26	99.16	105.70
1	1A	762	G	N3-C4-N9	7.26	130.36	126.00
1	1A	1310	G	C5-C6-N1	7.26	115.13	111.50
1	1A	2579	G	C4-C5-N7	-7.26	107.89	110.80
32	2a	1060	C	C6-N1-C2	-7.26	117.40	120.30
1	1A	2497	G	C5-C6-N1	-7.26	107.87	111.50
32	2a	990	C	N1-C2-O2	7.26	123.26	118.90
1	1A	80	G	O5'-P-OP2	-7.26	99.17	105.70
1	1A	2277	U	N3-C4-C5	-7.26	110.25	114.60
32	1a	339	C	C5-C6-N1	-7.26	117.37	121.00
32	2a	372	C	C6-N1-C2	7.26	123.20	120.30
32	2a	1499	A	O5'-P-OP2	-7.26	99.17	105.70
32	2a	550	G	C5-C6-O6	-7.25	124.25	128.60
1	1A	2260	C	O5'-P-OP2	-7.25	99.17	105.70
1	2A	178	G	N1-C6-O6	-7.25	115.55	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	530	G	N3-C4-N9	7.25	130.35	126.00
1	1A	2044	U	O5'-P-OP2	7.25	119.40	110.70
1	1A	2609	G	C2-N3-C4	-7.25	108.28	111.90
1	1A	2638	C	C5-C4-N4	-7.25	115.12	120.20
1	1A	565	C	N3-C4-C5	7.25	124.80	121.90
1	1A	2155	G	C8-N9-C1'	7.25	136.42	127.00
32	1a	177	C	O5'-P-OP1	-7.24	99.18	105.70
1	1A	877	G	C5-C6-O6	7.24	132.94	128.60
1	1A	1038	C	C5-C6-N1	-7.24	117.38	121.00
1	1A	2512	U	C2-N3-C4	-7.24	122.66	127.00
32	1a	1021	G	N3-C4-C5	-7.24	124.98	128.60
1	2A	2399	G	N1-C6-O6	-7.24	115.56	119.90
1	1A	925	A	C5-C6-N1	-7.24	114.08	117.70
1	1A	1375	U	C5-C4-O4	7.24	130.24	125.90
1	1A	1690	G	N7-C8-N9	-7.24	109.48	113.10
32	1a	220	G	C8-N9-C4	-7.24	103.50	106.40
32	1a	811	C	C6-N1-C2	7.24	123.19	120.30
1	2A	2447	G	C6-N1-C2	-7.24	120.76	125.10
1	1A	45	C	N1-C2-O2	-7.24	114.56	118.90
32	1a	912	C	C5-C6-N1	-7.24	117.38	121.00
32	2a	833	U	O5'-P-OP2	-7.24	99.19	105.70
1	1A	2366	G	N1-C6-O6	-7.23	115.56	119.90
1	1A	2552	C	N3-C4-N4	-7.23	112.94	118.00
2	1B	93	G	N1-C6-O6	-7.23	115.56	119.90
2	1B	98	G	N1-C6-O6	7.23	124.24	119.90
32	2a	291	C	C6-N1-C2	7.23	123.19	120.30
1	1A	766	C	N3-C4-C5	7.23	124.79	121.90
1	1A	1307	C	C2-N3-C4	-7.23	116.28	119.90
1	1A	2326	C	C6-N1-C2	7.23	123.19	120.30
1	1A	2358	A	C4-C5-C6	7.23	120.61	117.00
1	1A	2533	C	N1-C2-O2	-7.23	114.56	118.90
1	1A	2596	U	C6-N1-C2	7.23	125.34	121.00
1	1A	2795	G	C8-N9-C4	7.23	109.29	106.40
1	1A	2347	A	O5'-P-OP1	-7.23	99.19	105.70
1	1A	333	G	O5'-P-OP1	-7.22	99.20	105.70
1	1A	2346	G	N1-C6-O6	7.22	124.23	119.90
2	1B	100	A	OP1-P-OP2	7.22	130.43	119.60
1	1A	34	C	C6-N1-C2	-7.22	117.41	120.30
1	1A	1518	A	O5'-P-OP1	-7.22	99.20	105.70
1	1A	198	C	N3-C4-C5	7.22	124.79	121.90
1	1A	590	A	C5-N7-C8	-7.22	100.29	103.90
1	1A	1054	C	C6-N1-C2	-7.22	117.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	276	G	C8-N9-C4	-7.22	103.51	106.40
1	2A	679	C	N1-C2-O2	-7.22	114.57	118.90
1	2A	2331	G	O5'-P-OP2	-7.21	99.21	105.70
1	1A	1724	A	N1-C2-N3	7.21	132.91	129.30
1	2A	689	A	O5'-P-OP2	-7.21	99.21	105.70
1	1A	2883	A	OP1-P-OP2	7.21	130.41	119.60
32	1a	1169	A	C8-N9-C4	-7.21	102.92	105.80
1	2A	390	A	C8-N9-C4	7.21	108.68	105.80
1	1A	2597	U	OP1-P-OP2	-7.21	108.79	119.60
1	2A	2240	C	C6-N1-C2	-7.21	117.42	120.30
1	1A	2612	A	N1-C2-N3	7.21	132.90	129.30
1	1A	2326	C	O5'-P-OP2	-7.20	99.22	105.70
1	1A	2823	A	N1-C6-N6	-7.20	114.28	118.60
32	1a	830	G	O5'-P-OP1	-7.20	99.22	105.70
1	1A	1041	C	N1-C2-O2	7.20	123.22	118.90
1	2A	2823	A	C5-C6-N1	-7.20	114.10	117.70
1	1A	758	G	N1-C6-O6	7.20	124.22	119.90
1	1A	151	C	C5-C4-N4	-7.20	115.16	120.20
1	1A	174	U	C5-C4-O4	-7.20	121.58	125.90
1	1A	1285	G	C2-N3-C4	-7.20	108.30	111.90
1	1A	1603	C	C6-N1-C2	-7.20	117.42	120.30
1	1A	1850	A	C5-C6-N1	-7.20	114.10	117.70
1	1A	2497	G	N3-C4-C5	7.20	132.20	128.60
1	1A	519	G	N9-C4-C5	7.20	108.28	105.40
1	1A	1035	G	C6-N1-C2	-7.20	120.78	125.10
1	2A	2827	C	C5-C6-N1	-7.20	117.40	121.00
1	2A	869	G	O5'-P-OP2	-7.20	99.22	105.70
1	1A	519	G	N7-C8-N9	7.19	116.70	113.10
1	1A	2707	C	N3-C4-C5	7.19	124.78	121.90
1	1A	1390	G	N1-C6-O6	7.19	124.21	119.90
1	1A	1661	C	N3-C2-O2	-7.19	116.87	121.90
1	1A	150	C	C2-N3-C4	-7.19	116.31	119.90
1	1A	2879	G	C5-C6-N1	-7.19	107.91	111.50
1	2A	2318	G	C4-C5-N7	7.19	113.67	110.80
1	1A	423	G	N9-C4-C5	-7.19	102.53	105.40
32	1a	1492	A	O4'-C1'-N9	7.18	113.95	108.20
32	1a	1523	G	C8-N9-C4	-7.18	103.53	106.40
1	1A	2265	G	C8-N9-C4	7.18	109.27	106.40
32	2a	354	G	C6-C5-N7	-7.18	126.09	130.40
1	1A	1690	G	C5-N7-C8	7.18	107.89	104.30
1	1A	1720	U	C5-C4-O4	-7.18	121.59	125.90
1	1A	193	A	OP1-P-O3'	7.18	121.00	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1633	A	C2-N3-C4	7.18	114.19	110.60
1	2A	2362	G	C5-C6-O6	-7.18	124.29	128.60
32	2a	1391	U	N3-C2-O2	-7.18	117.17	122.20
1	2A	2139	C	N1-C2-O2	7.18	123.21	118.90
1	1A	553	A	N3-C4-C5	-7.18	121.78	126.80
1	1A	729	G	O5'-P-OP1	-7.18	99.24	105.70
32	1a	204	U	C2-N1-C1'	7.18	126.31	117.70
1	2A	1139	G	N1-C6-O6	7.18	124.21	119.90
2	2B	1	U	C5-C6-N1	7.18	126.29	122.70
1	1A	1666	G	C4-C5-N7	-7.17	107.93	110.80
1	2A	2172	U	O4'-C1'-N1	7.17	113.94	108.20
1	1A	2373	A	C5-C6-N1	-7.17	114.11	117.70
1	1A	991	G	O5'-P-OP2	7.17	119.30	110.70
1	1A	962	G	N9-C4-C5	-7.17	102.53	105.40
1	1A	2155	G	O4'-C1'-N9	7.17	113.94	108.20
1	2A	2591	C	N1-C2-O2	-7.17	114.60	118.90
2	2B	109	C	O5'-P-OP2	-7.17	99.25	105.70
1	1A	1996	C	O5'-P-OP2	-7.17	99.25	105.70
32	1a	1495	U	C5-C6-N1	7.17	126.28	122.70
1	1A	841	G	C5-C6-O6	7.16	132.90	128.60
1	2A	1156	A	O5'-P-OP2	-7.16	99.25	105.70
1	2A	788	A	N1-C6-N6	7.16	122.90	118.60
1	1A	1485	A	N1-C2-N3	7.16	132.88	129.30
1	1A	2556	G	N3-C2-N2	-7.16	114.89	119.90
1	2A	2502	G	O4'-C1'-N9	7.16	113.93	108.20
1	1A	31	C	N1-C2-O2	-7.16	114.61	118.90
1	1A	213	G	O5'-P-OP2	-7.16	99.26	105.70
1	1A	1875	C	N3-C4-C5	7.16	124.76	121.90
1	1A	2072	C	N3-C2-O2	7.16	126.91	121.90
32	1a	912	C	N1-C2-O2	-7.16	114.61	118.90
1	1A	472	G	C5-N7-C8	-7.16	100.72	104.30
1	1A	770	G	N1-C2-N2	-7.16	109.76	116.20
1	1A	2093	A	N1-C2-N3	7.16	132.88	129.30
1	2A	2828	C	C5-C6-N1	-7.16	117.42	121.00
32	1a	142	G	C4-N9-C1'	-7.15	117.20	126.50
1	1A	1690	G	C4-C5-N7	-7.15	107.94	110.80
32	1a	1486	G	N1-C6-O6	7.15	124.19	119.90
1	1A	664	U	O5'-P-OP2	-7.15	99.27	105.70
1	2A	918	A	O5'-P-OP1	-7.15	99.27	105.70
32	1a	402	G	O5'-P-OP2	-7.15	99.27	105.70
1	2A	1597	A	O5'-P-OP2	-7.15	99.27	105.70
32	1a	1113	C	C5-C6-N1	7.14	124.57	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	988	A	C5-N7-C8	-7.14	100.33	103.90
32	2a	1125	U	N3-C4-O4	-7.14	114.40	119.40
1	2A	363(E)	U	C5-C4-O4	-7.14	121.61	125.90
1	1A	2320	G	C5-N7-C8	-7.14	100.73	104.30
1	1A	2882	G	N1-C2-N2	-7.14	109.78	116.20
1	1A	828	A	N1-C6-N6	-7.14	114.32	118.60
1	1A	594	A	C5-C6-N1	7.13	121.27	117.70
32	1a	690	G	OP1-P-OP2	7.13	130.30	119.60
1	1A	1148	C	O5'-P-OP1	7.13	119.26	110.70
32	1a	563	A	N7-C8-N9	7.13	117.37	113.80
32	2a	436	C	O5'-P-OP1	-7.13	99.28	105.70
1	1A	481	C	N1-C2-O2	-7.13	114.62	118.90
1	1A	731	G	C2-N3-C4	7.13	115.46	111.90
1	1A	2455	C	N1-C2-O2	-7.13	114.62	118.90
32	1a	825	G	N1-C6-O6	-7.13	115.62	119.90
1	1A	253	C	N1-C2-O2	7.13	123.17	118.90
1	2A	383	U	N3-C2-O2	-7.13	117.21	122.20
1	1A	283	G	N9-C4-C5	7.12	108.25	105.40
1	1A	826	U	N1-C2-O2	-7.12	117.81	122.80
1	1A	1611	C	O5'-P-OP2	-7.12	99.29	105.70
1	1A	2171	G	C4-N9-C1'	-7.12	117.24	126.50
1	1A	2598	C	N1-C2-O2	-7.12	114.62	118.90
1	1A	836	A	N1-C6-N6	7.12	122.87	118.60
1	1A	2006	G	N1-C6-O6	-7.12	115.63	119.90
1	2A	92	A	N1-C6-N6	7.12	122.87	118.60
32	2a	44	G	C2-N3-C4	-7.12	108.34	111.90
32	2a	523	A	N1-C6-N6	7.12	122.87	118.60
32	1a	676	A	C2-N3-C4	-7.12	107.04	110.60
32	1a	355	C	C6-N1-C2	-7.12	117.45	120.30
1	1A	418	G	N1-C2-N3	7.11	128.17	123.90
1	1A	2879	G	N9-C4-C5	7.11	108.25	105.40
1	2A	571	A	N1-C6-N6	-7.11	114.33	118.60
1	2A	960	A	N1-C6-N6	7.11	122.87	118.60
1	1A	1116	A	O4'-C1'-N9	7.11	113.89	108.20
1	1A	2790	G	C5-C6-N1	7.11	115.06	111.50
1	2A	1253	A	N7-C8-N9	-7.11	110.25	113.80
1	1A	334	A	C2-N3-C4	-7.11	107.05	110.60
1	1A	2903	G	C4-N9-C1'	-7.11	117.26	126.50
1	2A	2035	G	N3-C4-N9	-7.11	121.73	126.00
1	2A	2586	C	N1-C2-O2	7.11	123.16	118.90
32	2a	346	G	C5-C6-N1	7.11	115.05	111.50
1	2A	1988	C	N3-C4-N4	7.10	122.97	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2057	G	C8-N9-C4	-7.10	103.56	106.40
1	1A	2086	C	N3-C4-C5	-7.10	119.06	121.90
20	1Y	11	ASP	CB-CG-OD1	-7.10	111.91	118.30
1	1A	107	G	C5-N7-C8	7.10	107.85	104.30
1	1A	2110	G	C5-C6-O6	-7.10	124.34	128.60
1	1A	2586	G	N1-C6-O6	-7.10	115.64	119.90
32	1a	120	A	O5'-P-OP2	7.10	119.22	110.70
32	2a	1259	C	C6-N1-C2	-7.10	117.46	120.30
1	1A	1747	A	N7-C8-N9	-7.10	110.25	113.80
1	1A	2194	U	N3-C4-O4	-7.10	114.43	119.40
1	2A	61	G	C4-C5-N7	7.10	113.64	110.80
1	1A	2217	C	OP1-P-O3'	7.09	120.81	105.20
2	1B	99	G	C8-N9-C4	7.09	109.24	106.40
1	2A	2062	A	N7-C8-N9	-7.09	110.25	113.80
32	1a	498	U	C5-C4-O4	7.09	130.15	125.90
1	1A	2173	G	N9-C1'-C2'	-7.09	104.20	112.00
32	1a	1417	G	N3-C4-N9	7.09	130.25	126.00
1	2A	353	G	N1-C6-O6	7.09	124.15	119.90
1	2A	572	A	N1-C6-N6	-7.09	114.35	118.60
1	2A	2112	G	C4-N9-C1'	-7.09	117.29	126.50
1	1A	1461	U	C5-C4-O4	7.08	130.15	125.90
1	1A	214	A	O5'-P-OP1	7.08	119.20	110.70
1	1A	1011	G	N1-C6-O6	-7.08	115.65	119.90
1	2A	660	G	C5-C6-O6	7.08	132.85	128.60
1	1A	138	G	N7-C8-N9	-7.08	109.56	113.10
1	2A	2318	G	C8-N9-C1'	-7.08	117.80	127.00
32	2a	189(J)	G	C8-N9-C4	7.08	109.23	106.40
1	1A	1747	A	O5'-P-OP2	7.08	119.19	110.70
1	2A	912	C	N3-C2-O2	-7.08	116.95	121.90
1	2A	2140	C	C5-C6-N1	7.08	124.54	121.00
1	1A	1626	A	N1-C6-N6	7.07	122.84	118.60
32	2a	454	C	N1-C2-O2	7.07	123.14	118.90
1	1A	12	U	N1-C2-O2	7.07	127.75	122.80
1	1A	1357	G	O5'-P-OP2	-7.07	99.34	105.70
32	2a	266	G	O5'-P-OP2	-7.07	99.34	105.70
1	1A	1035	G	C5-C6-N1	7.07	115.03	111.50
1	1A	1806	U	C5-C4-O4	-7.07	121.66	125.90
1	1A	1814	A	C2-N3-C4	7.07	114.13	110.60
1	2A	2023	G	C5-C6-O6	-7.07	124.36	128.60
1	2A	2467	C	N3-C2-O2	-7.07	116.95	121.90
1	2A	2467	C	C5-C6-N1	7.07	124.53	121.00
1	1A	1072	U	O4'-C1'-N1	7.06	113.85	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1094	U	C5-C4-O4	7.06	130.14	125.90
1	1A	1439	A	N1-C6-N6	-7.06	114.36	118.60
1	1A	1042	A	C8-N9-C4	7.06	108.62	105.80
1	1A	1347	A	C5-N7-C8	-7.06	100.37	103.90
1	1A	1620	G	C4-C5-N7	7.06	113.62	110.80
1	1A	826	U	C4-C5-C6	7.06	123.93	119.70
1	1A	2903	G	C8-N9-C1'	7.06	136.18	127.00
2	1B	32	C	C6-N1-C2	7.06	123.12	120.30
1	2A	1652	A	OP1-P-OP2	7.06	130.19	119.60
1	2A	2804	C	C6-N1-C2	-7.06	117.48	120.30
1	1A	494	G	C2-N3-C4	-7.06	108.37	111.90
1	1A	787	U	C2-N3-C4	-7.06	122.77	127.00
32	2a	23	C	O5'-P-OP2	7.06	119.17	110.70
1	1A	1405	A	N1-C2-N3	-7.05	125.77	129.30
1	1A	1970	G	O5'-P-OP1	-7.05	99.35	105.70
1	1A	588	C	C6-N1-C2	-7.05	117.48	120.30
1	1A	2496	G	C8-N9-C4	7.05	109.22	106.40
1	1A	2518	U	O4'-C1'-N1	7.05	113.84	108.20
1	1A	2544	G	OP2-P-O3'	7.05	120.71	105.20
1	2A	2501	C	OP1-P-OP2	-7.05	109.03	119.60
32	2a	694	A	O5'-P-OP2	7.05	119.16	110.70
1	1A	888	A	N1-C6-N6	7.05	122.83	118.60
1	1A	1835	C	C6-N1-C2	7.05	123.12	120.30
1	1A	2227	G	N3-C4-C5	7.05	132.12	128.60
32	2a	1125	U	C2-N1-C1'	7.05	126.16	117.70
1	1A	728	G	N1-C2-N3	7.05	128.13	123.90
1	1A	1700	G	O4'-C1'-N9	-7.05	102.56	108.20
1	2A	1663	C	C6-N1-C2	7.05	123.12	120.30
1	1A	1316	C	C2-N3-C4	-7.04	116.38	119.90
32	1a	421	U	N1-C2-O2	7.04	127.73	122.80
32	2a	630	G	C8-N9-C4	-7.04	103.58	106.40
1	1A	180	A	OP1-P-O3'	-7.04	89.70	105.20
1	1A	2298	A	C6-N1-C2	-7.04	114.37	118.60
1	1A	2642	G	C5-C6-O6	-7.04	124.37	128.60
1	2A	2894	G	C6-C5-N7	7.04	134.63	130.40
1	1A	591	U	C5-C4-O4	-7.04	121.67	125.90
1	2A	1988	C	C5-C4-N4	-7.04	115.27	120.20
32	2a	138	G	N3-C4-C5	7.04	132.12	128.60
32	2a	1515	C	C6-N1-C2	7.04	123.12	120.30
32	2a	458	C	N1-C2-O2	7.04	123.12	118.90
1	1A	472	G	C2-N3-C4	-7.04	108.38	111.90
1	1A	2657	G	C4-C5-N7	7.04	113.61	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1418	U	N3-C4-O4	7.04	124.33	119.40
1	1A	2607	G	N9-C4-C5	7.04	108.22	105.40
1	1A	1196	C	OP1-P-OP2	-7.04	109.05	119.60
1	1A	2405	A	OP1-P-OP2	7.04	130.15	119.60
1	1A	2667	G	O4'-C1'-N9	7.04	113.83	108.20
1	2A	1363	C	N3-C4-C5	7.04	124.71	121.90
1	1A	533	G	OP1-P-OP2	7.03	130.15	119.60
32	1a	768	A	O5'-P-OP2	-7.03	99.37	105.70
1	1A	250	G	C4-C5-N7	7.03	113.61	110.80
1	1A	1662	A	O5'-P-OP2	7.03	119.14	110.70
32	1a	325	A	C8-N9-C4	7.03	108.61	105.80
1	1A	1985	U	C6-N1-C1'	-7.03	111.36	121.20
1	1A	581	G	N3-C2-N2	7.03	124.82	119.90
1	1A	1635	C	N3-C4-C5	7.03	124.71	121.90
1	1A	630	U	O5'-P-OP1	-7.03	99.38	105.70
1	1A	642	G	O5'-P-OP2	-7.03	99.38	105.70
1	1A	1007	G	N3-C4-C5	-7.03	125.09	128.60
1	1A	2047	C	N1-C2-O2	-7.03	114.68	118.90
1	1A	2093	A	O5'-P-OP2	7.03	119.13	110.70
32	1a	1228	C	C5-C6-N1	7.02	124.51	121.00
1	1A	102	U	N3-C2-O2	7.02	127.11	122.20
1	1A	239	G	C8-N9-C4	-7.02	103.59	106.40
32	1a	880	C	O5'-P-OP2	-7.02	99.38	105.70
1	1A	849	A	C8-N9-C4	-7.02	102.99	105.80
1	1A	1232	G	N1-C6-O6	-7.02	115.69	119.90
1	1A	800	C	N3-C4-N4	-7.02	113.09	118.00
32	2a	630	G	N7-C8-N9	7.02	116.61	113.10
32	2a	802	A	C5-C6-N6	-7.02	118.09	123.70
1	1A	50	G	O5'-P-OP2	-7.02	99.39	105.70
1	1A	1329	G	O5'-P-OP2	-7.02	99.39	105.70
32	2a	299	G	N1-C6-O6	7.02	124.11	119.90
32	2a	500	G	O5'-P-OP2	-7.02	99.39	105.70
1	2A	2269	A	N9-C4-C5	-7.01	102.99	105.80
1	2A	2427	C	O5'-P-OP2	7.01	119.12	110.70
1	1A	837	C	C6-N1-C2	7.01	123.11	120.30
1	1A	2587	C	N3-C4-N4	-7.01	113.09	118.00
1	1A	2274	U	N1-C2-O2	-7.01	117.89	122.80
1	1A	569	G	N3-C4-N9	-7.01	121.79	126.00
1	1A	2531	U	C5-C4-O4	-7.01	121.69	125.90
1	1A	731	G	N3-C4-N9	7.01	130.21	126.00
1	1A	1821	C	N3-C4-N4	7.01	122.91	118.00
1	1A	1314	A	C2-N3-C4	-7.01	107.10	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1401	G	C5-C6-O6	7.01	132.80	128.60
2	1B	1	U	C2-N1-C1'	7.01	126.11	117.70
1	1A	2835	C	N3-C4-C5	7.00	124.70	121.90
1	2A	2553	G	C8-N9-C4	7.00	109.20	106.40
1	2A	2886	G	N3-C2-N2	-7.00	115.00	119.90
32	2a	938	A	C8-N9-C4	-7.00	103.00	105.80
32	1a	1184	G	C5-C6-O6	-7.00	124.40	128.60
1	1A	2072	C	N1-C2-O2	-7.00	114.70	118.90
1	1A	2290	A	OP2-P-O3'	7.00	120.60	105.20
1	1A	2561	G	OP1-P-O3'	-7.00	89.80	105.20
1	1A	2797	C	N3-C4-N4	7.00	122.90	118.00
32	2a	1508	G	O5'-P-OP2	-7.00	99.40	105.70
1	1A	2464	C	C2-N3-C4	-7.00	116.40	119.90
1	2A	113	G	C4-N9-C1'	-7.00	117.40	126.50
1	2A	2017	U	O5'-P-OP1	-7.00	99.40	105.70
1	1A	2537	G	N9-C4-C5	-7.00	102.60	105.40
1	1A	1021	G	N3-C2-N2	-6.99	115.00	119.90
1	1A	2238	C	C2-N3-C4	-6.99	116.40	119.90
1	2A	566	U	OP2-P-O3'	6.99	120.58	105.20
1	2A	2499	C	N1-C2-O2	-6.99	114.70	118.90
1	1A	1076	G	N7-C8-N9	-6.99	109.61	113.10
1	1A	2836	A	C2-N3-C4	-6.99	107.11	110.60
1	2A	1670	C	C4-C5-C6	6.99	120.89	117.40
1	1A	2264	G	N1-C6-O6	6.99	124.09	119.90
1	1A	2419	G	C4-N9-C1'	6.99	135.58	126.50
32	1a	343	U	O4'-C1'-N1	6.99	113.79	108.20
1	2A	1328	G	C5-C6-O6	-6.99	124.41	128.60
32	2a	30	U	O5'-P-OP1	-6.99	99.41	105.70
32	2a	316	G	C8-N9-C4	-6.99	103.61	106.40
1	1A	832	G	O5'-P-OP2	-6.99	99.41	105.70
1	2A	948	G	O5'-P-OP1	-6.99	99.41	105.70
13	2R	67	LEU	CA-CB-CG	6.99	131.37	115.30
1	1A	795	G	C6-N1-C2	-6.99	120.91	125.10
1	1A	1865	U	O5'-P-OP1	-6.99	99.41	105.70
1	1A	2067	C	C6-N1-C2	6.99	123.09	120.30
1	2A	2648	C	C6-N1-C2	6.99	123.09	120.30
1	1A	600	G	OP2-P-O3'	6.98	120.56	105.20
32	2a	533	A	N1-C2-N3	6.98	132.79	129.30
1	1A	816	G	C8-N9-C4	6.98	109.19	106.40
1	2A	1537	G	N3-C4-C5	-6.98	125.11	128.60
1	1A	1000	C	N3-C4-N4	-6.98	113.11	118.00
1	1A	2550	C	N3-C4-N4	-6.98	113.11	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	16	A	N1-C6-N6	-6.98	114.41	118.60
32	2a	320	C	C6-N1-C2	6.98	123.09	120.30
1	1A	351	G	O5'-P-OP2	-6.98	99.42	105.70
1	1A	1848	G	N1-C6-O6	-6.98	115.71	119.90
1	1A	2047	C	N3-C2-O2	6.98	126.78	121.90
32	2a	411	A	C8-N9-C4	-6.98	103.01	105.80
1	1A	34	C	N3-C4-C5	-6.98	119.11	121.90
1	1A	35	G	N7-C8-N9	-6.97	109.61	113.10
1	1A	1725	G	C4-C5-N7	6.97	113.59	110.80
1	1A	2007	G	O5'-P-OP2	-6.97	99.42	105.70
1	2A	12	U	C6-N1-C2	-6.97	116.82	121.00
1	1A	2074	G	OP1-P-OP2	-6.97	109.14	119.60
1	2A	1925	C	N1-C2-O2	-6.97	114.72	118.90
1	1A	2627	U	N1-C2-N3	6.97	119.08	114.90
1	1A	2629	C	C2-N3-C4	6.97	123.38	119.90
1	2A	2023	G	N1-C6-O6	6.97	124.08	119.90
1	1A	1925	G	OP2-P-O3'	6.97	120.53	105.20
1	1A	36	G	C4-C5-N7	-6.97	108.01	110.80
1	2A	30	G	O5'-P-OP2	-6.97	99.43	105.70
32	2a	295	C	C6-N1-C2	6.97	123.09	120.30
1	1A	659	C	OP2-P-O3'	6.96	120.52	105.20
1	2A	1078	U	O4'-C1'-N1	6.96	113.77	108.20
1	2A	2137	C	C5-C6-N1	6.96	124.48	121.00
32	1a	135	C	O5'-P-OP1	6.96	119.06	110.70
1	1A	2720	G	C8-N9-C4	6.96	109.19	106.40
4	1E	101	ARG	NE-CZ-NH1	-6.96	116.82	120.30
32	1a	1370	G	N1-C6-O6	6.96	124.08	119.90
1	1A	1518	A	N7-C8-N9	6.96	117.28	113.80
1	1A	2082	A	C5-N7-C8	-6.96	100.42	103.90
1	2A	9	U	C5-C6-N1	6.96	126.18	122.70
1	1A	2443	U	N3-C2-O2	-6.95	117.33	122.20
1	1A	2466	G	OP1-P-OP2	6.95	130.03	119.60
1	2A	1091	G	N3-C4-C5	-6.95	125.12	128.60
1	1A	2272	C	C6-N1-C2	6.95	123.08	120.30
1	1A	2446	A	N1-C2-N3	-6.95	125.82	129.30
1	1A	2461	U	N3-C4-O4	6.95	124.27	119.40
1	1A	1296	G	N9-C4-C5	6.95	108.18	105.40
32	2a	142	G	C8-N9-C4	-6.95	103.62	106.40
1	1A	545	G	C5-C6-O6	6.95	132.77	128.60
32	2a	1093	A	C5-C6-N6	-6.95	118.14	123.70
1	1A	251	A	C2-N3-C4	-6.95	107.13	110.60
1	1A	397	G	C5-C6-O6	-6.95	124.43	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	322	C	N3-C4-C5	6.95	124.68	121.90
1	2A	1791	A	OP1-P-OP2	-6.95	109.18	119.60
1	2A	1115	G	C8-N9-C4	6.94	109.18	106.40
1	1A	2005	C	C5-C6-N1	-6.94	117.53	121.00
1	1A	718	C	N3-C4-N4	-6.94	113.14	118.00
1	1A	975	U	OP1-P-O3'	6.94	120.47	105.20
1	2A	1826	G	N1-C6-O6	-6.94	115.74	119.90
2	2B	59	A	C5-C6-N1	6.94	121.17	117.70
1	1A	2762	A	N1-C6-N6	-6.94	114.44	118.60
2	2B	2	C	N1-C2-O2	6.94	123.06	118.90
32	2a	775	G	OP2-P-O3'	6.94	120.46	105.20
1	1A	837	C	N1-C2-O2	-6.94	114.74	118.90
1	2A	1647	G	N9-C4-C5	-6.94	102.62	105.40
1	1A	1015	C	C5-C6-N1	-6.93	117.53	121.00
1	1A	1025	G	N7-C8-N9	-6.93	109.63	113.10
1	1A	2357	G	C2-N3-C4	-6.93	108.43	111.90
1	1A	285	U	N3-C4-C5	6.93	118.76	114.60
1	1A	706	C	N3-C4-C5	6.93	124.67	121.90
1	1A	1317	G	N9-C4-C5	-6.93	102.63	105.40
1	1A	2495	C	N3-C4-C5	-6.93	119.13	121.90
1	1A	326	C	C6-N1-C2	-6.93	117.53	120.30
1	1A	1434	G	OP1-P-OP2	6.93	129.99	119.60
1	1A	932	C	C5-C6-N1	6.93	124.46	121.00
1	1A	1375	U	O5'-P-OP1	6.93	119.01	110.70
1	1A	1683	C	C5-C6-N1	-6.93	117.54	121.00
1	1A	1725	G	C5-N7-C8	-6.93	100.84	104.30
1	1A	2082	A	C6-N1-C2	6.93	122.76	118.60
32	1a	1151	A	OP1-P-OP2	6.93	129.99	119.60
32	1a	1211	U	C5-C6-N1	-6.93	119.24	122.70
1	2A	1272	A	O5'-P-OP1	6.93	119.01	110.70
1	2A	1660	C	O5'-P-OP2	-6.93	99.47	105.70
1	2A	1783	A	O4'-C1'-N9	-6.93	102.66	108.20
2	2B	30	C	O5'-P-OP1	-6.93	99.47	105.70
1	1A	1231	G	C8-N9-C4	6.92	109.17	106.40
1	1A	2273	C	N3-C2-O2	-6.92	117.05	121.90
1	1A	343	C	C6-N1-C2	-6.92	117.53	120.30
1	1A	779	C	N1-C2-O2	-6.92	114.75	118.90
1	1A	1376	C	C6-N1-C2	6.92	123.07	120.30
1	1A	2647	C	C2-N3-C4	-6.92	116.44	119.90
1	2A	459	U	N3-C2-O2	-6.92	117.35	122.20
1	1A	1130	A	C6-C5-N7	6.92	137.15	132.30
1	1A	2265	G	N3-C2-N2	-6.92	115.06	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	555	U	N3-C4-O4	6.92	124.25	119.40
1	2A	2390	U	C6-N1-C2	-6.92	116.85	121.00
1	1A	1008	U	O5'-P-OP1	-6.92	99.47	105.70
1	1A	461	U	N1-C2-O2	-6.92	117.96	122.80
1	1A	906	G	C8-N9-C4	6.92	109.17	106.40
1	1A	2595	G	C5-C6-O6	6.92	132.75	128.60
32	1a	142	G	C8-N9-C1'	6.92	135.99	127.00
1	2A	2356	C	C2-N3-C4	-6.92	116.44	119.90
1	1A	696	C	C6-N1-C2	-6.92	117.53	120.30
32	1a	815	A	C8-N9-C4	6.91	108.57	105.80
1	2A	1416	G	O4'-C1'-N9	6.91	113.73	108.20
1	2A	2166	G	C8-N9-C4	-6.91	103.64	106.40
1	1A	2176	G	N3-C4-N9	-6.91	121.85	126.00
1	2A	205	G	OP1-P-OP2	6.91	129.97	119.60
1	2A	311	A	OP1-P-OP2	-6.91	109.23	119.60
1	1A	1192	C	N1-C2-O2	-6.91	114.75	118.90
1	1A	1523	C	N1-C2-O2	-6.91	114.75	118.90
1	2A	2207	G	C8-N9-C1'	-6.91	118.02	127.00
1	1A	2523	U	C2-N3-C4	-6.91	122.86	127.00
1	2A	1605	C	N3-C4-C5	-6.91	119.14	121.90
1	1A	2443	U	C2-N3-C4	-6.91	122.86	127.00
1	1A	2171	G	C8-N9-C4	6.90	109.16	106.40
1	1A	2289	G	C4-C5-N7	-6.90	108.04	110.80
1	1A	122	G	C5-C6-O6	-6.90	124.46	128.60
1	1A	2544	G	C8-N9-C4	6.90	109.16	106.40
1	1A	958	C	C6-N1-C2	-6.90	117.54	120.30
1	1A	1013	G	C5-C6-O6	6.90	132.74	128.60
1	1A	1302	G	N7-C8-N9	-6.90	109.65	113.10
1	1A	1439	A	C5-C6-N1	6.90	121.15	117.70
1	1A	2092	G	N1-C2-N3	6.90	128.04	123.90
1	1A	2497	G	N9-C4-C5	-6.90	102.64	105.40
32	1a	1527	C	N1-C2-O2	-6.90	114.76	118.90
1	2A	192	C	N3-C4-N4	6.90	122.83	118.00
1	2A	2507	C	N1-C2-O2	6.90	123.04	118.90
1	1A	539	A	C8-N9-C4	6.89	108.56	105.80
1	1A	2409	G	C5-C6-O6	-6.89	124.46	128.60
1	1A	2506	G	C5-C6-O6	6.89	132.74	128.60
1	2A	2025	C	C6-N1-C2	-6.89	117.54	120.30
1	1A	174	U	C2-N3-C4	-6.89	122.86	127.00
1	1A	1000	C	C5-C6-N1	-6.89	117.55	121.00
1	1A	2155	G	C4-N9-C1'	-6.89	117.54	126.50
32	2a	915	A	O5'-P-OP2	-6.89	99.50	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1623	U	OP2-P-O3'	6.89	120.36	105.20
1	2A	634	C	C6-N1-C2	-6.89	117.55	120.30
1	2A	1170	G	N1-C6-O6	6.89	124.03	119.90
2	2B	24	G	N3-C4-N9	6.89	130.13	126.00
1	1A	1297	C	N3-C4-C5	6.89	124.65	121.90
1	1A	1347	A	OP1-P-OP2	-6.88	109.27	119.60
1	1A	994	C	N1-C2-O2	-6.88	114.77	118.90
1	2A	1653	G	OP1-P-OP2	6.88	129.93	119.60
1	1A	1707	C	N3-C2-O2	-6.88	117.08	121.90
1	1A	2188	G	N3-C4-C5	6.88	132.04	128.60
1	2A	2609	U	C5-C6-N1	-6.88	119.26	122.70
32	2a	1532	U	N3-C2-O2	6.88	127.02	122.20
1	1A	107	G	N7-C8-N9	-6.88	109.66	113.10
1	1A	973	G	OP1-P-O3'	6.88	120.33	105.20
32	1a	869	G	C8-N9-C4	6.88	109.15	106.40
1	2A	1071	G	N1-C6-O6	6.88	124.03	119.90
1	2A	2563	U	N3-C2-O2	-6.88	117.39	122.20
1	1A	89	U	N3-C2-O2	-6.88	117.39	122.20
1	1A	715	G	OP2-P-O3'	6.88	120.33	105.20
1	1A	1069	U	N3-C4-O4	6.88	124.21	119.40
1	1A	2524	C	N3-C2-O2	6.88	126.71	121.90
1	2A	50	U	C6-N1-C2	6.87	125.12	121.00
1	1A	575	G	C5-C6-O6	6.87	132.72	128.60
1	1A	2052	A	N1-C6-N6	6.87	122.72	118.60
1	1A	2717	A	C2-N3-C4	-6.87	107.16	110.60
1	1A	981	C	C5-C4-N4	-6.87	115.39	120.20
1	2A	2083	G	C2-N3-C4	-6.87	108.47	111.90
1	1A	38	A	C5-C6-N1	6.87	121.13	117.70
32	1a	233	C	C5-C6-N1	6.87	124.43	121.00
32	1a	1181	G	C6-N1-C2	6.87	129.22	125.10
1	1A	1522	G	N3-C2-N2	-6.87	115.09	119.90
1	2A	1783	A	N1-C6-N6	-6.87	114.48	118.60
1	2A	2508	G	O5'-P-OP2	6.87	118.94	110.70
1	1A	1543	U	N3-C4-O4	-6.86	114.60	119.40
1	1A	52	A	C2-N3-C4	-6.86	107.17	110.60
1	1A	985	G	N3-C4-C5	-6.86	125.17	128.60
1	1A	1068	G	N3-C4-C5	6.86	132.03	128.60
32	1a	896	C	N3-C4-C5	6.86	124.64	121.90
32	1a	1486	G	N3-C4-C5	6.86	132.03	128.60
1	2A	1249	U	O5'-P-OP1	-6.86	99.53	105.70
1	1A	2103	C	OP1-P-OP2	6.86	129.89	119.60
32	2a	768	A	C4-C5-C6	6.86	120.43	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	200	A	OP1-P-O3'	-6.86	90.11	105.20
2	1B	99	G	N7-C8-N9	-6.86	109.67	113.10
1	1A	335	A	OP1-P-OP2	-6.86	109.32	119.60
1	1A	995	G	N1-C2-N2	-6.86	110.03	116.20
2	1B	79	C	C6-N1-C2	-6.86	117.56	120.30
32	1a	23	C	N3-C4-C5	-6.86	119.16	121.90
1	1A	1244	U	N3-C2-O2	-6.85	117.40	122.20
32	2a	372	C	N1-C2-N3	-6.85	114.40	119.20
1	1A	979	G	C4-C5-N7	-6.85	108.06	110.80
1	2A	1373	A	C8-N9-C4	6.85	108.54	105.80
32	2a	1137	C	C6-N1-C2	-6.85	117.56	120.30
1	1A	1265	A	O5'-P-OP2	-6.85	99.54	105.70
32	1a	757	U	C6-N1-C2	6.85	125.11	121.00
1	2A	1239	G	N1-C6-O6	6.85	124.01	119.90
1	1A	234	G	C5-C6-O6	-6.84	124.49	128.60
32	1a	183	G	C8-N9-C4	-6.84	103.66	106.40
32	1a	618	C	O5'-P-OP1	-6.84	99.54	105.70
1	2A	277	C	N1-C2-O2	6.84	123.01	118.90
1	1A	1412	A	C5-C6-N6	-6.84	118.23	123.70
32	2a	334	C	N3-C4-C5	6.84	124.64	121.90
32	2a	726	C	O5'-P-OP1	-6.84	99.54	105.70
1	1A	1821	C	C2-N3-C4	-6.84	116.48	119.90
1	1A	2606	C	C2-N3-C4	-6.84	116.48	119.90
32	1a	831	U	C6-N1-C2	-6.84	116.90	121.00
32	1a	889	A	OP1-P-OP2	6.84	129.86	119.60
32	1a	1103	C	O5'-P-OP2	-6.84	99.55	105.70
1	1A	2282	G	N3-C2-N2	-6.84	115.11	119.90
1	1A	2719	G	N9-C4-C5	-6.83	102.67	105.40
1	2A	1071	G	C5-N7-C8	-6.83	100.88	104.30
1	1A	2498	G	C5-N7-C8	6.83	107.72	104.30
32	1a	770	C	O5'-P-OP2	-6.83	99.55	105.70
1	2A	948	G	O5'-P-OP2	6.83	118.90	110.70
1	2A	1005	C	O5'-P-OP1	-6.83	99.55	105.70
1	1A	1178	A	OP1-P-OP2	6.83	129.85	119.60
1	1A	1868	C	O5'-P-OP1	-6.83	99.55	105.70
32	1a	1505	G	N3-C2-N2	-6.83	115.12	119.90
1	2A	61	G	C5-N7-C8	-6.83	100.88	104.30
32	2a	945	G	C5-C6-O6	-6.83	124.50	128.60
1	1A	1299	A	C4-C5-C6	6.83	120.41	117.00
1	1A	1977	U	C2-N3-C4	-6.83	122.91	127.00
1	2A	1501	C	N3-C4-C5	-6.83	119.17	121.90
1	1A	593	G	C5-C6-O6	-6.82	124.50	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1043	G	OP1-P-OP2	-6.82	109.36	119.60
2	1B	24	G	C4-N9-C1'	6.82	135.37	126.50
1	1A	1106	U	C5-C6-N1	6.82	126.11	122.70
1	1A	1268	C	C5-C6-N1	-6.82	117.59	121.00
1	1A	50	G	N3-C4-C5	-6.82	125.19	128.60
1	1A	1396	C	N3-C4-C5	6.82	124.63	121.90
1	2A	213	A	C4-C5-C6	-6.82	113.59	117.00
1	2A	385	C	O5'-P-OP1	-6.82	99.56	105.70
1	1A	1186	U	O4'-C1'-N1	6.82	113.66	108.20
1	1A	1297	C	C6-N1-C2	6.82	123.03	120.30
1	2A	1793	C	N3-C4-C5	6.82	124.63	121.90
32	2a	230	G	C4-C5-N7	-6.82	108.07	110.80
1	1A	548	C	N3-C4-C5	6.82	124.63	121.90
1	1A	1485	A	O5'-P-OP1	-6.82	99.56	105.70
1	1A	1742	G	C4-C5-N7	6.82	113.53	110.80
1	1A	2767	U	N1-C2-O2	6.82	127.57	122.80
1	2A	614	U	N3-C2-O2	-6.82	117.43	122.20
1	2A	988	A	C4-C5-N7	6.82	114.11	110.70
32	2a	1026	G	C8-N9-C4	-6.82	103.67	106.40
1	1A	2222	C	O5'-P-OP2	-6.82	99.57	105.70
32	1a	836	G	C5-C6-O6	-6.82	124.51	128.60
1	1A	71	U	C6-N1-C2	6.81	125.09	121.00
1	2A	1065	U	P-O3'-C3'	6.81	127.88	119.70
1	1A	423	G	C8-N9-C4	6.81	109.12	106.40
1	1A	1517	G	N1-C6-O6	6.81	123.99	119.90
1	1A	2496	G	C4-C5-N7	6.81	113.53	110.80
2	2B	8	U	C5-C6-N1	6.81	126.11	122.70
1	1A	1343	C	O5'-P-OP1	6.81	118.87	110.70
1	1A	665	C	N3-C2-O2	6.81	126.67	121.90
1	1A	2024	G	C4-C5-N7	-6.81	108.08	110.80
1	1A	2378	A	N1-C6-N6	6.81	122.68	118.60
1	1A	98	U	N1-C2-O2	6.81	127.56	122.80
1	1A	880	U	N3-C2-O2	6.81	126.96	122.20
1	1A	1178	A	N9-C4-C5	6.81	108.52	105.80
1	1A	86	C	N3-C4-C5	6.80	124.62	121.90
1	1A	1318	A	O4'-C1'-N9	6.80	113.64	108.20
1	1A	1377	A	OP2-P-O3'	6.80	120.17	105.20
1	1A	2701	U	OP1-P-O3'	6.80	120.17	105.20
1	1A	913	A	O5'-P-OP1	-6.80	99.58	105.70
1	1A	189	U	C5-C6-N1	-6.80	119.30	122.70
1	1A	196	A	C4-C5-N7	6.80	114.10	110.70
1	1A	2110	G	N3-C4-C5	6.80	132.00	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1830	G	N7-C8-N9	-6.80	109.70	113.10
1	1A	336	G	O5'-P-OP1	-6.80	99.58	105.70
1	1A	2514	G	N1-C2-N2	-6.80	110.08	116.20
1	2A	1775	U	N1-C2-N3	6.80	118.98	114.90
1	1A	445	G	O5'-P-OP1	-6.79	99.58	105.70
1	1A	1446	G	OP2-P-O3'	6.79	120.15	105.20
32	1a	773	G	N3-C4-N9	-6.79	121.92	126.00
32	2a	332	G	C8-N9-C4	6.79	109.12	106.40
1	1A	189	U	O5'-P-OP2	-6.79	99.59	105.70
1	1A	565	C	N1-C2-O2	-6.79	114.83	118.90
1	1A	1386	U	N3-C4-C5	6.79	118.67	114.60
32	1a	47	C	C6-N1-C2	6.79	123.02	120.30
32	1a	784	C	C6-N1-C2	6.79	123.02	120.30
1	2A	2741	A	N1-C2-N3	-6.79	125.90	129.30
1	1A	872	C	C6-N1-C2	6.79	123.02	120.30
1	1A	1175	A	O5'-P-OP2	-6.79	99.59	105.70
1	1A	1207	C	OP2-P-O3'	6.79	120.13	105.20
1	2A	1087	G	N3-C4-N9	-6.79	121.93	126.00
1	1A	984	G	C8-N9-C4	-6.79	103.69	106.40
1	1A	2608	U	C5-C6-N1	-6.79	119.31	122.70
1	1A	1299	A	N7-C8-N9	-6.79	110.41	113.80
1	1A	2524	C	N1-C2-O2	-6.78	114.83	118.90
1	2A	1100	C	C6-N1-C2	-6.78	117.59	120.30
1	1A	239	G	N7-C8-N9	6.78	116.49	113.10
1	1A	2357	G	N1-C2-N2	-6.78	110.10	116.20
32	1a	1495	U	C2-N3-C4	6.78	131.07	127.00
1	2A	677	A	N9-C4-C5	-6.78	103.09	105.80
1	2A	1839	G	C8-N9-C4	6.78	109.11	106.40
32	2a	902	G	N1-C6-O6	-6.78	115.83	119.90
1	1A	144	C	C4-C5-C6	6.78	120.79	117.40
1	1A	791	G	N3-C2-N2	6.78	124.65	119.90
1	1A	1307	C	C5-C6-N1	-6.78	117.61	121.00
1	1A	1724	A	O5'-P-OP2	-6.78	99.60	105.70
1	1A	2009	G	N1-C6-O6	6.78	123.97	119.90
32	1a	18	C	O5'-P-OP2	6.78	118.84	110.70
32	1a	914	A	C8-N9-C4	-6.78	103.09	105.80
1	2A	1678	G	C4-C5-C6	6.78	122.87	118.80
1	2A	2092	U	C5-C4-O4	-6.78	121.83	125.90
1	2A	2261	C	C6-N1-C2	6.78	123.01	120.30
1	1A	483	A	C6-N1-C2	6.78	122.67	118.60
1	1A	2401	G	C5-C6-O6	6.78	132.67	128.60
32	2a	1158	C	C6-N1-C2	-6.78	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1041	C	N3-C2-O2	-6.78	117.16	121.90
1	1A	1612	C	O5'-P-OP2	-6.78	99.60	105.70
1	1A	1655	A	N7-C8-N9	-6.78	110.41	113.80
32	2a	638	G	O5'-P-OP2	-6.78	99.60	105.70
1	1A	2826	C	OP1-P-OP2	6.77	129.76	119.60
1	1A	725	C	O5'-P-OP2	-6.77	99.61	105.70
1	1A	961	C	N1-C2-O2	6.77	122.96	118.90
1	1A	1110	C	C6-N1-C2	-6.77	117.59	120.30
1	1A	1611	C	N3-C4-N4	-6.77	113.26	118.00
32	1a	569	C	O5'-P-OP2	-6.77	99.61	105.70
1	2A	2324	C	N3-C4-C5	6.77	124.61	121.90
1	1A	1832	G	N1-C6-O6	6.77	123.96	119.90
1	1A	2257	U	C6-N1-C2	6.77	125.06	121.00
1	1A	2446	A	C6-N1-C2	6.77	122.66	118.60
1	1A	2471	A	C2-N3-C4	6.77	113.98	110.60
1	1A	2783	G	C5-C6-O6	-6.77	124.54	128.60
32	2a	899	C	C6-N1-C2	6.77	123.01	120.30
2	1B	117	G	O5'-P-OP1	6.77	118.82	110.70
1	2A	2319	G	O4'-C1'-N9	6.77	113.61	108.20
1	1A	2411	G	O5'-P-OP2	-6.76	99.61	105.70
32	1a	1370	G	C4-C5-N7	6.76	113.50	110.80
1	2A	956	G	C5-C6-N1	-6.76	108.12	111.50
1	1A	2628	C	N3-C2-O2	-6.76	117.17	121.90
1	1A	1838	G	C2-N3-C4	-6.76	108.52	111.90
1	1A	2700	U	N3-C4-O4	6.76	124.13	119.40
1	2A	2283	C	N1-C2-O2	-6.76	114.84	118.90
32	2a	1259	C	C5-C6-N1	6.76	124.38	121.00
1	1A	1359	U	O5'-P-OP2	6.76	118.81	110.70
1	1A	1194	A	O5'-P-OP2	-6.76	99.62	105.70
1	1A	2607	G	O5'-P-OP2	-6.76	99.62	105.70
1	2A	1669	A	O5'-P-OP2	-6.76	99.62	105.70
1	2A	1794	U	C5-C6-N1	-6.76	119.32	122.70
32	2a	7	G	N1-C6-O6	6.76	123.95	119.90
1	1A	151	C	C2-N3-C4	-6.76	116.52	119.90
1	1A	403	C	C5-C6-N1	-6.76	117.62	121.00
1	1A	1455	C	OP2-P-O3'	6.76	120.06	105.20
1	1A	1816	A	C5-N7-C8	-6.76	100.52	103.90
1	1A	185	A	N7-C8-N9	6.75	117.18	113.80
1	1A	203	G	O4'-C1'-N9	6.75	113.60	108.20
1	1A	239	G	OP1-P-OP2	-6.75	109.47	119.60
1	1A	489	G	N1-C6-O6	-6.75	115.85	119.90
1	1A	722	A	N9-C4-C5	-6.75	103.10	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1452	U	C2-N3-C4	-6.75	122.95	127.00
1	1A	1514	C	OP1-P-OP2	-6.75	109.47	119.60
1	1A	1537	G	C5-N7-C8	6.75	107.68	104.30
1	1A	2882	G	N3-C2-N2	6.75	124.63	119.90
32	1a	577	G	OP2-P-O3'	6.75	120.06	105.20
1	2A	363(C)	G	N7-C8-N9	-6.75	109.72	113.10
1	2A	1246	A	C2-N3-C4	-6.75	107.22	110.60
1	2A	1076	C	N3-C2-O2	-6.75	117.17	121.90
1	1A	139	A	N7-C8-N9	-6.75	110.42	113.80
1	2A	1760	A	N7-C8-N9	-6.75	110.42	113.80
1	1A	798	A	C6-N1-C2	-6.75	114.55	118.60
1	1A	1187	U	C2-N1-C1'	6.75	125.80	117.70
1	1A	2618	C	N1-C2-O2	-6.75	114.85	118.90
1	2A	297	C	N3-C2-O2	-6.75	117.17	121.90
1	2A	845	G	N3-C4-C5	-6.75	125.23	128.60
1	2A	1863	G	N1-C6-O6	6.75	123.95	119.90
1	2A	1351	C	OP1-P-O3'	6.75	120.04	105.20
1	2A	2069	G	N7-C8-N9	-6.75	109.73	113.10
1	1A	1859	G	C6-C5-N7	-6.75	126.35	130.40
1	2A	1216	G	C8-N9-C4	-6.75	103.70	106.40
1	2A	2319	G	C4-C5-N7	6.75	113.50	110.80
32	2a	1396	A	OP1-P-OP2	6.75	129.72	119.60
1	1A	1184	G	O5'-P-OP2	-6.74	99.63	105.70
2	1B	79	C	C2-N3-C4	-6.74	116.53	119.90
32	1a	398	C	C6-N1-C2	6.74	123.00	120.30
32	1a	912	C	N3-C2-O2	6.74	126.62	121.90
1	2A	2574	G	C5-C6-O6	-6.74	124.56	128.60
1	1A	716	G	C8-N9-C4	6.74	109.09	106.40
1	2A	1790	C	P-O3'-C3'	6.74	127.78	119.70
1	2A	1934	C	N3-C4-N4	-6.74	113.28	118.00
1	1A	244	A	N1-C2-N3	6.74	132.67	129.30
32	1a	560	U	C5-C6-N1	6.74	126.07	122.70
1	2A	1516	C	C6-N1-C2	6.74	122.99	120.30
32	1a	187	C	C6-N1-C2	-6.73	117.61	120.30
1	2A	2207	G	C4-C5-C6	6.73	122.84	118.80
1	1A	108	G	N1-C6-O6	-6.73	115.86	119.90
1	1A	130	G	C4-C5-N7	-6.73	108.11	110.80
1	1A	1508	G	O5'-P-OP1	-6.73	99.64	105.70
1	2A	887	A	C8-N9-C4	6.73	108.49	105.80
1	1A	727	G	O5'-P-OP1	-6.73	99.64	105.70
13	2R	103	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	1A	418	G	N3-C2-N2	-6.73	115.19	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2111	U	N3-C4-C5	6.73	118.64	114.60
1	2A	2570	G	C4-C5-N7	-6.73	108.11	110.80
1	1A	1728	G	C5-N7-C8	-6.73	100.94	104.30
1	1A	1948	U	O5'-P-OP2	-6.73	99.64	105.70
1	1A	1206	G	C8-N9-C4	6.73	109.09	106.40
1	1A	1613	A	C6-N1-C2	6.73	122.64	118.60
1	1A	501	U	C4-C5-C6	6.72	123.73	119.70
1	1A	1838	G	C5-C6-O6	-6.72	124.56	128.60
1	2A	1702	G	C6-C5-N7	6.72	134.44	130.40
1	1A	770	G	N3-C2-N2	6.72	124.61	119.90
1	2A	1312	U	C5-C4-O4	6.72	129.93	125.90
1	2A	2454	G	C5-C6-O6	6.72	132.63	128.60
32	2a	811	C	N3-C2-O2	6.72	126.61	121.90
1	1A	1708	G	N7-C8-N9	-6.72	109.74	113.10
1	1A	1487	G	O5'-P-OP2	-6.72	99.65	105.70
32	2a	142	G	N3-C4-C5	-6.72	125.24	128.60
1	1A	1281	G	C2-N3-C4	-6.72	108.54	111.90
1	1A	2277	U	OP1-P-OP2	-6.72	109.53	119.60
32	1a	869	G	N3-C4-C5	6.72	131.96	128.60
1	2A	1902	C	O5'-P-OP2	6.72	118.76	110.70
32	1a	771	G	OP2-P-O3'	6.71	119.97	105.20
1	2A	1987	G	N1-C6-O6	6.71	123.93	119.90
1	2A	2378	A	N9-C4-C5	-6.71	103.11	105.80
32	2a	302	G	C8-N9-C4	6.71	109.09	106.40
1	1A	760	G	N1-C6-O6	6.71	123.93	119.90
1	1A	1541	A	O5'-P-OP2	-6.71	99.66	105.70
1	1A	398	A	C5-C6-N6	-6.71	118.33	123.70
1	1A	1110	C	N1-C2-O2	6.71	122.92	118.90
1	1A	2704	C	C2-N3-C4	-6.71	116.55	119.90
1	1A	2472	U	N3-C2-O2	-6.71	117.51	122.20
1	2A	1573	G	N9-C4-C5	6.71	108.08	105.40
1	2A	1334	G	C4-C5-N7	-6.70	108.12	110.80
32	2a	851	G	C8-N9-C4	-6.70	103.72	106.40
1	1A	1447	G	C5-C6-N1	-6.70	108.15	111.50
1	1A	2258	G	N7-C8-N9	-6.70	109.75	113.10
1	1A	2521	G	N1-C6-O6	-6.70	115.88	119.90
32	1a	148	G	N3-C4-N9	6.70	130.02	126.00
1	1A	250	G	C5-N7-C8	-6.70	100.95	104.30
1	1A	2033	U	N1-C2-O2	-6.70	118.11	122.80
1	1A	2331	G	N9-C4-C5	6.70	108.08	105.40
1	1A	2461	U	C5-C4-O4	-6.70	121.88	125.90
2	1B	33	G	O5'-P-OP2	-6.70	99.67	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	769	G	OP1-P-O3'	6.70	119.94	105.20
1	2A	1459	G	N1-C6-O6	-6.70	115.88	119.90
1	2A	2517	C	O4'-C1'-N1	6.70	113.56	108.20
1	1A	176	G	N9-C4-C5	6.70	108.08	105.40
1	1A	821	A	C8-N9-C4	-6.70	103.12	105.80
1	1A	2579	G	C5-C6-O6	6.70	132.62	128.60
32	1a	802	A	N1-C6-N6	6.70	122.62	118.60
32	1a	1442	G	C8-N9-C4	-6.70	103.72	106.40
1	1A	2125	C	C2-N3-C4	6.70	123.25	119.90
1	1A	1159	U	N3-C2-O2	6.70	126.89	122.20
1	1A	1728	G	N3-C4-C5	6.70	131.95	128.60
1	2A	1126	A	O5'-P-OP1	-6.70	99.67	105.70
1	2A	2823	A	C2-N3-C4	-6.70	107.25	110.60
32	2a	715	A	C2-N3-C4	-6.70	107.25	110.60
1	1A	2049	G	N1-C2-N2	-6.69	110.17	116.20
32	1a	139	G	C8-N9-C4	-6.69	103.72	106.40
1	1A	147	U	C6-N1-C2	6.69	125.02	121.00
1	1A	2622	C	C4-C5-C6	6.69	120.75	117.40
32	1a	560	U	C6-N1-C2	-6.69	116.98	121.00
1	2A	2508	G	O5'-P-OP1	-6.69	99.68	105.70
1	1A	103	C	N3-C4-C5	6.69	124.58	121.90
1	1A	1453	C	C2-N3-C4	-6.69	116.56	119.90
1	1A	2244	U	O5'-P-OP2	-6.69	99.68	105.70
1	1A	2262	G	N1-C6-O6	-6.69	115.89	119.90
32	1a	737	A	O5'-P-OP2	6.69	118.73	110.70
1	2A	416	C	O5'-P-OP1	6.69	118.73	110.70
1	1A	590	A	N9-C4-C5	6.69	108.47	105.80
1	1A	1742	G	O5'-P-OP1	-6.69	99.68	105.70
1	1A	2220	A	OP1-P-OP2	-6.69	109.57	119.60
32	1a	1513	A	C5-C6-N6	-6.69	118.35	123.70
1	2A	1246	A	C8-N9-C4	6.69	108.47	105.80
1	1A	82	G	C5-C6-O6	-6.68	124.59	128.60
1	1A	916	G	O5'-P-OP2	-6.68	99.68	105.70
1	1A	490	U	OP1-P-OP2	-6.68	109.58	119.60
1	1A	668	A	C8-N9-C4	6.68	108.47	105.80
1	1A	1664	A	C4-C5-N7	-6.68	107.36	110.70
32	1a	187	C	C2-N1-C1'	6.68	126.15	118.80
1	2A	2084	C	C6-N1-C2	6.68	122.97	120.30
1	2A	2230	G	C5-C6-N1	-6.68	108.16	111.50
1	1A	2238	C	N3-C2-O2	6.68	126.58	121.90
1	2A	247	G	N3-C4-C5	6.68	131.94	128.60
1	2A	1108	U	N3-C4-O4	6.68	124.08	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1780	A	C8-N9-C4	-6.68	103.13	105.80
1	1A	1828	C	C5-C6-N1	-6.68	117.66	121.00
1	1A	2802	C	C5-C6-N1	-6.68	117.66	121.00
1	2A	1904	G	C4-C5-N7	-6.68	108.13	110.80
1	1A	537	G	N1-C6-O6	6.67	123.91	119.90
1	1A	2094	G	N1-C6-O6	-6.67	115.90	119.90
32	1a	114	U	OP1-P-OP2	6.67	129.61	119.60
1	2A	323	G	C5-C6-O6	-6.67	124.60	128.60
1	2A	1420	U	P-O3'-C3'	6.67	127.71	119.70
1	2A	2896	C	N1-C2-O2	6.67	122.91	118.90
32	1a	266	G	C5-N7-C8	-6.67	100.96	104.30
32	2a	1452	C	N1-C2-O2	6.67	122.90	118.90
1	1A	1375	U	N3-C4-O4	-6.67	114.73	119.40
1	2A	1020	A	C8-N9-C4	6.67	108.47	105.80
1	2A	2319	G	N3-C4-N9	-6.67	122.00	126.00
1	1A	2361	G	OP1-P-OP2	6.67	129.60	119.60
1	1A	2768	C	C6-N1-C2	-6.67	117.63	120.30
1	2A	1369	G	C5-C6-N1	6.67	114.83	111.50
1	1A	2802	C	C6-N1-C2	6.67	122.97	120.30
32	2a	857	C	O5'-P-OP2	-6.67	99.70	105.70
1	1A	1169	C	C5-C4-N4	-6.66	115.53	120.20
1	1A	1661	C	C6-N1-C2	-6.66	117.64	120.30
1	1A	1710	C	C5-C6-N1	-6.66	117.67	121.00
1	1A	2476	C	N3-C4-C5	6.66	124.56	121.90
32	1a	962	C	C6-N1-C2	6.66	122.97	120.30
1	1A	624	C	C5-C6-N1	-6.66	117.67	121.00
32	2a	1054	C	C6-N1-C1'	-6.66	112.81	120.80
1	1A	2068	G	N1-C6-O6	-6.66	115.90	119.90
1	1A	1051	C	C5-C4-N4	6.66	124.86	120.20
1	1A	2331	G	C4-C5-N7	6.66	113.46	110.80
32	1a	655	A	O5'-P-OP2	-6.66	99.71	105.70
1	2A	1079	C	N3-C2-O2	-6.66	117.24	121.90
1	2A	1354	A	O5'-P-OP2	-6.66	99.71	105.70
32	2a	32	A	C2-N3-C4	6.66	113.93	110.60
1	1A	715	G	C8-N9-C4	6.66	109.06	106.40
1	1A	1510	C	O5'-P-OP1	-6.66	99.71	105.70
1	1A	1685	C	N1-C2-O2	-6.66	114.91	118.90
32	1a	454	C	O4'-C1'-N1	6.66	113.53	108.20
1	2A	2257	U	O5'-P-OP1	-6.66	99.71	105.70
1	1A	2577	A	C5-C6-N1	6.66	121.03	117.70
32	1a	1492	A	N9-C4-C5	6.66	108.46	105.80
32	2a	115	G	P-O3'-C3'	6.66	127.69	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	719	C	N3-C4-C5	6.65	124.56	121.90
1	1A	2735	G	N3-C4-N9	6.65	129.99	126.00
1	2A	186	G	N3-C2-N2	-6.65	115.24	119.90
1	2A	2852	G	C8-N9-C4	6.65	109.06	106.40
32	2a	1024	G	N9-C4-C5	6.65	108.06	105.40
1	1A	975	U	C6-N1-C2	6.65	124.99	121.00
1	1A	733	G	C4-C5-N7	6.65	113.46	110.80
1	1A	1283	A	N9-C4-C5	6.65	108.46	105.80
1	2A	1758	G	C8-N9-C4	6.65	109.06	106.40
32	2a	1476	G	O5'-P-OP2	6.65	118.68	110.70
1	1A	792	G	N9-C4-C5	-6.65	102.74	105.40
1	1A	2807	C	C6-N1-C2	-6.65	117.64	120.30
1	2A	2041	U	N3-C4-O4	6.65	124.05	119.40
1	1A	1431	G	O4'-C1'-N9	6.65	113.52	108.20
1	1A	2324	U	O5'-P-OP2	6.65	118.68	110.70
1	2A	988	A	C5-C6-N6	-6.65	118.38	123.70
1	1A	203	G	O5'-P-OP2	-6.65	99.72	105.70
1	1A	314	G	O5'-P-OP1	-6.65	99.72	105.70
32	2a	451	A	OP1-P-OP2	6.65	129.57	119.60
32	1a	899	C	N1-C2-O2	-6.64	114.91	118.90
1	1A	826	U	C5-C4-O4	-6.64	121.91	125.90
2	1B	5	C	C6-N1-C2	6.64	122.96	120.30
32	1a	57	G	C8-N9-C4	-6.64	103.74	106.40
1	1A	1522	G	N9-C4-C5	6.64	108.06	105.40
32	1a	1183	A	OP1-P-O3'	6.64	119.81	105.20
1	2A	741	G	N3-C4-N9	-6.64	122.02	126.00
32	2a	1057	G	C8-N9-C4	6.64	109.06	106.40
1	1A	553	A	N7-C8-N9	6.64	117.12	113.80
1	1A	718	C	N1-C2-N3	6.64	123.85	119.20
1	1A	1571	G	OP1-P-OP2	6.64	129.56	119.60
32	1a	515	G	C8-N9-C4	-6.64	103.74	106.40
1	2A	354	G	C8-N9-C4	6.64	109.06	106.40
32	1a	189(G)	G	N3-C2-N2	-6.64	115.25	119.90
1	2A	1603	A	C2-N3-C4	6.64	113.92	110.60
1	1A	217	A	C8-N9-C1'	6.64	139.65	127.70
1	1A	1854	G	C2-N3-C4	-6.64	108.58	111.90
1	1A	2344	U	C5-C6-N1	-6.64	119.38	122.70
1	2A	744	G	N1-C6-O6	-6.64	115.92	119.90
1	2A	2894	G	C5-C6-O6	6.64	132.58	128.60
1	1A	1640	G	N3-C4-N9	-6.63	122.02	126.00
1	2A	2334	G	C5-C6-O6	-6.63	124.62	128.60
1	1A	960	C	O5'-P-OP2	-6.63	99.73	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	5	C	C5-C6-N1	-6.63	117.68	121.00
1	2A	374	A	N1-C6-N6	6.63	122.58	118.60
1	1A	731	G	O5'-P-OP2	-6.63	99.73	105.70
32	1a	813	U	OP1-P-OP2	-6.63	109.65	119.60
32	1a	1224	G	N1-C6-O6	-6.63	115.92	119.90
1	2A	1759	A	N1-C2-N3	6.63	132.62	129.30
32	2a	305	G	C5-C6-O6	6.63	132.58	128.60
32	2a	662	G	N1-C6-O6	6.63	123.88	119.90
32	2a	778	G	C5-C6-O6	-6.63	124.62	128.60
1	1A	1013	G	N1-C6-O6	-6.63	115.92	119.90
1	2A	562	U	N3-C2-O2	-6.63	117.56	122.20
32	2a	833	U	N3-C2-O2	-6.63	117.56	122.20
1	2A	2008	C	O5'-P-OP2	-6.63	99.73	105.70
1	1A	322	G	C5-N7-C8	6.63	107.61	104.30
1	1A	999	G	C4-C5-N7	-6.63	108.15	110.80
1	1A	2320	G	C4-C5-N7	6.63	113.45	110.80
1	2A	1460	A	O4'-C1'-N9	6.63	113.50	108.20
1	1A	150	C	C5-C6-N1	-6.62	117.69	121.00
1	1A	202	A	OP2-P-O3'	6.62	119.78	105.20
1	1A	848	G	C5-C6-O6	6.62	132.57	128.60
1	1A	405	C	C2-N3-C4	-6.62	116.59	119.90
1	1A	1727	U	N3-C4-O4	-6.62	114.76	119.40
1	2A	1899	G	C4-C5-N7	6.62	113.45	110.80
1	1A	843	C	C2-N3-C4	-6.62	116.59	119.90
1	1A	1692	G	C2-N3-C4	6.62	115.21	111.90
1	1A	2041	A	C2-N3-C4	-6.62	107.29	110.60
1	1A	2285	A	N1-C6-N6	6.62	122.57	118.60
1	1A	2858	G	N1-C6-O6	-6.62	115.93	119.90
1	1A	2249	G	C2-N3-C4	-6.62	108.59	111.90
1	1A	2728	C	C2-N3-C4	-6.62	116.59	119.90
32	1a	236	G	O5'-P-OP2	-6.62	99.74	105.70
32	1a	280	C	N3-C4-C5	6.62	124.55	121.90
32	2a	346	G	N3-C4-C5	-6.62	125.29	128.60
1	1A	343	C	N3-C4-C5	-6.62	119.25	121.90
1	1A	1033	G	C8-N9-C4	-6.62	103.75	106.40
32	1a	1385	G	O5'-P-OP2	-6.62	99.74	105.70
1	2A	2269	A	N1-C6-N6	6.62	122.57	118.60
1	1A	1397	C	O5'-P-OP1	6.62	118.64	110.70
1	1A	2298	A	C4-C5-C6	6.62	120.31	117.00
1	1A	2590	G	C6-C5-N7	6.62	134.37	130.40
1	2A	1992	G	P-O3'-C3'	6.62	127.64	119.70
32	2a	995	C	N1-C2-O2	6.62	122.87	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1995	G	N1-C2-N3	6.62	127.87	123.90
1	2A	1045	A	C5-N7-C8	-6.62	100.59	103.90
1	1A	906	G	N3-C4-C5	6.61	131.91	128.60
1	1A	1787	G	O5'-P-OP2	-6.61	99.75	105.70
1	2A	391	G	C8-N9-C1'	-6.61	118.40	127.00
1	2A	1063	G	N3-C4-C5	-6.61	125.29	128.60
1	2A	1690	A	C5-C6-N6	-6.61	118.41	123.70
32	2a	266	G	C6-C5-N7	-6.61	126.43	130.40
32	2a	1395	C	N3-C4-C5	-6.61	119.25	121.90
1	1A	1031	C	N3-C4-N4	-6.61	113.37	118.00
1	1A	262	C	C5-C6-N1	-6.61	117.69	121.00
1	1A	1110	C	N3-C2-O2	-6.61	117.27	121.90
1	1A	2189	U	O4'-C1'-N1	6.61	113.49	108.20
1	1A	2877	G	C5-C6-O6	-6.61	124.63	128.60
1	1A	1461	U	N3-C4-O4	-6.61	114.77	119.40
1	2A	768	G	O5'-P-OP2	-6.61	99.75	105.70
1	1A	1184	G	C4-C5-N7	-6.61	108.16	110.80
1	1A	2323	A	N1-C6-N6	-6.61	114.64	118.60
2	1B	50	G	C6-C5-N7	6.61	134.36	130.40
1	2A	2032	G	C5-N7-C8	6.61	107.60	104.30
1	1A	1474	C	O5'-P-OP1	-6.60	99.76	105.70
32	1a	664	G	C8-N9-C4	-6.60	103.76	106.40
1	1A	223	C	N1-C2-O2	6.60	122.86	118.90
1	1A	1033	G	N3-C4-N9	-6.60	122.04	126.00
1	1A	1232	G	N3-C2-N2	6.60	124.52	119.90
1	1A	1617	A	N1-C6-N6	6.60	122.56	118.60
1	1A	2108	U	N1-C2-O2	6.60	127.42	122.80
1	1A	2498	G	C4-C5-N7	-6.60	108.16	110.80
32	1a	1106	G	C8-N9-C4	-6.60	103.76	106.40
32	1a	1181	G	C8-N9-C4	6.60	109.04	106.40
1	2A	1848	A	C8-N9-C4	6.60	108.44	105.80
32	2a	1067	A	P-O3'-C3'	6.60	127.62	119.70
1	1A	2028	C	N3-C4-C5	6.60	124.54	121.90
1	1A	1254	G	N1-C2-N2	6.60	122.14	116.20
1	1A	1664	A	C5-N7-C8	6.60	107.20	103.90
1	1A	2610	A	OP2-P-O3'	6.60	119.72	105.20
32	1a	510	A	O5'-P-OP2	-6.60	99.76	105.70
1	2A	2755	C	C5-C6-N1	6.60	124.30	121.00
1	1A	127	C	O5'-P-OP2	-6.60	99.76	105.70
1	1A	1220	U	O4'-C1'-N1	6.60	113.48	108.20
1	1A	1405	A	C2-N3-C4	6.60	113.90	110.60
32	1a	1151	A	O5'-P-OP2	-6.60	99.76	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2726	U	C6-N1-C2	6.60	124.96	121.00
32	2a	1030(B)	C	N1-C2-O2	6.60	122.86	118.90
1	1A	1052	C	N1-C2-O2	-6.60	114.94	118.90
1	1A	1450	C	OP1-P-OP2	6.59	129.49	119.60
1	1A	1202	A	O4'-C1'-N9	-6.59	102.93	108.20
1	1A	1515	C	N1-C2-O2	-6.59	114.94	118.90
27	15	15	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	1A	1112	U	C6-N1-C2	-6.59	117.05	121.00
1	1A	1655	A	C5-C6-N6	-6.59	118.43	123.70
1	1A	2049	G	N1-C2-N3	6.59	127.85	123.90
32	1a	1348	U	O5'-P-OP2	-6.59	99.77	105.70
1	2A	1987	G	C8-N9-C4	6.59	109.04	106.40
1	2A	2042	A	C8-N9-C4	6.59	108.44	105.80
1	2A	2574	G	N1-C6-O6	6.59	123.85	119.90
1	1A	25	U	C5-C4-O4	-6.59	121.95	125.90
1	2A	2861	G	N3-C2-N2	-6.59	115.29	119.90
32	2a	140	A	C8-N9-C4	-6.59	103.17	105.80
1	1A	1306	G	C2-N3-C4	-6.59	108.61	111.90
1	1A	1686	U	N3-C4-O4	-6.59	114.79	119.40
1	2A	1035	U	C5-C4-O4	6.59	129.85	125.90
1	1A	348	A	O5'-P-OP1	6.58	118.60	110.70
1	2A	2706	G	N7-C8-N9	-6.58	109.81	113.10
1	1A	2529	C	N1-C2-O2	-6.58	114.95	118.90
1	1A	2537	G	C8-N9-C4	6.58	109.03	106.40
1	2A	571	A	N9-C4-C5	6.58	108.43	105.80
1	2A	2041	U	C2-N3-C4	-6.58	123.05	127.00
1	2A	2596	U	C5-C6-N1	-6.58	119.41	122.70
32	2a	357	G	N3-C2-N2	-6.58	115.29	119.90
32	1a	1286	A	N1-C6-N6	-6.58	114.65	118.60
1	2A	271(L)	U	C2-N1-C1'	6.58	125.60	117.70
1	1A	359	C	C5-C6-N1	6.58	124.29	121.00
1	2A	581	C	N3-C4-N4	-6.58	113.39	118.00
1	2A	1378	A	O5'-P-OP1	-6.58	99.78	105.70
1	2A	33	U	N3-C2-O2	-6.58	117.60	122.20
1	1A	20	C	N3-C4-C5	6.58	124.53	121.90
1	1A	660	C	N1-C2-N3	6.58	123.80	119.20
1	1A	1298	G	N3-C4-C5	6.58	131.89	128.60
1	1A	1783	C	N1-C2-O2	-6.58	114.95	118.90
2	1B	74	U	O5'-P-OP2	-6.58	99.78	105.70
1	2A	1244	G	C8-N9-C4	6.58	109.03	106.40
32	2a	26	A	O5'-P-OP2	-6.58	99.78	105.70
1	1A	354	A	N1-C2-N3	6.57	132.59	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1778	U	C6-N1-C2	6.57	124.94	121.00
1	2A	2166	G	N9-C4-C5	6.57	108.03	105.40
1	1A	61	C	C5-C6-N1	-6.57	117.71	121.00
32	2a	1530	G	C4-N9-C1'	-6.57	117.96	126.50
1	1A	176	G	C8-N9-C4	-6.57	103.77	106.40
1	1A	2392	C	C2-N3-C4	-6.57	116.61	119.90
1	2A	2690	C	N1-C2-O2	-6.57	114.96	118.90
32	2a	1532	U	N1-C2-O2	-6.57	118.20	122.80
1	1A	1381	U	C4-C5-C6	6.57	123.64	119.70
1	1A	2092	G	C6-C5-N7	-6.57	126.46	130.40
1	1A	2453	C	N1-C2-N3	6.57	123.80	119.20
1	2A	391	G	N3-C4-N9	6.57	129.94	126.00
1	1A	565	C	C2-N3-C4	-6.57	116.62	119.90
1	1A	1456	G	OP2-P-O3'	6.57	119.65	105.20
1	1A	2386	C	C5-C6-N1	-6.57	117.72	121.00
1	1A	2609	G	O5'-P-OP1	6.57	118.58	110.70
1	2A	1899	G	C5-N7-C8	-6.57	101.02	104.30
1	2A	573	G	OP1-P-O3'	6.56	119.64	105.20
1	1A	2001	C	N3-C4-C5	6.56	124.52	121.90
1	1A	2620	G	N1-C6-O6	6.56	123.84	119.90
1	2A	2629	A	C5-C6-N1	-6.56	114.42	117.70
1	1A	1985	U	O4'-C1'-N1	-6.56	102.95	108.20
32	1a	1168	A	C8-N9-C4	-6.56	103.18	105.80
1	2A	1721	G	N3-C4-N9	6.56	129.94	126.00
32	1a	687	A	P-O3'-C3'	6.56	127.57	119.70
32	2a	1406	U	O5'-P-OP1	6.56	118.57	110.70
1	1A	2348	A	N1-C2-N3	-6.55	126.02	129.30
1	1A	2428	C	N3-C4-N4	-6.55	113.41	118.00
1	2A	2564	A	N1-C6-N6	6.55	122.53	118.60
32	2a	509	A	C8-N9-C4	-6.55	103.18	105.80
1	1A	1358	U	C4-C5-C6	6.55	123.63	119.70
1	1A	2879	G	N1-C6-O6	6.55	123.83	119.90
1	1A	1696	G	C8-N9-C4	-6.55	103.78	106.40
1	2A	2794	C	C5-C6-N1	6.55	124.28	121.00
1	1A	99	G	C8-N9-C4	6.55	109.02	106.40
1	1A	1655	A	C8-N9-C4	6.55	108.42	105.80
1	1A	697	C	C5-C6-N1	6.55	124.27	121.00
1	2A	1075	C	C5-C6-N1	6.55	124.27	121.00
32	2a	411	A	O5'-P-OP2	-6.55	99.81	105.70
1	1A	2713	C	N1-C2-O2	-6.54	114.97	118.90
1	1A	476	G	OP1-P-OP2	6.54	129.42	119.60
1	1A	850	U	C5-C6-N1	-6.54	119.43	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1298	G	N3-C4-N9	-6.54	122.07	126.00
1	1A	1921	G	N9-C4-C5	-6.54	102.78	105.40
1	1A	2593	G	N9-C4-C5	-6.54	102.78	105.40
1	1A	2599	A	O5'-P-OP2	-6.54	99.81	105.70
20	1Y	50	ARG	NE-CZ-NH1	6.54	123.57	120.30
32	1a	945	G	C5-C6-O6	-6.54	124.67	128.60
1	2A	749	C	C2-N3-C4	6.54	123.17	119.90
1	1A	923	C	O5'-P-OP2	6.54	118.55	110.70
1	1A	2346	G	OP2-P-O3'	6.54	119.59	105.20
32	1a	635	G	O5'-P-OP2	6.54	118.55	110.70
32	1a	625	G	O5'-P-OP1	-6.54	99.81	105.70
1	1A	756	U	O5'-P-OP1	6.54	118.55	110.70
1	1A	1472	G	C8-N9-C4	6.54	109.02	106.40
1	1A	857	U	C5-C4-O4	-6.54	121.98	125.90
1	1A	1433	C	O5'-P-OP2	-6.54	99.82	105.70
1	2A	363(E)	U	N3-C4-O4	6.54	123.98	119.40
1	2A	1973	G	C8-N9-C4	6.54	109.02	106.40
1	1A	889	G	OP2-P-O3'	6.54	119.58	105.20
1	1A	2392	C	C6-N1-C2	6.54	122.91	120.30
1	2A	1377	G	N3-C4-C5	-6.54	125.33	128.60
1	1A	1097	G	C5-C6-N1	-6.53	108.23	111.50
1	1A	2034	G	C5-C6-O6	6.53	132.52	128.60
1	1A	2623	U	O5'-P-OP2	6.53	118.54	110.70
1	2A	2339	G	O5'-P-OP2	-6.53	99.82	105.70
1	2A	1937	A	N7-C8-N9	-6.53	110.53	113.80
1	1A	1329	G	OP1-P-OP2	6.53	129.40	119.60
1	1A	1723	A	C8-N9-C4	6.53	108.41	105.80
1	1A	1823	G	N1-C6-O6	-6.53	115.98	119.90
32	1a	879	C	C6-N1-C2	6.53	122.91	120.30
32	1a	1522	U	OP1-P-OP2	6.53	129.40	119.60
1	2A	249	C	N3-C2-O2	6.53	126.47	121.90
1	2A	1647	G	C5-C6-N1	6.53	114.77	111.50
1	1A	548	C	C6-N1-C2	6.53	122.91	120.30
1	1A	747	G	N1-C6-O6	-6.53	115.98	119.90
1	1A	1832	G	N9-C4-C5	-6.53	102.79	105.40
2	1B	24	G	N3-C4-C5	-6.53	125.34	128.60
1	2A	1858	G	N1-C6-O6	-6.53	115.98	119.90
32	2a	483	C	C6-N1-C2	6.53	122.91	120.30
1	1A	2728	C	C5-C6-N1	-6.52	117.74	121.00
1	1A	1969	C	O5'-P-OP1	-6.52	99.83	105.70
1	1A	2458	G	C6-N1-C2	6.52	129.01	125.10
32	1a	78	G	O4'-C1'-N9	6.52	113.42	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1998	G	C5-C6-O6	6.52	132.51	128.60
1	2A	2689	U	N3-C2-O2	-6.52	117.63	122.20
1	2A	2721	A	O5'-P-OP1	-6.52	99.83	105.70
1	1A	1724	A	C2-N3-C4	-6.52	107.34	110.60
1	1A	2499	G	C4-C5-N7	6.52	113.41	110.80
1	2A	2877	G	C8-N9-C4	6.52	109.01	106.40
1	1A	1052	C	C4-C5-C6	6.52	120.66	117.40
1	1A	2410	U	OP2-P-O3'	6.52	119.54	105.20
1	1A	2546	A	C5-C6-N6	-6.52	118.48	123.70
1	1A	2641	A	O4'-C1'-N9	6.52	113.42	108.20
1	2A	1186	G	OP1-P-O3'	6.52	119.54	105.20
32	2a	454	C	N3-C2-O2	-6.52	117.34	121.90
1	1A	399	G	O4'-C1'-N9	6.52	113.41	108.20
1	1A	1358	U	N3-C4-C5	-6.52	110.69	114.60
1	1A	2606	C	C6-N1-C2	6.52	122.91	120.30
32	1a	799	G	C4-C5-N7	-6.52	108.19	110.80
1	1A	424	G	C8-N9-C4	6.51	109.01	106.40
1	1A	1277	G	N1-C6-O6	6.51	123.81	119.90
4	1E	119	ARG	NE-CZ-NH1	6.51	123.56	120.30
11	1P	41	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	2A	749	C	C5-C6-N1	6.51	124.26	121.00
1	1A	623	G	C5-C6-N1	-6.51	108.24	111.50
1	1A	1822	A	OP2-P-O3'	6.51	119.53	105.20
1	1A	2625	U	N3-C2-O2	-6.51	117.64	122.20
1	2A	9	U	N3-C4-C5	-6.51	110.69	114.60
1	1A	2586	G	C5-C6-N1	6.51	114.76	111.50
32	1a	558	G	N1-C6-O6	6.51	123.81	119.90
1	1A	649	C	N3-C4-C5	6.51	124.50	121.90
1	1A	2081	A	N9-C4-C5	6.51	108.40	105.80
32	1a	1052	U	N1-C2-O2	6.51	127.36	122.80
32	2a	746	A	O5'-P-OP2	-6.51	99.84	105.70
1	1A	181	C	C2-N3-C4	-6.51	116.65	119.90
1	1A	856	G	N1-C6-O6	-6.51	116.00	119.90
1	1A	260	A	C8-N9-C4	6.51	108.40	105.80
1	1A	1193	C	C6-N1-C2	6.51	122.90	120.30
1	1A	1958	A	O4'-C1'-N9	6.51	113.40	108.20
1	2A	761	A	C5-N7-C8	6.51	107.15	103.90
32	2a	649	G	N3-C4-C5	6.51	131.85	128.60
32	2a	1093	A	C4-C5-N7	6.51	113.95	110.70
32	2a	561	U	N1-C2-O2	-6.50	118.25	122.80
1	2A	2431	U	O5'-P-OP2	-6.50	99.85	105.70
1	1A	350	G	N7-C8-N9	-6.50	109.85	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1021	G	N1-C2-N2	6.50	122.05	116.20
1	2A	1077	A	O5'-P-OP1	-6.50	99.85	105.70
1	2A	2834	G	N1-C6-O6	-6.50	116.00	119.90
1	1A	702	A	C2-N3-C4	-6.50	107.35	110.60
1	1A	1790	A	C6-C5-N7	-6.50	127.75	132.30
1	1A	2358	A	N1-C2-N3	6.50	132.55	129.30
32	2a	1436	U	C5-C4-O4	-6.50	122.00	125.90
1	1A	1171	G	N1-C2-N3	6.50	127.80	123.90
32	1a	266	G	N1-C6-O6	6.50	123.80	119.90
1	2A	312	G	O5'-P-OP1	-6.50	99.85	105.70
1	1A	128	C	N3-C4-C5	6.50	124.50	121.90
1	1A	981	C	N1-C2-O2	-6.50	115.00	118.90
1	1A	1200	G	OP1-P-OP2	-6.50	109.86	119.60
1	1A	1816	A	N7-C8-N9	6.50	117.05	113.80
1	1A	1922	A	C2-N3-C4	6.50	113.85	110.60
1	2A	1615	C	N3-C4-C5	-6.50	119.30	121.90
32	2a	1024	G	N1-C2-N2	6.50	122.05	116.20
1	1A	1720	U	C2-N3-C4	-6.50	123.10	127.00
1	2A	1547	C	C4-C5-C6	6.50	120.65	117.40
32	2a	400	C	C6-N1-C2	6.50	122.90	120.30
1	1A	125	A	C6-N1-C2	-6.49	114.70	118.60
1	1A	189	U	C4-C5-C6	6.49	123.60	119.70
1	1A	514	G	N1-C2-N3	6.49	127.80	123.90
1	1A	1218	G	O4'-C1'-N9	6.49	113.39	108.20
1	1A	1539	C	C4-C5-C6	6.49	120.65	117.40
32	1a	635	G	C5-C6-O6	-6.49	124.70	128.60
1	2A	178	G	O5'-P-OP2	-6.49	99.86	105.70
1	2A	2668	G	N1-C6-O6	-6.49	116.00	119.90
32	2a	1075	C	N3-C4-C5	-6.49	119.30	121.90
1	1A	1717	C	N3-C2-O2	6.49	126.44	121.90
1	1A	2006	G	OP2-P-O3'	6.49	119.48	105.20
1	2A	686	G	C5-C6-N1	6.49	114.75	111.50
32	2a	562	C	N1-C2-O2	-6.49	115.00	118.90
1	1A	1346	U	N1-C2-N3	6.49	118.79	114.90
1	2A	747	U	N3-C4-O4	6.49	123.94	119.40
32	1a	804	U	N1-C2-N3	6.49	118.79	114.90
32	2a	1027	C	N3-C2-O2	-6.49	117.36	121.90
1	1A	542	C	OP2-P-O3'	6.49	119.47	105.20
32	1a	1030	C	C5-C6-N1	6.49	124.24	121.00
1	1A	1652	G	C8-N9-C4	6.49	108.99	106.40
1	1A	1742	G	C6-C5-N7	-6.49	126.51	130.40
1	1A	1959	A	O4'-C1'-N9	6.49	113.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1134	G	C8-N9-C4	-6.49	103.81	106.40
1	1A	243	G	C5-N7-C8	6.48	107.54	104.30
1	1A	1264	G	C4-C5-N7	6.48	113.39	110.80
1	1A	1299	A	C6-N1-C2	-6.48	114.71	118.60
1	1A	2279	A	OP1-P-OP2	6.48	129.32	119.60
32	1a	479	C	N3-C4-C5	-6.48	119.31	121.90
32	1a	557	G	N3-C2-N2	6.48	124.44	119.90
1	1A	601	A	C4-C5-C6	6.48	120.24	117.00
1	1A	1353	A	N1-C6-N6	6.48	122.49	118.60
1	1A	2619	G	C8-N9-C4	-6.48	103.81	106.40
2	1B	79	C	N1-C2-N3	6.48	123.73	119.20
1	1A	841	G	N1-C2-N2	-6.48	110.37	116.20
32	1a	794	A	C2-N3-C4	-6.48	107.36	110.60
2	2B	1	U	C2-N1-C1'	6.48	125.47	117.70
1	1A	271	U	C2-N1-C1'	-6.47	109.93	117.70
1	1A	2316	G	O5'-P-OP1	-6.47	99.87	105.70
1	1A	2434	A	C8-N9-C4	-6.47	103.21	105.80
32	1a	1458	G	N3-C4-N9	-6.47	122.11	126.00
1	2A	2144	U	C2-N1-C1'	6.47	125.47	117.70
1	2A	2476	A	C8-N9-C4	-6.47	103.21	105.80
32	2a	190	U	N1-C2-N3	6.47	118.78	114.90
1	1A	857	U	O5'-P-OP2	-6.47	99.88	105.70
1	1A	990	A	O4'-C1'-N9	-6.47	103.02	108.20
1	2A	786	C	N3-C2-O2	6.47	126.43	121.90
1	2A	2269	A	O5'-P-OP1	-6.47	99.88	105.70
1	1A	2509	A	N7-C8-N9	-6.47	110.56	113.80
1	2A	188	G	OP1-P-OP2	6.47	129.31	119.60
1	2A	1091	G	N3-C4-N9	6.47	129.88	126.00
1	2A	1799	G	N3-C4-N9	6.47	129.88	126.00
1	1A	1537	G	N7-C8-N9	-6.47	109.87	113.10
1	1A	2069	U	N3-C4-C5	6.47	118.48	114.60
1	1A	2427	G	N3-C2-N2	-6.47	115.37	119.90
1	2A	1848	A	N7-C8-N9	-6.47	110.57	113.80
1	1A	1028	C	C5-C4-N4	-6.47	115.67	120.20
1	2A	226	G	O4'-C1'-N9	6.47	113.37	108.20
1	2A	2894	G	N1-C6-O6	-6.47	116.02	119.90
1	1A	350	G	C5-N7-C8	6.47	107.53	104.30
1	1A	640	A	O5'-P-OP2	-6.47	99.88	105.70
1	1A	2346	G	N9-C4-C5	-6.47	102.81	105.40
2	1B	98	G	OP1-P-OP2	6.47	129.30	119.60
32	1a	174	C	C6-N1-C2	-6.47	117.71	120.30
32	1a	623	C	C5-C6-N1	6.47	124.23	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1647	G	O4'-C1'-N9	-6.47	103.03	108.20
1	2A	2444	G	N3-C2-N2	-6.47	115.37	119.90
32	2a	561	U	N3-C2-O2	6.47	126.73	122.20
1	1A	1320	A	C4-C5-C6	6.46	120.23	117.00
1	1A	2139	A	N1-C6-N6	-6.46	114.72	118.60
1	1A	2603	C	C6-N1-C2	-6.46	117.71	120.30
1	1A	2783	G	O5'-P-OP1	6.46	118.46	110.70
32	2a	305	G	C4-C5-N7	-6.46	108.21	110.80
1	1A	893	C	OP1-P-OP2	6.46	129.29	119.60
1	1A	1977	U	C5-C6-N1	-6.46	119.47	122.70
1	1A	2082	A	N9-C4-C5	6.46	108.39	105.80
32	1a	623	C	O5'-P-OP1	6.46	118.45	110.70
1	2A	677	A	N1-C6-N6	6.46	122.48	118.60
1	2A	2363	C	O5'-P-OP2	-6.46	99.88	105.70
1	1A	529	U	O5'-P-OP1	-6.46	99.89	105.70
1	2A	2318	G	C5-N7-C8	-6.46	101.07	104.30
1	1A	1994	A	C5-N7-C8	-6.46	100.67	103.90
1	1A	2445	A	N9-C4-C5	-6.46	103.22	105.80
1	2A	567	A	C5-N7-C8	-6.46	100.67	103.90
1	2A	738	G	N1-C6-O6	-6.46	116.03	119.90
1	1A	655	G	N1-C6-O6	6.46	123.77	119.90
1	1A	1803	G	N7-C8-N9	-6.46	109.87	113.10
32	1a	189(E)	U	O5'-P-OP2	-6.46	99.89	105.70
32	1a	190	U	OP1-P-OP2	-6.46	109.92	119.60
1	2A	983	A	C8-N9-C4	6.46	108.38	105.80
1	1A	1370	G	C5-C6-O6	6.45	132.47	128.60
1	1A	1757	C	N3-C2-O2	6.45	126.42	121.90
1	1A	1757	C	C5-C6-N1	-6.45	117.78	121.00
1	1A	2420	U	OP2-P-O3'	6.45	119.39	105.20
1	2A	2828	C	C6-N1-C2	6.45	122.88	120.30
1	1A	563	G	C2-N3-C4	6.45	115.12	111.90
1	1A	1237	G	N3-C4-C5	6.45	131.82	128.60
1	2A	542	C	C6-N1-C2	6.45	122.88	120.30
1	2A	1082	U	N1-C2-O2	6.45	127.31	122.80
1	2A	2162	G	C4-N9-C1'	6.45	134.88	126.50
1	1A	801	C	C6-N1-C2	6.45	122.88	120.30
1	1A	735	U	C4-C5-C6	6.45	123.57	119.70
1	2A	178	G	C5-C6-N1	6.45	114.72	111.50
1	2A	1212	G	C8-N9-C4	6.45	108.98	106.40
32	2a	560	U	C5-C6-N1	6.45	125.92	122.70
1	1A	499	G	OP2-P-O3'	6.44	119.38	105.20
1	1A	2070	G	C8-N9-C4	-6.44	103.82	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	29	GLY	N-CA-C	-6.44	96.99	113.10
1	1A	641	G	N3-C2-N2	6.44	124.41	119.90
1	1A	655	G	C4-C5-N7	6.44	113.38	110.80
1	1A	1911	A	OP1-P-OP2	6.44	129.26	119.60
2	1B	6	C	N3-C4-C5	6.44	124.48	121.90
1	2A	1632	A	N7-C8-N9	-6.44	110.58	113.80
1	1A	589	U	OP2-P-O3'	6.44	119.37	105.20
1	1A	623	G	N9-C4-C5	6.44	107.97	105.40
1	1A	1860	A	O5'-P-OP2	-6.44	99.91	105.70
1	1A	1894	G	O5'-P-OP2	-6.44	99.91	105.70
1	1A	2073	A	C5-N7-C8	6.44	107.12	103.90
1	2A	1992	G	C2-N3-C4	6.44	115.12	111.90
1	2A	2164	C	C6-N1-C2	-6.44	117.73	120.30
32	1a	1372	U	C6-N1-C2	-6.43	117.14	121.00
1	2A	2629	A	C5-C6-N6	6.43	128.85	123.70
1	1A	67	G	C2-N3-C4	6.43	115.12	111.90
1	2A	837	C	C6-N1-C2	-6.43	117.73	120.30
1	1A	188	A	N1-C6-N6	-6.43	114.74	118.60
32	1a	834	C	O5'-P-OP2	-6.43	99.91	105.70
1	2A	510	C	OP1-P-O3'	6.43	119.35	105.20
1	1A	322	G	N3-C4-C5	-6.43	125.39	128.60
1	1A	2402	U	N3-C4-C5	-6.43	110.74	114.60
32	1a	404	U	C5-C4-O4	6.43	129.76	125.90
1	2A	2362	G	C4-C5-N7	6.43	113.37	110.80
2	2B	65	C	O5'-P-OP2	6.43	118.42	110.70
1	2A	1206	G	O5'-P-OP1	-6.43	99.92	105.70
1	2A	1351	C	N1-C2-O2	-6.43	115.05	118.90
3	2D	60	ARG	NE-CZ-NH1	-6.43	117.09	120.30
32	2a	398	C	C5-C4-N4	6.43	124.70	120.20
1	1A	1102	G	C4-C5-N7	6.42	113.37	110.80
1	1A	2593	G	N1-C2-N2	-6.42	110.42	116.20
1	2A	56	A	N1-C6-N6	-6.42	114.75	118.60
1	1A	1828	C	N3-C4-C5	6.42	124.47	121.90
1	1A	2082	A	N1-C2-N3	-6.42	126.09	129.30
1	1A	2187	G	C6-C5-N7	6.42	134.25	130.40
1	2A	2440	C	O5'-P-OP2	-6.42	99.92	105.70
32	2a	811	C	N1-C2-O2	-6.42	115.05	118.90
1	1A	830	A	N1-C6-N6	-6.42	114.75	118.60
1	1A	1237	G	C4-C5-N7	-6.42	108.23	110.80
1	1A	2050	U	N3-C4-C5	6.42	118.45	114.60
1	2A	90	U	C5-C4-O4	6.42	129.75	125.90
1	2A	569	U	N1-C2-O2	-6.42	118.31	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1386	U	N1-C2-N3	6.42	118.75	114.90
32	2a	898	G	C2-N3-C4	-6.42	108.69	111.90
1	1A	1853	G	C5-C6-O6	6.42	132.45	128.60
1	1A	2639	G	N3-C4-N9	6.42	129.85	126.00
32	1a	673	G	C8-N9-C4	-6.42	103.83	106.40
1	2A	1904	G	N9-C4-C5	6.42	107.97	105.40
1	1A	130	G	C5-C6-O6	6.42	132.45	128.60
1	1A	355	A	N1-C6-N6	6.42	122.45	118.60
1	1A	585	U	O5'-P-OP1	-6.42	99.93	105.70
1	2A	2879	C	N3-C4-N4	6.42	122.49	118.00
1	2A	2891	G	N1-C6-O6	6.42	123.75	119.90
1	1A	2093	A	OP1-P-OP2	-6.41	109.98	119.60
1	1A	2511	C	C6-N1-C2	-6.41	117.73	120.30
32	2a	704	A	C2-N3-C4	6.41	113.81	110.60
1	1A	1814	A	OP1-P-O3'	6.41	119.31	105.20
5	1F	195	ASP	CB-CA-C	-6.41	97.58	110.40
32	1a	821	G	C5-C6-O6	-6.41	124.75	128.60
1	1A	788	G	N9-C4-C5	6.41	107.96	105.40
1	1A	2511	C	N1-C2-O2	-6.41	115.05	118.90
1	2A	2554	U	C5-C4-O4	6.41	129.75	125.90
32	2a	810	C	N3-C4-C5	6.41	124.47	121.90
1	1A	793	A	O5'-P-OP2	6.41	118.39	110.70
1	1A	1024	G	C4-C5-N7	-6.41	108.24	110.80
1	1A	1067	A	OP2-P-O3'	6.41	119.30	105.20
1	1A	1414	G	C6-C5-N7	6.41	134.25	130.40
1	1A	2187	G	C4-C5-N7	-6.41	108.24	110.80
32	2a	574	A	C4-C5-N7	6.41	113.90	110.70
1	2A	1963	U	N1-C2-O2	6.41	127.28	122.80
1	1A	40	C	N3-C2-O2	6.41	126.38	121.90
1	1A	96	C	OP1-P-OP2	6.41	129.21	119.60
1	1A	554	A	C8-N9-C4	-6.41	103.24	105.80
1	1A	2591	C	N3-C2-O2	-6.41	117.42	121.90
1	1A	1522	G	N1-C2-N2	6.40	121.96	116.20
1	1A	1206	G	N1-C2-N3	-6.40	120.06	123.90
1	1A	1257	G	O5'-P-OP2	-6.40	99.94	105.70
1	1A	2031	G	N3-C2-N2	-6.40	115.42	119.90
1	1A	2043	C	N1-C2-O2	-6.40	115.06	118.90
1	2A	76	C	C5-C6-N1	6.40	124.20	121.00
1	2A	408	G	O5'-P-OP2	-6.40	99.94	105.70
1	2A	2577	A	C6-N1-C2	6.40	122.44	118.60
32	2a	719	C	N3-C4-N4	6.40	122.48	118.00
1	1A	1690	G	C6-C5-N7	6.40	134.24	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2751	G	N3-C4-C5	6.40	131.80	128.60
32	2a	832	C	C6-N1-C2	-6.40	117.74	120.30
32	1a	1021	G	C5-C6-N1	6.40	114.70	111.50
1	1A	421	A	N1-C6-N6	-6.40	114.76	118.60
1	1A	709	G	C4-C5-N7	-6.40	108.24	110.80
1	1A	1406	A	N1-C6-N6	6.40	122.44	118.60
1	1A	1683	C	OP1-P-O3'	6.40	119.27	105.20
1	1A	1959	A	C5-C6-N6	6.40	128.82	123.70
1	1A	2084	A	N7-C8-N9	-6.40	110.60	113.80
32	1a	753	A	OP1-P-O3'	6.40	119.28	105.20
1	1A	824	A	N1-C2-N3	6.40	132.50	129.30
32	1a	460	G	N7-C8-N9	6.40	116.30	113.10
32	2a	572	A	C8-N9-C4	6.40	108.36	105.80
1	1A	1015	C	N3-C4-C5	6.39	124.46	121.90
1	1A	2063	U	N1-C2-O2	-6.39	118.32	122.80
1	1A	2110	G	N9-C4-C5	-6.39	102.84	105.40
1	1A	2390	A	N1-C6-N6	6.39	122.44	118.60
1	1A	2735	G	C5-C6-O6	-6.39	124.76	128.60
1	1A	45	C	N3-C4-C5	6.39	124.46	121.90
1	1A	965	G	OP2-P-O3'	6.39	119.27	105.20
1	1A	1170	C	N3-C4-C5	6.39	124.46	121.90
32	1a	324	G	OP2-P-O3'	6.39	119.26	105.20
32	2a	812	C	C6-N1-C2	-6.39	117.74	120.30
1	1A	2761	A	C8-N9-C4	6.39	108.36	105.80
32	2a	1432	G	C5-C6-O6	6.39	132.43	128.60
1	1A	2303	U	N1-C2-O2	-6.39	118.33	122.80
32	1a	802	A	C8-N9-C4	6.39	108.36	105.80
1	2A	981	A	N1-C6-N6	-6.39	114.77	118.60
1	2A	1837	C	N1-C2-O2	-6.39	115.07	118.90
1	1A	2761	A	N9-C4-C5	-6.39	103.25	105.80
32	1a	1065	U	O5'-P-OP1	-6.39	99.95	105.70
1	2A	1764	G	C5-C6-O6	6.39	132.43	128.60
1	2A	2527	C	O5'-P-OP2	-6.39	99.95	105.70
1	2A	2579	C	C4-C5-C6	-6.39	114.21	117.40
32	2a	1149	C	C6-N1-C2	-6.39	117.75	120.30
1	1A	877	G	N1-C6-O6	-6.38	116.07	119.90
1	1A	1907	A	O5'-P-OP1	6.38	118.36	110.70
1	1A	2095	C	C6-N1-C2	-6.38	117.75	120.30
32	1a	903	G	C8-N9-C4	6.38	108.95	106.40
1	2A	2541	A	N1-C6-N6	6.38	122.43	118.60
32	2a	245	C	O5'-P-OP2	6.38	118.36	110.70
1	1A	472	G	C5-C6-O6	-6.38	124.77	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	548	C	OP2-P-O3'	6.38	119.24	105.20
1	1A	1735	U	OP1-P-OP2	6.38	129.17	119.60
1	1A	2595	G	C8-N9-C4	6.38	108.95	106.40
1	2A	743	G	C4-C5-N7	-6.38	108.25	110.80
1	2A	272(E)	G	C8-N9-C4	6.38	108.95	106.40
32	2a	1486	G	C8-N9-C4	6.38	108.95	106.40
1	1A	406	G	N7-C8-N9	-6.38	109.91	113.10
1	1A	1274	G	N3-C2-N2	-6.38	115.44	119.90
32	1a	914	A	O5'-P-OP1	-6.38	99.96	105.70
1	2A	127	A	O5'-P-OP2	-6.38	99.96	105.70
1	2A	528	A	N7-C8-N9	6.38	116.99	113.80
32	2a	902	G	C5-C6-N1	6.38	114.69	111.50
1	1A	2068	G	C5-C6-O6	6.38	132.43	128.60
1	1A	2654	G	C8-N9-C4	-6.38	103.85	106.40
32	1a	590	C	O5'-P-OP1	6.38	118.35	110.70
1	2A	192	C	C5-C4-N4	-6.38	115.74	120.20
1	2A	1430	C	N3-C4-C5	-6.38	119.35	121.90
32	1a	697	U	C2-N3-C4	-6.38	123.17	127.00
1	2A	906	G	C6-N1-C2	6.38	128.93	125.10
1	1A	74	G	OP1-P-OP2	6.37	129.16	119.60
1	1A	832	G	C5-C6-O6	6.37	132.42	128.60
1	1A	1020	C	OP1-P-OP2	-6.37	110.04	119.60
1	2A	988	A	N7-C8-N9	6.37	116.99	113.80
1	2A	1092	C	N3-C2-O2	-6.37	117.44	121.90
1	2A	2496	C	O5'-P-OP1	-6.37	99.96	105.70
1	2A	2894	G	N3-C4-N9	-6.37	122.17	126.00
1	1A	1614	A	C5-C6-N6	6.37	128.80	123.70
1	2A	2581	G	O4'-C1'-N9	6.37	113.30	108.20
32	2a	771	G	C5-C6-N1	-6.37	108.31	111.50
1	2A	2074	U	N1-C2-O2	-6.37	118.34	122.80
1	1A	1082	G	N7-C8-N9	-6.37	109.92	113.10
1	1A	1244	U	N1-C2-O2	6.37	127.26	122.80
1	1A	2247	G	C5-C6-N1	-6.37	108.32	111.50
1	1A	479	C	N3-C4-N4	-6.37	113.54	118.00
1	1A	666	C	N3-C4-N4	6.37	122.46	118.00
1	1A	1014	U	N3-C4-C5	6.37	118.42	114.60
1	1A	1370	G	N1-C6-O6	-6.37	116.08	119.90
1	1A	1442	U	N3-C2-O2	-6.37	117.74	122.20
1	1A	1725	G	OP1-P-OP2	6.37	129.15	119.60
1	1A	1441	A	O5'-P-OP1	-6.36	99.97	105.70
1	1A	1796	C	O5'-P-OP2	-6.36	99.97	105.70
1	2A	2427	C	N3-C2-O2	6.36	126.36	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	354	G	N1-C6-O6	6.36	123.72	119.90
1	1A	2454	C	N3-C4-C5	6.36	124.44	121.90
32	2a	1127	G	N7-C8-N9	-6.36	109.92	113.10
1	1A	1378	G	N1-C2-N3	6.36	127.72	123.90
1	1A	2459	G	C5-C6-N1	6.36	114.68	111.50
32	1a	903	G	N7-C8-N9	-6.36	109.92	113.10
32	2a	539	A	C8-N9-C4	-6.36	103.26	105.80
1	1A	129	G	C5-C6-N1	6.36	114.68	111.50
1	1A	1143	U	C5-C6-N1	6.36	125.88	122.70
1	1A	780	G	C5-N7-C8	6.36	107.48	104.30
1	1A	1569	U	O5'-P-OP2	6.36	118.33	110.70
32	1a	199	G	O5'-P-OP1	-6.36	99.98	105.70
32	1a	1442	G	N1-C6-O6	-6.36	116.09	119.90
1	2A	669	G	C5-C6-O6	-6.36	124.78	128.60
1	2A	2143	C	C5-C6-N1	6.36	124.18	121.00
1	1A	1200	G	O5'-P-OP1	6.36	118.33	110.70
1	1A	2344	U	OP2-P-O3'	6.36	119.18	105.20
1	2A	1617	C	C6-N1-C2	-6.36	117.76	120.30
1	2A	1699	G	N9-C4-C5	6.36	107.94	105.40
32	2a	1491	G	N9-C1'-C2'	-6.36	105.01	112.00
1	1A	733	G	N1-C6-O6	6.35	123.71	119.90
1	1A	2193	A	O4'-C1'-N9	6.35	113.28	108.20
32	1a	115	G	P-O3'-C3'	6.35	127.32	119.70
1	1A	1921	G	C6-N1-C2	-6.35	121.29	125.10
9	1N	25	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	2A	1618	A	N1-C6-N6	-6.35	114.79	118.60
32	2a	640	A	C8-N9-C4	-6.35	103.26	105.80
32	2a	768	A	C2-N3-C4	-6.35	107.42	110.60
1	2A	1065	U	O4'-C1'-N1	6.35	113.28	108.20
1	1A	2858	G	N3-C4-N9	-6.35	122.19	126.00
1	1A	2858	G	O5'-P-OP1	6.35	118.32	110.70
32	1a	1524	C	N1-C2-O2	-6.35	115.09	118.90
1	2A	1681	G	C4-C5-N7	6.35	113.34	110.80
32	1a	841	U	C6-N1-C2	-6.35	117.19	121.00
1	2A	570	G	C5-C6-O6	6.35	132.41	128.60
1	2A	2056	G	O4'-C1'-N9	-6.35	103.12	108.20
20	2Y	73	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	1A	789	G	N7-C8-N9	-6.35	109.93	113.10
32	1a	836	G	C8-N9-C4	6.35	108.94	106.40
1	2A	271(D)	G	O5'-P-OP2	-6.35	99.99	105.70
1	2A	858	U	O5'-P-OP2	-6.35	99.99	105.70
1	2A	1658	C	C6-N1-C2	-6.35	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1515	C	O5'-P-OP2	-6.35	99.99	105.70
1	1A	410	U	N1-C2-O2	6.34	127.24	122.80
1	2A	600	G	O5'-P-OP1	-6.34	99.99	105.70
1	2A	1899	G	N7-C8-N9	6.34	116.27	113.10
1	1A	1237	G	C2-N3-C4	-6.34	108.73	111.90
1	1A	1666	G	C5-N7-C8	6.34	107.47	104.30
1	1A	1853	G	N1-C2-N2	-6.34	110.49	116.20
32	2a	560	U	C6-N1-C2	-6.34	117.19	121.00
1	1A	2443	U	N1-C2-N3	6.34	118.70	114.90
32	2a	190	U	C6-N1-C2	-6.34	117.20	121.00
1	1A	2387	G	N7-C8-N9	-6.34	109.93	113.10
1	1A	1999	A	O5'-P-OP1	-6.34	100.00	105.70
1	1A	2548	G	C5-C6-N1	-6.34	108.33	111.50
32	1a	781	A	N9-C4-C5	-6.34	103.27	105.80
1	2A	567	A	N1-C6-N6	6.34	122.40	118.60
1	2A	2863	C	O5'-P-OP2	-6.33	100.00	105.70
1	1A	718	C	N3-C2-O2	-6.33	117.47	121.90
1	2A	2106	G	N3-C4-C5	-6.33	125.43	128.60
32	2a	555	C	N3-C4-C5	-6.33	119.37	121.90
1	1A	1353	A	C5-C6-N6	-6.33	118.64	123.70
1	1A	1392	G	N7-C8-N9	-6.33	109.94	113.10
1	1A	2886	G	C4-C5-N7	6.33	113.33	110.80
32	1a	404	U	C2-N3-C4	6.33	130.80	127.00
32	2a	902	G	C6-N1-C2	-6.33	121.30	125.10
1	1A	623	G	C5-C6-O6	6.33	132.40	128.60
1	1A	1257	G	O4'-C1'-N9	6.33	113.26	108.20
1	1A	1313	U	C2-N3-C4	-6.33	123.20	127.00
1	1A	1376	C	N3-C4-C5	6.33	124.43	121.90
1	1A	1625	U	O5'-P-OP2	-6.33	100.00	105.70
1	1A	1826	C	C6-N1-C2	6.33	122.83	120.30
1	1A	1921	G	N3-C4-N9	6.33	129.80	126.00
1	1A	225	C	C5-C6-N1	-6.33	117.84	121.00
1	1A	977	G	N1-C2-N2	-6.33	110.50	116.20
1	1A	1043	G	N3-C2-N2	6.33	124.33	119.90
1	1A	1846	A	N1-C2-N3	6.33	132.47	129.30
1	1A	2013	U	C5-C6-N1	-6.33	119.53	122.70
1	1A	2254	G	C5-N7-C8	6.33	107.47	104.30
1	1A	2738	A	N1-C2-N3	6.33	132.47	129.30
32	1a	1097	C	C6-N1-C2	-6.33	117.77	120.30
32	2a	1505	G	N9-C4-C5	6.33	107.93	105.40
1	1A	2499	G	C8-N9-C4	6.33	108.93	106.40
1	1A	1099	C	C2-N3-C4	6.33	123.06	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1143	U	C6-N1-C2	-6.33	117.20	121.00
1	1A	2320	G	N7-C8-N9	6.33	116.26	113.10
1	2A	390	A	N9-C4-C5	-6.33	103.27	105.80
15	2T	96	ARG	CG-CD-NE	-6.33	98.52	111.80
1	1A	360	C	C4-C5-C6	6.32	120.56	117.40
1	1A	837	C	N3-C2-O2	6.32	126.33	121.90
2	2B	41	U	C2-N1-C1'	6.32	125.29	117.70
32	2a	721	G	O5'-P-OP1	6.32	118.29	110.70
32	2a	754	C	C2-N1-C1'	6.32	125.75	118.80
32	2a	1501	C	C6-N1-C2	6.32	122.83	120.30
1	1A	106	U	C5-C6-N1	-6.32	119.54	122.70
1	1A	821	A	C2-N3-C4	6.32	113.76	110.60
1	1A	2138	G	C4-N9-C1'	6.32	134.72	126.50
1	1A	906	G	C4-N9-C1'	-6.32	118.28	126.50
1	2A	1837	C	O5'-P-OP2	6.32	118.28	110.70
32	2a	46	G	C8-N9-C4	6.32	108.93	106.40
1	1A	60	G	N3-C2-N2	-6.32	115.48	119.90
1	2A	1899	G	C5-C6-O6	-6.32	124.81	128.60
50	2s	30	LEU	CA-CB-CG	6.32	129.83	115.30
1	1A	1019	G	N9-C4-C5	6.32	107.93	105.40
1	1A	1055	A	N7-C8-N9	-6.32	110.64	113.80
1	1A	1476	C	O5'-P-OP2	-6.32	100.02	105.70
1	1A	2100	C	C5-C6-N1	-6.32	117.84	121.00
1	1A	2395	G	C5-C6-O6	6.32	132.39	128.60
1	2A	2378	A	C8-N9-C1'	-6.32	116.33	127.70
1	1A	557	A	N1-C6-N6	-6.31	114.81	118.60
1	1A	2088	C	O5'-P-OP1	-6.31	100.02	105.70
1	1A	2568	C	O5'-P-OP1	-6.31	100.02	105.70
2	1B	24	G	C8-N9-C1'	-6.31	118.80	127.00
1	2A	2365	G	C5-C6-O6	-6.31	124.81	128.60
1	2A	2444	G	N3-C4-N9	-6.31	122.21	126.00
1	1A	347	G	N1-C2-N2	-6.31	110.52	116.20
1	1A	1387	U	C5-C6-N1	6.31	125.86	122.70
1	1A	1973	U	C5-C6-N1	-6.31	119.55	122.70
1	1A	2033	U	N3-C4-C5	-6.31	110.81	114.60
1	1A	2134	G	C8-N9-C1'	-6.31	118.80	127.00
1	1A	2195	A	N1-C2-N3	6.31	132.46	129.30
1	1A	2869	G	N9-C4-C5	6.31	107.92	105.40
1	2A	1373	A	N7-C8-N9	-6.31	110.65	113.80
1	1A	1795	G	N1-C2-N2	-6.31	110.52	116.20
1	1A	1852	A	C2-N3-C4	6.31	113.75	110.60
1	1A	2566	U	N1-C2-O2	-6.31	118.39	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	353	A	OP2-P-O3'	6.31	119.08	105.20
1	2A	1375	C	N1-C2-O2	6.31	122.68	118.90
1	2A	2549	G	OP1-P-OP2	6.31	129.06	119.60
1	2A	2612	C	O5'-P-OP2	-6.31	100.02	105.70
1	1A	167	G	N9-C4-C5	6.31	107.92	105.40
1	1A	16	G	N7-C8-N9	-6.30	109.95	113.10
1	1A	389	G	N9-C4-C5	-6.30	102.88	105.40
1	1A	2074	G	C8-N9-C4	-6.30	103.88	106.40
1	1A	2619	G	C2-N3-C4	-6.30	108.75	111.90
32	1a	266	G	P-O3'-C3'	6.30	127.27	119.70
32	1a	776	G	N9-C4-C5	-6.30	102.88	105.40
1	2A	1073	A	P-O3'-C3'	6.30	127.27	119.70
1	1A	2351	G	O5'-P-OP2	-6.30	100.03	105.70
32	2a	1528	U	C6-N1-C2	6.30	124.78	121.00
1	1A	115	G	O5'-P-OP2	-6.30	100.03	105.70
1	1A	1794	G	N9-C4-C5	6.30	107.92	105.40
1	1A	1832	G	OP1-P-OP2	6.30	129.05	119.60
1	1A	2385	G	C2-N3-C4	-6.30	108.75	111.90
1	2A	1292	U	O5'-P-OP2	-6.30	100.03	105.70
1	1A	1307	C	N1-C2-O2	-6.30	115.12	118.90
1	1A	2632	C	N1-C2-O2	6.30	122.68	118.90
1	2A	1108	U	C5-C6-N1	6.30	125.85	122.70
1	1A	857	U	O5'-P-OP1	6.30	118.26	110.70
1	1A	2638	C	N3-C2-O2	6.30	126.31	121.90
1	2A	446	G	C8-N9-C4	6.30	108.92	106.40
32	2a	1041	A	O4'-C1'-N9	-6.30	103.16	108.20
1	1A	725	C	C5-C6-N1	-6.30	117.85	121.00
1	1A	753	A	C2-N3-C4	-6.30	107.45	110.60
2	2B	71	C	O5'-P-OP1	-6.30	100.03	105.70
1	2A	1986	A	C2-N3-C4	-6.29	107.45	110.60
1	2A	261	G	N3-C2-N2	-6.29	115.50	119.90
1	2A	484	C	O5'-P-OP1	6.29	118.25	110.70
1	2A	1992	G	N7-C8-N9	6.29	116.25	113.10
32	2a	1517	G	O5'-P-OP2	-6.29	100.03	105.70
1	1A	1397	C	OP1-P-OP2	-6.29	110.16	119.60
1	1A	1862	G	N3-C2-N2	-6.29	115.50	119.90
32	1a	204	U	N1-C2-O2	6.29	127.20	122.80
1	2A	529	A	N7-C8-N9	6.29	116.94	113.80
1	2A	2599	G	N1-C6-O6	-6.29	116.13	119.90
32	2a	218	C	N3-C4-C5	-6.29	119.38	121.90
1	1A	888	A	C2-N3-C4	-6.29	107.45	110.60
2	1B	62	C	OP1-P-OP2	6.29	129.03	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2852	G	N9-C4-C5	-6.29	102.88	105.40
1	1A	809	U	C2-N1-C1'	6.29	125.25	117.70
1	1A	2657	G	N7-C8-N9	6.29	116.24	113.10
32	1a	138	G	N1-C6-O6	6.29	123.67	119.90
1	2A	1071	G	C4-C5-C6	6.29	122.57	118.80
1	2A	1075	C	C2-N1-C1'	6.29	125.72	118.80
2	2B	27	C	N1-C2-O2	6.29	122.67	118.90
1	1A	1520	G	N3-C2-N2	6.29	124.30	119.90
1	1A	1976	G	N1-C6-O6	6.29	123.67	119.90
1	1A	2137	G	N3-C4-C5	-6.29	125.46	128.60
1	2A	2895	U	C5-C6-N1	6.29	125.84	122.70
1	1A	540	A	C6-N1-C2	-6.29	114.83	118.60
1	1A	2525	G	C2-N3-C4	-6.29	108.76	111.90
1	2A	178	G	O5'-P-OP1	6.29	118.24	110.70
1	2A	250	G	C8-N9-C4	-6.29	103.89	106.40
1	1A	1673	G	O5'-P-OP2	-6.28	100.04	105.70
1	1A	2336	C	N3-C2-O2	6.28	126.30	121.90
32	1a	824	C	OP2-P-O3'	6.28	119.02	105.20
1	2A	157	U	N1-C2-O2	6.28	127.20	122.80
1	2A	541	C	O5'-P-OP1	-6.28	100.04	105.70
1	2A	961	C	C6-N1-C2	6.28	122.81	120.30
1	2A	2250	G	OP1-P-OP2	6.28	129.03	119.60
1	1A	2839	C	C5-C6-N1	6.28	124.14	121.00
1	2A	956	G	C2-N3-C4	-6.28	108.76	111.90
1	1A	70	A	N1-C2-N3	-6.28	126.16	129.30
1	1A	507	G	O5'-P-OP2	-6.28	100.05	105.70
1	1A	855	G	C6-N1-C2	-6.28	121.33	125.10
1	1A	1982	A	N1-C2-N3	-6.28	126.16	129.30
1	1A	2807	C	N3-C4-C5	-6.28	119.39	121.90
1	2A	251	A	C4-C5-C6	6.28	120.14	117.00
32	2a	458	C	C6-N1-C2	-6.28	117.79	120.30
1	1A	2776	G	OP2-P-O3'	6.28	119.01	105.20
1	2A	912	C	N1-C2-O2	6.28	122.67	118.90
1	2A	2564	A	C5-C6-N6	-6.28	118.68	123.70
1	1A	35	G	C5-N7-C8	6.28	107.44	104.30
1	1A	1369	U	C2-N3-C4	-6.28	123.23	127.00
1	1A	2030	C	N1-C2-N3	6.28	123.59	119.20
1	1A	2082	A	C5-C6-N6	6.28	128.72	123.70
32	1a	156	G	N7-C8-N9	6.28	116.24	113.10
32	2a	36	C	N1-C2-O2	-6.28	115.14	118.90
1	1A	2641	A	C5-N7-C8	-6.27	100.76	103.90
32	1a	1183	A	P-O3'-C3'	6.27	127.23	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	592	U	N3-C4-O4	6.27	123.79	119.40
1	1A	2531	U	N3-C4-O4	6.27	123.79	119.40
1	1A	1353	A	N9-C4-C5	-6.27	103.29	105.80
32	1a	893	C	C6-N1-C1'	-6.27	113.28	120.80
32	1a	1093	A	OP1-P-OP2	-6.27	110.19	119.60
1	2A	936	C	C6-N1-C2	6.27	122.81	120.30
2	1B	115	G	C2-N3-C4	-6.27	108.77	111.90
1	2A	271(O)	C	C6-N1-C2	-6.27	117.79	120.30
1	2A	486	C	O5'-P-OP2	6.27	118.22	110.70
1	2A	1268	A	C5-N7-C8	6.27	107.03	103.90
1	2A	2596	U	N1-C2-O2	-6.27	118.41	122.80
1	2A	2877	G	N3-C4-C5	6.27	131.74	128.60
1	1A	2549	U	O5'-P-OP2	-6.27	100.06	105.70
1	2A	2378	A	C5-C6-N6	-6.27	118.69	123.70
32	2a	910	C	C6-N1-C2	6.27	122.81	120.30
32	1a	558	G	O5'-P-OP2	6.27	118.22	110.70
1	2A	1005	C	OP1-P-OP2	6.27	129.00	119.60
1	1A	98	U	O4'-C1'-N1	6.26	113.21	108.20
1	1A	1980	C	N1-C2-O2	-6.26	115.14	118.90
1	2A	1445(A)	C	N1-C2-O2	6.26	122.66	118.90
1	2A	2444	G	C2-N3-C4	-6.26	108.77	111.90
1	2A	2814	C	N1-C2-O2	-6.26	115.14	118.90
2	2B	8	U	C4-C5-C6	-6.26	115.94	119.70
1	1A	1991	A	OP1-P-O3'	6.26	118.98	105.20
1	1A	2100	C	OP1-P-OP2	6.26	128.99	119.60
1	2A	795	C	N3-C4-N4	-6.26	113.62	118.00
32	2a	316	G	N7-C8-N9	6.26	116.23	113.10
1	1A	243	G	C5-C6-O6	6.26	132.36	128.60
1	1A	812	G	OP2-P-O3'	6.26	118.97	105.20
32	1a	681	C	N1-C2-O2	-6.26	115.14	118.90
1	2A	944	G	C8-N9-C1'	-6.26	118.86	127.00
1	2A	1790	C	OP1-P-O3'	6.26	118.98	105.20
32	2a	980	C	C6-N1-C2	6.26	122.81	120.30
1	1A	2585	C	N3-C4-N4	6.26	122.38	118.00
1	1A	2639	G	N1-C6-O6	6.26	123.66	119.90
32	1a	168	G	N9-C4-C5	-6.26	102.90	105.40
1	2A	2035	G	C8-N9-C1'	6.26	135.14	127.00
32	2a	800	G	OP2-P-O3'	6.26	118.97	105.20
32	2a	848	C	C5-C6-N1	6.26	124.13	121.00
32	2a	1119	C	C6-N1-C2	-6.26	117.80	120.30
1	1A	2308	U	N3-C4-C5	-6.26	110.84	114.60
1	2A	2447	G	C5-C6-O6	-6.26	124.84	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1241	G	O5'-P-OP2	-6.26	100.07	105.70
1	1A	1814	A	N9-C4-C5	6.26	108.30	105.80
1	1A	1862	G	C5-C6-O6	6.26	132.35	128.60
1	1A	2019	G	OP1-P-OP2	-6.26	110.22	119.60
1	1A	2459	G	OP1-P-OP2	-6.26	110.22	119.60
32	1a	767	A	N1-C2-N3	6.26	132.43	129.30
32	2a	1253	G	O5'-P-OP2	-6.26	100.07	105.70
1	1A	839	G	N1-C6-O6	-6.25	116.15	119.90
1	1A	1986	G	N3-C2-N2	6.25	124.28	119.90
1	1A	2497	G	N3-C2-N2	6.25	124.28	119.90
1	1A	398	A	C6-C5-N7	-6.25	127.92	132.30
1	1A	726	C	O5'-P-OP1	-6.25	100.07	105.70
1	1A	1132	A	N7-C8-N9	6.25	116.93	113.80
1	1A	1532	A	O5'-P-OP2	-6.25	100.07	105.70
1	1A	1753	U	O5'-P-OP1	-6.25	100.07	105.70
1	1A	1794	G	N3-C2-N2	-6.25	115.52	119.90
32	1a	894	G	C8-N9-C4	6.25	108.90	106.40
1	2A	1678	G	C6-C5-N7	-6.25	126.65	130.40
32	2a	1024	G	C8-N9-C4	-6.25	103.90	106.40
1	1A	177	G	C5-C6-O6	6.25	132.35	128.60
1	2A	1251	C	O5'-P-OP1	-6.25	100.07	105.70
1	2A	1583	A	O5'-P-OP2	-6.25	100.07	105.70
1	2A	2378	A	N3-C4-N9	6.25	132.40	127.40
1	1A	1266	C	C4-C5-C6	6.25	120.53	117.40
1	1A	1630	A	C8-N9-C4	6.25	108.30	105.80
1	1A	2244	U	OP1-P-OP2	6.25	128.97	119.60
1	2A	1094	U	O4'-C1'-N1	6.25	113.20	108.20
1	1A	1628	G	O5'-P-OP2	-6.25	100.08	105.70
1	1A	1986	G	N1-C2-N2	-6.25	110.58	116.20
32	1a	498	U	N3-C4-O4	-6.25	115.03	119.40
1	2A	831	G	O5'-P-OP1	-6.25	100.08	105.70
1	2A	2705	A	C2-N3-C4	-6.25	107.47	110.60
1	2A	2805	G	N1-C6-O6	-6.25	116.15	119.90
1	1A	449	A	O5'-P-OP2	6.25	118.20	110.70
1	1A	654	G	C4-C5-N7	-6.25	108.30	110.80
1	1A	1300	A	C2-N3-C4	6.25	113.72	110.60
1	1A	1896	G	N1-C6-O6	6.25	123.65	119.90
1	1A	2110	G	C4-C5-N7	6.25	113.30	110.80
1	1A	2463	A	N9-C4-C5	6.25	108.30	105.80
1	2A	2004	G	OP2-P-O3'	6.25	118.94	105.20
1	2A	2178	C	C6-N1-C2	-6.25	117.80	120.30
32	2a	1037	C	C6-N1-C2	-6.25	117.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	88	G	N3-C2-N2	-6.25	115.53	119.90
1	1A	2439	C	C2-N1-C1'	-6.25	111.93	118.80
1	2A	2678	C	OP2-P-O3'	6.25	118.94	105.20
1	1A	1648	U	N3-C4-O4	-6.24	115.03	119.40
1	1A	2070	G	N9-C4-C5	6.24	107.90	105.40
1	1A	2227	G	C8-N9-C1'	6.24	135.12	127.00
1	1A	2698	G	C4-C5-N7	6.24	113.30	110.80
1	2A	312	G	N1-C6-O6	6.24	123.65	119.90
32	1a	120	A	C2-N3-C4	-6.24	107.48	110.60
27	25	15	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	1A	883	G	C8-N9-C4	-6.24	103.90	106.40
1	1A	1071	G	C5-C6-O6	6.24	132.34	128.60
1	1A	1234	A	O5'-P-OP2	-6.24	100.08	105.70
1	1A	1319	U	N3-C4-O4	-6.24	115.03	119.40
1	1A	1812	C	N1-C2-O2	6.24	122.64	118.90
1	1A	2343	G	C8-N9-C4	6.24	108.90	106.40
1	1A	2481	A	OP1-P-OP2	6.24	128.96	119.60
3	1D	48	ARG	NE-CZ-NH1	-6.24	117.18	120.30
32	1a	1158	C	C5-C6-N1	-6.24	117.88	121.00
1	1A	514	G	N3-C2-N2	-6.24	115.53	119.90
32	1a	260	G	C5-C6-N1	-6.24	108.38	111.50
32	1a	1475	G	C8-N9-C4	-6.24	103.91	106.40
1	2A	188	G	N3-C4-C5	6.24	131.72	128.60
1	2A	1634	A	C2-N3-C4	6.24	113.72	110.60
32	1a	553	A	O5'-P-OP1	6.24	118.18	110.70
1	1A	423	G	C5-C6-O6	-6.24	124.86	128.60
1	1A	748	G	OP2-P-O3'	6.24	118.92	105.20
1	1A	799	A	C5-C6-N1	-6.24	114.58	117.70
1	1A	2264	G	C4-C5-N7	6.24	113.29	110.80
32	1a	1065	U	P-O3'-C3'	6.24	127.18	119.70
1	2A	2049	G	N3-C4-N9	-6.24	122.26	126.00
1	2A	2541	A	C5-C6-N6	-6.24	118.71	123.70
1	2A	2571	C	N3-C2-O2	-6.24	117.53	121.90
1	1A	569	G	N7-C8-N9	6.23	116.22	113.10
1	2A	1340	U	N3-C4-O4	6.23	123.76	119.40
1	1A	620	U	N1-C2-O2	-6.23	118.44	122.80
1	1A	1619	A	C5-C6-N1	-6.23	114.58	117.70
1	2A	1130	U	OP1-P-OP2	6.23	128.95	119.60
1	1A	342	C	N1-C2-O2	-6.23	115.16	118.90
1	2A	1658	C	C2-N1-C1'	6.23	125.65	118.80
1	1A	1628	G	OP2-P-O3'	6.23	118.90	105.20
1	1A	1807	G	C6-C5-N7	-6.23	126.66	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2627	U	C5-C4-O4	6.23	129.64	125.90
1	1A	554	A	N7-C8-N9	6.23	116.91	113.80
1	1A	1035	G	N7-C8-N9	-6.23	109.99	113.10
1	1A	2082	A	C4-C5-C6	-6.23	113.89	117.00
1	1A	2521	G	C5-C6-O6	6.23	132.34	128.60
1	1A	2081	A	N1-C6-N6	-6.23	114.86	118.60
1	1A	2262	G	C5-C6-O6	6.23	132.34	128.60
1	2A	713	G	N9-C4-C5	-6.23	102.91	105.40
1	2A	2271	G	N3-C4-C5	-6.23	125.49	128.60
32	2a	675	A	OP1-P-O3'	6.23	118.90	105.20
1	1A	94	G	C5-C6-O6	6.22	132.33	128.60
1	1A	127	C	C5-C4-N4	-6.22	115.84	120.20
1	1A	1728	G	N3-C4-N9	-6.22	122.27	126.00
1	1A	2062	C	N1-C2-N3	-6.22	114.84	119.20
1	2A	2681	C	N3-C2-O2	-6.22	117.54	121.90
1	1A	347	G	N3-C2-N2	6.22	124.26	119.90
1	1A	739	C	OP1-P-OP2	-6.22	110.27	119.60
1	1A	1134	A	O4'-C1'-N9	6.22	113.18	108.20
1	2A	61	G	C5-C6-O6	-6.22	124.87	128.60
32	2a	34	C	N3-C4-C5	6.22	124.39	121.90
1	1A	801	C	N3-C2-O2	6.22	126.25	121.90
1	2A	1092	C	C2-N3-C4	6.22	123.01	119.90
1	2A	1313	U	O4'-C1'-N1	6.22	113.18	108.20
1	1A	196	A	C8-N9-C4	6.22	108.29	105.80
1	1A	330	U	N3-C4-C5	-6.22	110.87	114.60
32	1a	266	G	C4-N9-C1'	6.22	134.59	126.50
1	2A	1700	A	C8-N9-C4	6.22	108.29	105.80
32	2a	904	C	C5-C4-N4	-6.22	115.85	120.20
1	1A	237	G	N3-C2-N2	6.22	124.25	119.90
1	1A	839	G	N3-C2-N2	6.22	124.25	119.90
1	1A	1076	G	C8-N9-C4	6.22	108.89	106.40
1	1A	1664	A	N7-C8-N9	-6.22	110.69	113.80
32	1a	574	A	C8-N9-C4	6.22	108.29	105.80
32	2a	883	C	C4-C5-C6	6.22	120.51	117.40
1	1A	2596	U	N3-C4-O4	-6.22	115.05	119.40
1	1A	2691	A	O5'-P-OP2	-6.22	100.11	105.70
1	1A	592	U	C4-C5-C6	6.21	123.43	119.70
1	1A	1837	C	OP2-P-O3'	6.21	118.87	105.20
1	1A	141	C	N3-C4-C5	6.21	124.39	121.90
1	1A	830	A	C2-N3-C4	6.21	113.71	110.60
1	1A	1664	A	C5-C6-N6	6.21	128.67	123.70
1	1A	2439	C	N1-C2-O2	-6.21	115.17	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	243	G	N1-C6-O6	-6.21	116.17	119.90
1	1A	935	C	P-O3'-C3'	6.21	127.15	119.70
1	2A	1652	A	C2-N3-C4	-6.21	107.50	110.60
1	1A	627	G	C5'-C4'-O4'	6.21	116.55	109.10
1	1A	1919	G	N9-C4-C5	-6.21	102.92	105.40
1	1A	2050	U	N3-C4-O4	-6.21	115.06	119.40
1	1A	2270	C	N3-C4-N4	6.21	122.34	118.00
32	1a	341	C	C6-N1-C2	6.21	122.78	120.30
1	2A	1638	C	C5-C6-N1	-6.21	117.90	121.00
32	2a	134	A	C8-N9-C4	6.21	108.28	105.80
32	2a	1190	G	C8-N9-C4	-6.21	103.92	106.40
1	1A	668	A	N1-C6-N6	6.21	122.32	118.60
1	1A	1059	C	O5'-P-OP2	-6.21	100.11	105.70
1	1A	2577	A	C6-N1-C2	-6.20	114.88	118.60
1	2A	1426	G	C2-N3-C4	-6.20	108.80	111.90
1	2A	2328	A	C8-N9-C4	6.20	108.28	105.80
1	2A	906	G	C6-C5-N7	6.20	134.12	130.40
1	1A	1080	G	C8-N9-C4	6.20	108.88	106.40
1	1A	1723	A	O5'-P-OP2	-6.20	100.12	105.70
1	1A	1816	A	C4-C5-N7	6.20	113.80	110.70
1	1A	2597	U	O4'-C1'-N1	6.20	113.16	108.20
1	1A	2734	A	C8-N9-C4	6.20	108.28	105.80
32	1a	1030	C	C2-N3-C4	6.20	123.00	119.90
32	2a	1158	C	N1-C2-O2	6.20	122.62	118.90
1	1A	1316	C	OP2-P-O3'	6.20	118.84	105.20
1	1A	1921	G	C5-C6-N1	6.20	114.60	111.50
1	1A	2881	C	N3-C4-C5	6.20	124.38	121.90
32	1a	501	C	OP2-P-O3'	6.20	118.84	105.20
1	2A	748	G	N1-C6-O6	-6.20	116.18	119.90
1	1A	1859	G	N1-C6-O6	6.20	123.62	119.90
1	1A	2569	G	C4-C5-N7	-6.20	108.32	110.80
1	1A	709	G	N9-C4-C5	6.20	107.88	105.40
1	1A	2354	C	O5'-P-OP1	-6.20	100.12	105.70
1	1A	2867	G	OP1-P-OP2	6.20	128.89	119.60
1	2A	95	G	N1-C6-O6	6.20	123.62	119.90
1	2A	531	C	C5-C6-N1	-6.20	117.90	121.00
32	2a	1279	A	N7-C8-N9	6.20	116.90	113.80
1	1A	617	U	N3-C4-O4	-6.19	115.07	119.40
1	1A	835	A	C5-N7-C8	6.19	107.00	103.90
1	1A	1822	A	OP1-P-OP2	-6.19	110.32	119.60
2	1B	36	C	N1-C2-O2	-6.19	115.19	118.90
4	1E	16	ARG	NE-CZ-NH1	-6.19	117.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1991	A	OP1-P-OP2	-6.19	110.32	119.60
1	2A	2697	G	C5-C6-O6	6.19	132.31	128.60
32	2a	12	U	C5-C4-O4	6.19	129.61	125.90
1	1A	393	A	N1-C6-N6	-6.18	114.89	118.60
1	1A	731	G	OP1-P-OP2	6.18	128.88	119.60
1	1A	1739	U	C2-N3-C4	-6.18	123.29	127.00
1	1A	1924	C	OP2-P-O3'	6.18	118.81	105.20
1	2A	2162	G	C8-N9-C1'	-6.18	118.96	127.00
1	1A	43	A	C2-N3-C4	-6.18	107.51	110.60
1	1A	365	G	N1-C6-O6	-6.18	116.19	119.90
1	2A	1926	U	N1-C2-N3	6.18	118.61	114.90
1	1A	1981	G	C5-N7-C8	6.18	107.39	104.30
1	1A	2632	C	C5-C6-N1	-6.18	117.91	121.00
1	1A	984	G	N9-C4-C5	6.18	107.87	105.40
1	1A	2266	C	N1-C2-O2	-6.18	115.19	118.90
11	1P	33	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	2A	677	A	C5-C6-N6	-6.18	118.76	123.70
1	2A	2706	G	C8-N9-C4	6.18	108.87	106.40
3	2D	275	LYS	N-CA-C	-6.18	94.32	111.00
32	2a	1423	G	N3-C2-N2	-6.18	115.57	119.90
1	1A	2379	G	N7-C8-N9	-6.18	110.01	113.10
1	2A	570	G	N3-C2-N2	6.18	124.22	119.90
1	1A	881	C	O5'-P-OP2	-6.18	100.14	105.70
1	1A	2373	A	C5-C6-N6	6.18	128.64	123.70
1	2A	391	G	C8-N9-C4	6.18	108.87	106.40
1	2A	632	A	O5'-P-OP2	6.18	118.11	110.70
32	2a	305	G	N1-C6-O6	-6.18	116.19	119.90
32	2a	1477	C	OP2-P-O3'	6.18	118.79	105.20
1	1A	186	A	C5-N7-C8	-6.17	100.81	103.90
1	1A	1235	G	N7-C8-N9	-6.17	110.01	113.10
1	1A	2251	G	N3-C2-N2	6.17	124.22	119.90
1	1A	2579	G	C6-C5-N7	6.17	134.10	130.40
1	1A	2898	C	C6-N1-C2	-6.17	117.83	120.30
2	1B	57	A	C4-C5-N7	6.17	113.79	110.70
48	1q	98	LEU	CA-CB-CG	6.17	129.50	115.30
1	2A	705	A	N1-C6-N6	6.17	122.31	118.60
1	2A	1309	G	C8-N9-C4	6.17	108.87	106.40
1	1A	2625	U	O5'-P-OP2	-6.17	100.14	105.70
32	2a	360	A	O5'-P-OP2	-6.17	100.14	105.70
1	1A	354	A	N9-C1'-C2'	-6.17	105.21	112.00
1	1A	803	C	C2-N3-C4	-6.17	116.81	119.90
1	1A	999	G	C5-C6-O6	6.17	132.30	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2138	G	C8-N9-C4	-6.17	103.93	106.40
1	2A	601	C	OP2-P-O3'	6.17	118.78	105.20
1	2A	1459	G	C5-C6-O6	6.17	132.30	128.60
1	2A	1931	U	C5-C6-N1	6.17	125.78	122.70
1	2A	2733	A	C8-N9-C4	-6.17	103.33	105.80
1	2A	2896	C	C2-N1-C1'	6.17	125.59	118.80
1	1A	2475	C	C2-N3-C4	-6.17	116.81	119.90
1	2A	1385	G	O4'-C1'-N9	6.17	113.14	108.20
32	1a	818	G	O5'-P-OP1	-6.17	100.15	105.70
32	2a	869	G	O5'-P-OP1	-6.17	100.15	105.70
1	1A	505	A	N1-C6-N6	-6.17	114.90	118.60
1	1A	727	G	C8-N9-C4	-6.17	103.93	106.40
1	1A	925	A	C2-N3-C4	-6.17	107.52	110.60
1	1A	1708	G	C5-N7-C8	6.17	107.38	104.30
1	1A	2619	G	C5-C6-O6	6.17	132.30	128.60
2	1B	68	C	OP2-P-O3'	6.17	118.77	105.20
32	1a	561	U	C5-C6-N1	-6.17	119.62	122.70
1	2A	221	A	C5'-C4'-C3'	-6.17	106.14	116.00
1	2A	1128	A	N7-C8-N9	-6.17	110.72	113.80
1	2A	1651	G	C8-N9-C4	6.17	108.87	106.40
1	1A	1314	A	C4-C5-C6	6.17	120.08	117.00
1	1A	2517	G	C6-N1-C2	6.16	128.80	125.10
32	1a	331	G	OP1-P-O3'	6.16	118.76	105.20
32	1a	1107	C	C6-N1-C2	-6.16	117.83	120.30
1	2A	1858	G	C5-C6-O6	6.16	132.30	128.60
1	2A	2131	G	N7-C8-N9	6.16	116.18	113.10
1	2A	2318	G	C8-N9-C4	-6.16	103.94	106.40
1	2A	2429	G	O5'-P-OP2	-6.16	100.15	105.70
1	2A	2487	G	N9-C4-C5	-6.16	102.93	105.40
1	2A	2744	G	OP2-P-O3'	6.16	118.76	105.20
32	2a	504	C	C6-N1-C2	-6.16	117.83	120.30
1	1A	329	U	O5'-P-OP1	-6.16	100.16	105.70
1	1A	2235	G	N1-C6-O6	6.16	123.60	119.90
1	2A	1826	G	N1-C2-N2	-6.16	110.65	116.20
1	1A	2050	U	C6-N1-C2	6.16	124.70	121.00
1	2A	242	G	O5'-P-OP2	6.16	118.09	110.70
32	2a	721	G	N1-C6-O6	6.16	123.60	119.90
1	1A	86	C	C6-N1-C2	6.16	122.76	120.30
1	1A	1414	G	O5'-P-OP2	-6.16	100.16	105.70
1	1A	1807	G	C4-C5-N7	6.16	113.26	110.80
1	1A	1826	C	C5-C6-N1	-6.16	117.92	121.00
1	1A	2826	C	O5'-P-OP2	-6.16	100.16	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	7	G	C8-N9-C4	6.16	108.86	106.40
32	1a	267	C	OP2-P-O3'	6.16	118.75	105.20
32	1a	1211	U	C2-N1-C1'	-6.16	110.31	117.70
1	2A	96	G	OP1-P-OP2	6.16	128.84	119.60
1	1A	2756	C	C5-C6-N1	-6.16	117.92	121.00
1	2A	2611	U	OP2-P-O3'	6.16	118.75	105.20
1	1A	1151	U	C4-C5-C6	-6.16	116.01	119.70
1	1A	2459	G	C6-N1-C2	-6.16	121.41	125.10
2	1B	41	U	C5-C6-N1	-6.16	119.62	122.70
1	2A	2804	C	C5-C6-N1	6.16	124.08	121.00
1	1A	1637	G	N1-C6-O6	-6.15	116.21	119.90
1	1A	2572	C	N1-C2-N3	6.15	123.51	119.20
32	1a	738	C	N1-C2-O2	-6.15	115.21	118.90
1	1A	733	G	N9-C4-C5	-6.15	102.94	105.40
1	1A	2671	G	N3-C4-C5	6.15	131.68	128.60
32	1a	62	U	O5'-P-OP1	6.15	118.08	110.70
1	2A	586	A	N1-C6-N6	-6.15	114.91	118.60
1	2A	2444	G	C4-C5-N7	-6.15	108.34	110.80
1	2A	2558	C	N3-C4-C5	6.15	124.36	121.90
1	1A	732	A	N1-C2-N3	6.15	132.38	129.30
1	2A	482	A	O5'-P-OP1	6.15	118.08	110.70
1	2A	2199	A	OP1-P-OP2	-6.15	110.38	119.60
1	1A	148	C	C2-N3-C4	-6.15	116.83	119.90
1	1A	1006	C	N3-C4-C5	6.15	124.36	121.90
1	1A	1177	G	N9-C4-C5	6.15	107.86	105.40
1	1A	1312	G	N1-C6-O6	6.15	123.59	119.90
1	1A	1511	C	N1-C2-O2	-6.15	115.21	118.90
1	1A	2530	A	C5-C6-N1	-6.15	114.63	117.70
1	1A	2754	A	OP1-P-OP2	6.15	128.82	119.60
1	2A	882	G	C4-N9-C1'	-6.15	118.51	126.50
1	2A	1846	G	C5-C6-N1	-6.15	108.43	111.50
1	2A	2414	G	N1-C6-O6	6.15	123.59	119.90
32	1a	190	U	O5'-P-OP2	6.15	118.08	110.70
1	2A	819	A	N7-C8-N9	6.15	116.87	113.80
1	1A	561	A	N9-C4-C5	6.14	108.26	105.80
1	1A	1428	G	C5-C6-O6	-6.14	124.91	128.60
1	1A	1069	U	OP1-P-OP2	6.14	128.81	119.60
1	1A	2025	G	C8-N9-C4	6.14	108.86	106.40
2	1B	90	A	N9-C4-C5	-6.14	103.34	105.80
1	2A	348	G	O5'-P-OP2	-6.14	100.17	105.70
1	2A	1694	C	O5'-P-OP1	-6.14	100.17	105.70
1	2A	1826	G	C4-C5-N7	-6.14	108.34	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1989	G	N3-C2-N2	6.14	124.20	119.90
32	2a	550	G	C4-C5-N7	6.14	113.26	110.80
32	2a	811	C	C6-N1-C2	6.14	122.76	120.30
1	1A	2353	G	C8-N9-C4	-6.14	103.94	106.40
2	1B	31	C	N1-C2-O2	6.14	122.58	118.90
1	1A	2533	C	C2-N3-C4	-6.14	116.83	119.90
1	2A	207	A	N1-C2-N3	6.14	132.37	129.30
1	2A	740	U	N3-C2-O2	-6.14	117.90	122.20
1	2A	1047	G	C2-N3-C4	6.14	114.97	111.90
1	1A	2626	A	OP1-P-OP2	-6.14	110.39	119.60
1	1A	2271	G	C5-C6-N1	6.14	114.57	111.50
12	1Q	59	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	2A	154	G	N9-C4-C5	-6.14	102.95	105.40
32	2a	771	G	N3-C4-C5	6.14	131.67	128.60
1	1A	2513	C	OP1-P-OP2	-6.13	110.40	119.60
1	2A	2112	G	C8-N9-C1'	6.13	134.97	127.00
1	2A	2313	C	C6-N1-C2	-6.13	117.85	120.30
32	2a	563	A	C2-N3-C4	-6.13	107.53	110.60
32	2a	630	G	C4-N9-C1'	6.13	134.47	126.50
1	1A	1795	G	N3-C2-N2	6.13	124.19	119.90
13	1R	12	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	1A	696	C	C2-N3-C4	6.13	122.97	119.90
1	1A	1026	A	N1-C2-N3	-6.13	126.23	129.30
1	1A	1879	A	C8-N9-C4	6.13	108.25	105.80
1	1A	2241	C	C2-N3-C4	6.13	122.97	119.90
1	1A	2392	C	C5-C4-N4	-6.13	115.91	120.20
1	2A	238	C	N3-C4-C5	-6.13	119.45	121.90
1	2A	758	C	O5'-P-OP2	-6.13	100.18	105.70
1	1A	957	A	O5'-P-OP1	-6.13	100.18	105.70
32	1a	192	U	N3-C2-O2	-6.13	117.91	122.20
1	1A	1188	A	P-O3'-C3'	6.13	127.05	119.70
1	1A	1734	G	N9-C4-C5	6.13	107.85	105.40
1	1A	2245	U	O5'-P-OP2	-6.13	100.18	105.70
32	1a	118	U	O5'-P-OP1	-6.13	100.19	105.70
32	1a	670	G	C5-C6-O6	6.13	132.28	128.60
1	2A	1702	G	C4-C5-N7	-6.13	108.35	110.80
1	1A	95	G	C8-N9-C4	6.13	108.85	106.40
1	1A	562	C	C4-C5-C6	6.13	120.46	117.40
1	1A	653	G	O5'-P-OP2	-6.13	100.19	105.70
1	2A	2554	U	N3-C4-O4	-6.13	115.11	119.40
32	2a	1043	C	C2-N1-C1'	-6.13	112.06	118.80
1	1A	593	G	C5-C6-N1	6.12	114.56	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1220	U	P-O3'-C3'	6.12	127.05	119.70
1	1A	1354	A	C8-N9-C4	-6.12	103.35	105.80
1	1A	1033	G	C4-C5-N7	-6.12	108.35	110.80
1	1A	1135	G	C4-N9-C1'	6.12	134.46	126.50
1	1A	2346	G	C2-N3-C4	-6.12	108.84	111.90
32	1a	733	A	C8-N9-C4	6.12	108.25	105.80
32	1a	759	A	OP2-P-O3'	6.12	118.67	105.20
1	2A	90	U	N3-C4-O4	-6.12	115.11	119.40
1	2A	2606	C	C4-C5-C6	6.12	120.46	117.40
1	1A	553	A	C4-C5-C6	6.12	120.06	117.00
1	1A	1701	A	N9-C4-C5	-6.12	103.35	105.80
1	1A	2713	C	C2-N3-C4	-6.12	116.84	119.90
1	1A	1317	G	C8-N9-C4	6.12	108.85	106.40
1	1A	1749	G	N9-C4-C5	6.12	107.85	105.40
1	1A	2265	G	N1-C6-O6	6.12	123.57	119.90
1	2A	1662	C	N1-C2-O2	-6.12	115.23	118.90
1	1A	1863	C	C2-N3-C4	-6.12	116.84	119.90
1	1A	1250	U	C5-C4-O4	-6.12	122.23	125.90
1	1A	1710	C	C4-C5-C6	6.12	120.46	117.40
1	1A	2425	G	O5'-P-OP1	6.12	118.04	110.70
32	1a	1052	U	N3-C2-O2	-6.12	117.92	122.20
1	2A	652(T)	C	C2-N3-C4	6.12	122.96	119.90
32	2a	896	C	N3-C4-C5	6.12	124.35	121.90
1	1A	1667	U	N3-C4-O4	6.11	123.68	119.40
2	1B	38	C	N3-C4-C5	6.11	124.35	121.90
32	1a	1406	U	O5'-P-OP1	6.11	118.04	110.70
1	2A	329	G	O5'-P-OP1	-6.11	100.20	105.70
1	2A	1148	A	C8-N9-C4	-6.11	103.36	105.80
1	2A	1772	G	N1-C6-O6	-6.11	116.23	119.90
32	2a	1226	C	C6-N1-C2	-6.11	117.85	120.30
32	2a	1471	G	N1-C6-O6	-6.11	116.23	119.90
1	1A	217	A	C4-N9-C1'	-6.11	115.30	126.30
32	1a	893	C	N1-C2-O2	6.11	122.57	118.90
1	2A	415	A	O5'-P-OP1	6.11	118.03	110.70
1	2A	1139	G	O5'-P-OP2	-6.11	100.20	105.70
1	1A	1627	A	N1-C6-N6	6.11	122.27	118.60
1	1A	2520	G	N3-C4-C5	-6.11	125.54	128.60
1	1A	2595	G	N7-C8-N9	-6.11	110.05	113.10
1	1A	2630	G	C8-N9-C4	-6.11	103.96	106.40
32	2a	618	C	OP1-P-O3'	6.11	118.64	105.20
1	2A	2137	C	N1-C2-O2	6.11	122.56	118.90
1	2A	1296	G	C2-N3-C4	-6.11	108.85	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2372	G	C5-C6-O6	-6.11	124.94	128.60
2	2B	24	G	C5-C6-O6	-6.11	124.94	128.60
1	1A	1821	C	OP1-P-O3'	6.11	118.63	105.20
1	1A	1831	C	C5-C4-N4	6.11	124.47	120.20
1	1A	2045	G	O5'-P-OP2	6.11	118.03	110.70
1	1A	2289	G	C5-N7-C8	6.11	107.35	104.30
32	1a	73	G	C4-N9-C1'	-6.11	118.56	126.50
1	1A	121	G	N1-C6-O6	6.10	123.56	119.90
1	1A	1258	A	N1-C2-N3	6.10	132.35	129.30
1	1A	2095	C	OP1-P-OP2	-6.10	110.44	119.60
32	1a	557	G	N1-C2-N2	-6.10	110.71	116.20
32	1a	804	U	C6-N1-C1'	6.10	129.74	121.20
1	2A	2112	G	O4'-C1'-N9	6.10	113.08	108.20
1	1A	979	G	C8-N9-C4	6.10	108.84	106.40
1	1A	188	A	N9-C4-C5	6.10	108.24	105.80
1	1A	797	A	OP1-P-O3'	6.10	118.62	105.20
1	1A	2618	C	C4-C5-C6	6.10	120.45	117.40
32	1a	255	G	OP1-P-OP2	-6.10	110.45	119.60
1	2A	1525	G	O5'-P-OP2	-6.10	100.21	105.70
32	2a	44	G	C5-C6-O6	6.10	132.26	128.60
32	2a	1093	A	N9-C4-C5	-6.10	103.36	105.80
32	2a	1495	U	N3-C4-C5	-6.10	110.94	114.60
1	1A	1311	A	O5'-P-OP2	-6.10	100.21	105.70
1	1A	2103	C	C2-N3-C4	-6.10	116.85	119.90
2	1B	59	A	N1-C2-N3	6.10	132.35	129.30
1	2A	1632	A	C5-N7-C8	6.10	106.95	103.90
1	1A	815	G	N1-C2-N3	6.10	127.56	123.90
32	1a	1169	A	N7-C8-N9	6.10	116.85	113.80
32	1a	1006	C	N1-C2-O2	6.09	122.56	118.90
32	2a	441	A	N1-C6-N6	6.09	122.26	118.60
1	1A	1740	U	C5-C6-N1	-6.09	119.65	122.70
32	1a	204	U	C5-C6-N1	6.09	125.75	122.70
1	1A	1707	C	N1-C2-N3	6.09	123.47	119.20
32	1a	533	A	C4-C5-N7	6.09	113.75	110.70
1	2A	2240	C	N3-C2-O2	-6.09	117.64	121.90
32	2a	649	G	N3-C4-N9	-6.09	122.34	126.00
1	1A	393	A	N9-C4-C5	6.09	108.24	105.80
1	1A	1874	C	N3-C4-C5	6.09	124.33	121.90
1	1A	2638	C	C2-N3-C4	-6.09	116.86	119.90
32	1a	302	G	N9-C4-C5	6.09	107.84	105.40
1	2A	203	C	C5-C4-N4	-6.09	115.94	120.20
32	2a	889	A	N1-C6-N6	-6.09	114.95	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2590	G	O5'-P-OP1	-6.09	100.22	105.70
2	1B	55	U	OP1-P-OP2	6.09	128.73	119.60
1	1A	760	G	N3-C4-C5	6.09	131.64	128.60
1	1A	2573	A	N1-C6-N6	-6.09	114.95	118.60
1	1A	2708	U	C2-N3-C4	-6.09	123.35	127.00
1	1A	2722	C	N1-C2-O2	-6.09	115.25	118.90
2	1B	18	G	C5-C6-O6	-6.09	124.95	128.60
32	2a	138	G	N1-C6-O6	6.09	123.55	119.90
32	2a	513	C	C5-C6-N1	6.09	124.04	121.00
1	1A	619	G	C8-N9-C4	6.08	108.83	106.40
1	2A	701	G	N3-C4-C5	6.08	131.64	128.60
1	2A	754	C	N1-C2-O2	-6.08	115.25	118.90
1	2A	1047	G	N3-C4-C5	-6.08	125.56	128.60
1	1A	1665	G	C8-N9-C4	6.08	108.83	106.40
1	2A	398	G	C2-N3-C4	-6.08	108.86	111.90
1	2A	1283	G	N3-C2-N2	6.08	124.16	119.90
1	2A	2769	C	O5'-P-OP2	-6.08	100.22	105.70
1	1A	566	C	C2-N3-C4	-6.08	116.86	119.90
1	1A	727	G	C5-C6-O6	-6.08	124.95	128.60
1	1A	760	G	C4-C5-N7	6.08	113.23	110.80
1	1A	1238	G	N9-C4-C5	6.08	107.83	105.40
1	1A	2054	G	C5-N7-C8	6.08	107.34	104.30
1	2A	2020	A	OP2-P-O3'	6.08	118.58	105.20
1	2A	2063	C	O5'-P-OP2	-6.08	100.23	105.70
32	2a	1499	A	O5'-P-OP1	6.08	118.00	110.70
1	1A	1262	C	C2-N3-C4	-6.08	116.86	119.90
1	1A	2081	A	C4-C5-N7	-6.08	107.66	110.70
1	1A	539	A	OP1-P-OP2	6.08	128.72	119.60
1	1A	1725	G	O5'-P-OP2	-6.08	100.23	105.70
1	1A	2250	G	N3-C4-N9	6.08	129.65	126.00
1	1A	2294	G	N3-C2-N2	6.08	124.16	119.90
1	1A	2595	G	C4-C5-N7	-6.08	108.37	110.80
1	1A	2746	A	N1-C6-N6	6.08	122.25	118.60
32	1a	1529	G	C8-N9-C4	-6.08	103.97	106.40
1	2A	496	G	N1-C2-N3	6.08	127.55	123.90
1	2A	1321	A	N9-C4-C5	-6.08	103.37	105.80
1	2A	2516	G	C2-N3-C4	-6.08	108.86	111.90
32	2a	28	G	O5'-P-OP1	-6.08	100.23	105.70
32	2a	895	G	C2-N3-C4	-6.08	108.86	111.90
32	2a	901	A	C6-N1-C2	-6.08	114.95	118.60
32	2a	1504	G	N3-C4-C5	6.08	131.64	128.60
1	1A	1294	G	N9-C4-C5	-6.08	102.97	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1426	G	N9-C4-C5	-6.08	102.97	105.40
1	1A	996	C	N3-C4-N4	-6.08	113.75	118.00
1	1A	1067	A	C2-N3-C4	6.08	113.64	110.60
1	1A	1199	C	C5-C4-N4	-6.08	115.95	120.20
1	1A	2284	U	N1-C2-N3	6.08	118.55	114.90
1	1A	2484	G	C5-C6-N1	6.08	114.54	111.50
32	1a	819	A	N1-C6-N6	6.08	122.25	118.60
1	2A	1238	G	O5'-P-OP2	-6.08	100.23	105.70
1	2A	2466	C	C6-N1-C2	6.08	122.73	120.30
1	2A	2834	G	C5-C6-O6	6.08	132.25	128.60
32	2a	1436	U	N1-C2-N3	6.08	118.55	114.90
1	1A	672	G	N9-C4-C5	6.07	107.83	105.40
1	1A	1719	C	O5'-P-OP2	6.07	117.99	110.70
1	1A	1835	C	N3-C4-C5	6.07	124.33	121.90
1	1A	2018	C	C2-N3-C4	-6.07	116.86	119.90
1	1A	2034	G	N1-C2-N2	-6.07	110.73	116.20
32	1a	903	G	O5'-P-OP2	-6.07	100.23	105.70
1	1A	2535	G	C5-C6-O6	6.07	132.24	128.60
1	2A	976	C	N1-C2-O2	6.07	122.54	118.90
1	1A	1928	G	O5'-P-OP1	-6.07	100.24	105.70
32	1a	226	G	C8-N9-C4	6.07	108.83	106.40
1	2A	1079	C	C5'-C4'-O4'	6.07	116.39	109.10
1	2A	1848	A	C5-C6-N1	6.07	120.73	117.70
1	2A	1693	U	C5-C4-O4	-6.07	122.26	125.90
1	1A	856	G	C2-N3-C4	6.07	114.93	111.90
1	1A	940	C	C6-N1-C2	-6.07	117.87	120.30
1	1A	2030	C	N3-C2-O2	-6.07	117.65	121.90
1	1A	2067	C	C4-C5-C6	6.07	120.43	117.40
32	1a	113	G	N1-C6-O6	-6.07	116.26	119.90
32	1a	910	C	N3-C4-C5	6.07	124.33	121.90
1	2A	2346	A	N1-C2-N3	6.07	132.33	129.30
19	2X	57	LEU	CA-CB-CG	6.07	129.26	115.30
32	2a	687	A	P-O3'-C3'	6.07	126.98	119.70
1	1A	903	C	N1-C2-O2	-6.07	115.26	118.90
1	1A	1422	C	N3-C4-N4	-6.07	113.75	118.00
1	1A	1536	A	O5'-P-OP1	-6.07	100.24	105.70
1	1A	2220	A	O4'-C1'-N9	6.07	113.05	108.20
1	1A	2229	A	C8-N9-C4	-6.07	103.37	105.80
1	1A	2361	G	O5'-P-OP1	-6.07	100.24	105.70
32	2a	771	G	C2-N3-C4	-6.07	108.87	111.90
1	1A	201	G	N1-C6-O6	6.06	123.54	119.90
1	1A	2873	C	O5'-P-OP2	-6.06	100.24	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	595	C	N3-C4-N4	6.06	122.25	118.00
1	1A	340	C	OP2-P-O3'	6.06	118.54	105.20
1	1A	419	C	N1-C2-O2	-6.06	115.26	118.90
1	1A	1024	G	C5-C6-O6	6.06	132.24	128.60
1	2A	529	A	C5-C6-N6	-6.06	118.85	123.70
32	2a	904	C	N3-C4-N4	6.06	122.24	118.00
1	1A	126	C	C5-C6-N1	-6.06	117.97	121.00
1	1A	130	G	OP2-P-O3'	6.06	118.53	105.20
32	1a	476	G	N3-C4-N9	6.06	129.64	126.00
1	1A	281	G	C5-C6-O6	6.06	132.24	128.60
32	1a	693	G	N3-C4-N9	6.06	129.64	126.00
39	1h	112	LEU	CA-CB-CG	6.06	129.24	115.30
1	2A	692	C	C6-N1-C2	6.06	122.72	120.30
1	2A	871	U	C5-C4-O4	-6.06	122.26	125.90
1	2A	2058	A	N1-C2-N3	6.06	132.33	129.30
1	1A	265	U	O5'-P-OP1	-6.06	100.25	105.70
1	1A	731	G	N3-C4-C5	-6.06	125.57	128.60
1	1A	2627	U	C2-N3-C4	-6.06	123.36	127.00
1	1A	2822	G	N3-C2-N2	6.06	124.14	119.90
32	1a	786	G	C8-N9-C4	6.06	108.82	106.40
32	2a	618	C	N3-C4-C5	-6.06	119.48	121.90
1	1A	1419	A	N7-C8-N9	-6.06	110.77	113.80
32	2a	1252	A	O5'-P-OP2	-6.06	100.25	105.70
1	1A	128	C	C5-C4-N4	-6.05	115.96	120.20
1	1A	749	G	OP1-P-OP2	6.05	128.68	119.60
1	1A	859	C	C2-N3-C4	-6.05	116.87	119.90
1	1A	1281	G	O5'-P-OP2	-6.05	100.25	105.70
1	1A	1769	G	N9-C4-C5	6.05	107.82	105.40
1	1A	1807	G	O5'-P-OP2	-6.05	100.25	105.70
1	2A	65	C	C6-N1-C2	-6.05	117.88	120.30
1	2A	1899	G	C8-N9-C4	-6.05	103.98	106.40
1	2A	2330	G	N3-C2-N2	-6.05	115.66	119.90
1	1A	406	G	C8-N9-C4	6.05	108.82	106.40
1	1A	1986	G	O4'-C1'-N9	-6.05	103.36	108.20
1	1A	2250	G	OP2-P-O3'	6.05	118.52	105.20
1	1A	2578	A	OP1-P-O3'	6.05	118.52	105.20
1	1A	403	C	N3-C4-N4	-6.05	113.76	118.00
1	1A	740	C	N3-C4-N4	-6.05	113.76	118.00
1	2A	6	A	C8-N9-C4	-6.05	103.38	105.80
1	2A	2855	C	C5-C6-N1	6.05	124.03	121.00
1	1A	1006	C	C2-N3-C4	-6.05	116.88	119.90
1	1A	1256	U	C6-N1-C2	6.05	124.63	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	998	G	N3-C4-N9	-6.05	122.37	126.00
1	1A	352	U	C2-N1-C1'	6.05	124.96	117.70
1	1A	813	C	C4-C5-C6	6.05	120.42	117.40
1	1A	1729	G	N1-C6-O6	-6.05	116.27	119.90
1	1A	1827	U	C2-N3-C4	-6.05	123.37	127.00
1	1A	2342	G	N1-C6-O6	6.05	123.53	119.90
1	1A	2586	G	N3-C2-N2	6.05	124.13	119.90
1	1A	2735	G	N7-C8-N9	-6.05	110.08	113.10
32	1a	786	G	O5'-P-OP2	-6.05	100.26	105.70
1	1A	186	A	C5-C6-N1	-6.04	114.68	117.70
2	2B	2	C	N3-C2-O2	-6.04	117.67	121.90
32	2a	310	G	N3-C2-N2	-6.04	115.67	119.90
4	1E	119	ARG	NE-CZ-NH2	-6.04	117.28	120.30
32	1a	613	C	C6-N1-C2	-6.04	117.88	120.30
1	2A	1471	A	N7-C8-N9	6.04	116.82	113.80
1	2A	1901	A	N7-C8-N9	-6.04	110.78	113.80
32	2a	19	C	OP1-P-OP2	6.04	128.67	119.60
1	1A	147	U	C5-C4-O4	-6.04	122.28	125.90
1	1A	472	G	C6-C5-N7	-6.04	126.78	130.40
32	1a	699	C	C6-N1-C2	-6.04	117.88	120.30
32	2a	1495	U	C5-C6-N1	6.04	125.72	122.70
1	2A	1992	G	C6-N1-C2	-6.04	121.48	125.10
32	2a	1009	G	N1-C6-O6	6.04	123.52	119.90
1	1A	1766	G	N9-C4-C5	-6.04	102.98	105.40
1	1A	2459	G	O5'-P-OP2	6.04	117.95	110.70
1	1A	1572	G	O5'-P-OP2	-6.04	100.27	105.70
1	1A	2390	A	C4-C5-C6	6.04	120.02	117.00
32	2a	824	C	N3-C4-C5	-6.04	119.48	121.90
32	2a	831	U	C6-N1-C2	-6.04	117.38	121.00
1	1A	146	G	N1-C6-O6	-6.04	116.28	119.90
1	1A	828	A	N9-C4-C5	6.04	108.21	105.80
1	1A	1033	G	OP1-P-OP2	-6.04	110.55	119.60
1	1A	1692	G	N3-C4-C5	-6.04	125.58	128.60
1	1A	2728	C	N3-C4-C5	6.04	124.31	121.90
2	1B	80	U	O5'-P-OP2	6.04	117.94	110.70
1	2A	1536	C	N3-C4-C5	-6.04	119.49	121.90
1	2A	1801	G	C5-C6-N1	6.04	114.52	111.50
1	2A	1841	U	N1-C2-O2	6.04	127.02	122.80
1	2A	1938	A	O5'-P-OP2	-6.04	100.27	105.70
1	2A	2270	G	C4-C5-N7	6.04	113.21	110.80
1	1A	955	A	OP2-P-O3'	6.03	118.47	105.20
1	1A	1026	A	C4-C5-N7	6.03	113.72	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1522	G	C4-C5-N7	-6.03	108.39	110.80
1	2A	391	G	N9-C4-C5	-6.03	102.99	105.40
32	2a	773	G	O5'-P-OP2	-6.03	100.27	105.70
32	2a	1058	G	OP1-P-O3'	6.03	118.47	105.20
1	1A	369	A	C5-C6-N1	6.03	120.72	117.70
1	1A	2043	C	C6-N1-C2	6.03	122.71	120.30
1	2A	1074	G	O5'-P-OP1	6.03	117.94	110.70
32	2a	1131	G	N3-C4-C5	-6.03	125.58	128.60
1	1A	503	A	C8-N9-C4	6.03	108.21	105.80
1	1A	1421	C	C5-C4-N4	-6.03	115.98	120.20
32	1a	729	A	N1-C6-N6	-6.03	114.98	118.60
32	1a	732	C	N3-C4-N4	-6.03	113.78	118.00
1	2A	203	C	N3-C4-C5	6.03	124.31	121.90
1	2A	1236	G	O5'-P-OP2	6.03	117.94	110.70
1	1A	1784	G	C4-C5-N7	6.03	113.21	110.80
1	1A	2181	G	N3-C4-C5	-6.03	125.59	128.60
1	1A	2374	G	OP2-P-O3'	6.03	118.46	105.20
1	1A	2757	G	C8-N9-C4	6.03	108.81	106.40
32	1a	1530	G	N1-C2-N2	6.03	121.62	116.20
1	2A	789	A	C5-C6-N6	-6.03	118.88	123.70
1	2A	943	U	C5-C6-N1	-6.03	119.69	122.70
1	2A	2002	G	N7-C8-N9	-6.03	110.09	113.10
32	2a	656	C	C5-C6-N1	6.03	124.01	121.00
32	2a	811	C	C5-C4-N4	-6.03	115.98	120.20
1	1A	222	A	C8-N9-C4	6.03	108.21	105.80
1	1A	1686	U	O5'-P-OP2	-6.03	100.28	105.70
32	1a	573	A	O5'-P-OP1	6.03	117.93	110.70
32	1a	594	G	O5'-P-OP1	-6.03	100.28	105.70
1	2A	193	U	N1-C2-O2	-6.03	118.58	122.80
1	2A	1359	A	C2-N3-C4	6.03	113.61	110.60
32	2a	572	A	C4-N9-C1'	-6.03	115.45	126.30
32	1a	893	C	C5-C4-N4	-6.02	115.98	120.20
1	2A	451	C	C5-C4-N4	-6.02	115.98	120.20
1	2A	753	C	N3-C4-C5	6.02	124.31	121.90
1	1A	458	U	C5-C6-N1	-6.02	119.69	122.70
1	1A	2270	C	C5-C4-N4	-6.02	115.98	120.20
1	1A	2802	C	C5-C4-N4	6.02	124.42	120.20
32	1a	570	G	N1-C6-O6	6.02	123.51	119.90
1	2A	2346	A	O5'-P-OP1	-6.02	100.28	105.70
32	2a	1501	C	N1-C2-O2	-6.02	115.29	118.90
1	1A	1320	A	C5-C6-N1	-6.02	114.69	117.70
1	2A	1692	U	O5'-P-OP2	-6.02	100.28	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	88	G	N9-C4-C5	6.02	107.81	105.40
1	1A	2357	G	C5-C6-N1	-6.02	108.49	111.50
2	1B	41	U	C4-C5-C6	6.02	123.31	119.70
2	1B	104	U	C6-N1-C2	6.02	124.61	121.00
32	1a	299	G	C4-C5-N7	6.02	113.21	110.80
1	2A	50	U	N1-C2-N3	-6.02	111.29	114.90
1	2A	1699	G	O5'-P-OP1	-6.02	100.28	105.70
1	1A	1852	A	C5-C6-N1	6.02	120.71	117.70
1	1A	2510	C	N3-C4-N4	-6.02	113.79	118.00
1	1A	398	A	O5'-P-OP2	-6.02	100.28	105.70
32	1a	1283	G	C8-N9-C4	-6.02	103.99	106.40
1	2A	1207	C	N1-C2-O2	-6.02	115.29	118.90
1	2A	1853	A	O5'-P-OP1	-6.02	100.29	105.70
32	2a	833	U	OP2-P-O3'	6.01	118.43	105.20
1	2A	2143	C	N1-C2-O2	6.01	122.51	118.90
27	25	58	LEU	CA-CB-CG	6.01	129.13	115.30
1	1A	255	G	C5-C6-N1	6.01	114.51	111.50
1	1A	590	A	N3-C4-N9	-6.01	122.59	127.40
1	1A	840	A	C4-C5-N7	6.01	113.70	110.70
1	1A	1313	U	C5-C4-O4	-6.01	122.29	125.90
1	1A	1455	C	C5-C6-N1	-6.01	117.99	121.00
1	1A	1682	G	N1-C6-O6	6.01	123.51	119.90
1	1A	1726	U	N1-C2-O2	-6.01	118.59	122.80
1	2A	453	C	O5'-P-OP1	-6.01	100.29	105.70
1	2A	887	A	N9-C4-C5	-6.01	103.40	105.80
1	1A	1234	A	N1-C6-N6	6.01	122.20	118.60
1	1A	2435	U	O4'-C1'-N1	6.01	113.01	108.20
1	2A	458	G	N1-C6-O6	-6.01	116.30	119.90
1	1A	1814	A	N1-C2-N3	-6.01	126.30	129.30
1	2A	742	G	C5-C6-O6	6.01	132.21	128.60
1	2A	2358	G	O5'-P-OP2	-6.01	100.29	105.70
1	1A	1485	A	C2-N3-C4	-6.01	107.60	110.60
1	1A	2561	G	O5'-P-OP2	-6.01	100.29	105.70
1	2A	188	G	C4-C5-N7	6.01	113.20	110.80
1	2A	1537	G	C8-N9-C4	-6.01	104.00	106.40
1	1A	292	G	C4-C5-N7	6.00	113.20	110.80
1	1A	1366	C	N3-C4-N4	-6.00	113.80	118.00
1	1A	1656	A	C5-N7-C8	-6.00	100.90	103.90
1	1A	1947	C	O5'-P-OP1	-6.00	100.30	105.70
1	1A	2001	C	N1-C2-O2	-6.00	115.30	118.90
1	1A	2071	G	O5'-P-OP1	-6.00	100.30	105.70
1	1A	2502	G	N9-C4-C5	-6.00	103.00	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2105	C	N1-C2-O2	6.00	122.50	118.90
32	2a	1530	G	N7-C8-N9	-6.00	110.10	113.10
1	1A	2457	G	OP1-P-OP2	6.00	128.60	119.60
1	1A	2687	A	N1-C2-N3	-6.00	126.30	129.30
32	1a	734	G	OP2-P-O3'	6.00	118.40	105.20
33	1b	178	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	2A	1637	A	C5-C6-N1	-6.00	114.70	117.70
1	2A	1662	C	C5-C6-N1	-6.00	118.00	121.00
32	2a	902	G	O5'-P-OP1	6.00	117.90	110.70
1	1A	2517	G	OP2-P-O3'	6.00	118.40	105.20
1	2A	467	G	C5-N7-C8	6.00	107.30	104.30
1	2A	1212	G	N7-C8-N9	-6.00	110.10	113.10
1	1A	660	C	N3-C2-O2	-6.00	117.70	121.90
1	1A	1184	G	N3-C2-N2	-6.00	115.70	119.90
1	1A	1435	G	C5-C6-N1	-6.00	108.50	111.50
1	1A	1620	G	OP2-P-O3'	6.00	118.40	105.20
1	1A	1839	U	N1-C2-O2	-6.00	118.60	122.80
2	1B	13	A	C5-N7-C8	6.00	106.90	103.90
32	1a	142	G	O4'-C1'-N9	6.00	113.00	108.20
1	2A	147	U	N3-C2-O2	6.00	126.40	122.20
1	2A	1309	G	O5'-P-OP1	6.00	117.90	110.70
1	1A	448	U	C5-C6-N1	-6.00	119.70	122.70
1	1A	1606	G	OP1-P-O3'	6.00	118.39	105.20
1	1A	2319	G	N1-C6-O6	6.00	123.50	119.90
1	2A	1062	G	N7-C8-N9	6.00	116.10	113.10
1	2A	1404	C	OP1-P-OP2	6.00	128.59	119.60
1	2A	2894	G	C4-C5-N7	-6.00	108.40	110.80
1	1A	153	C	OP2-P-O3'	6.00	118.39	105.20
1	1A	261	A	O5'-P-OP1	6.00	117.89	110.70
1	1A	2131	U	N1-C2-N3	6.00	118.50	114.90
1	1A	2823	A	O5'-P-OP1	6.00	117.89	110.70
2	1B	113	G	C4-C5-N7	6.00	113.20	110.80
32	1a	818	G	N3-C4-C5	-6.00	125.60	128.60
1	1A	438	G	O5'-P-OP1	5.99	117.89	110.70
1	1A	908	A	O5'-P-OP2	5.99	117.89	110.70
1	1A	2284	U	OP2-P-O3'	5.99	118.39	105.20
2	1B	75	G	N7-C8-N9	-5.99	110.10	113.10
32	1a	1287	A	N3-C4-N9	-5.99	122.60	127.40
1	2A	251	A	N1-C2-N3	5.99	132.30	129.30
1	2A	496	G	C5-C6-O6	5.99	132.20	128.60
1	2A	1994	C	C6-N1-C2	5.99	122.70	120.30
1	2A	2451	A	N7-C8-N9	5.99	116.80	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2621	A	N3-C4-C5	5.99	131.00	126.80
1	2A	2817	G	C4-C5-N7	-5.99	108.40	110.80
32	1a	694	A	C8-N9-C4	5.99	108.20	105.80
1	1A	12	U	C6-N1-C2	-5.99	117.41	121.00
1	1A	851	A	C4-C5-C6	-5.99	114.00	117.00
1	1A	2043	C	O5'-P-OP2	-5.99	100.31	105.70
1	2A	2511	U	O5'-P-OP1	5.99	117.89	110.70
1	1A	616	G	OP1-P-OP2	5.99	128.58	119.60
1	2A	241	A	O5'-P-OP2	-5.99	100.31	105.70
1	2A	2538	C	O5'-P-OP1	-5.99	100.31	105.70
32	2a	798	G	O5'-P-OP2	5.99	117.89	110.70
1	1A	75	C	OP2-P-O3'	5.99	118.37	105.20
1	1A	545	G	N9-C4-C5	5.99	107.80	105.40
1	1A	1455	C	C6-N1-C2	5.99	122.69	120.30
1	2A	2061	G	O5'-P-OP2	-5.99	100.31	105.70
1	2A	2741	A	C8-N9-C4	5.99	108.19	105.80
32	2a	1527	C	O5'-P-OP2	-5.99	100.31	105.70
1	1A	639	G	O4'-C1'-N9	5.99	112.99	108.20
1	1A	808	A	N1-C2-N3	-5.99	126.31	129.30
1	1A	2663	C	C6-N1-C2	5.99	122.69	120.30
32	1a	266	G	C8-N9-C4	-5.99	104.01	106.40
32	1a	1036	G	O4'-C1'-N9	5.99	112.99	108.20
1	2A	307	G	OP1-P-OP2	5.99	128.58	119.60
1	2A	1244	G	N3-C4-C5	5.99	131.59	128.60
1	2A	2626	C	C6-N1-C2	5.99	122.69	120.30
32	2a	585	G	N1-C6-O6	-5.99	116.31	119.90
1	1A	2053	A	C2-N3-C4	-5.98	107.61	110.60
1	1A	2188	G	C5-C6-O6	5.98	132.19	128.60
1	2A	2046	G	N7-C8-N9	-5.98	110.11	113.10
1	1A	1836	U	N1-C2-N3	5.98	118.49	114.90
1	1A	1858	C	O5'-P-OP1	-5.98	100.32	105.70
1	1A	2451	A	O5'-P-OP2	-5.98	100.31	105.70
32	1a	1502	A	O5'-P-OP2	-5.98	100.32	105.70
1	2A	1427	A	C5-C6-N1	5.98	120.69	117.70
1	2A	2599	G	C5-C6-O6	5.98	132.19	128.60
1	1A	2137	G	N7-C8-N9	5.98	116.09	113.10
32	1a	693	G	N9-C4-C5	-5.98	103.01	105.40
1	2A	1650	G	N1-C2-N3	5.98	127.49	123.90
32	2a	686	U	N1-C2-N3	5.98	118.49	114.90
32	2a	1452	C	C6-N1-C2	-5.98	117.91	120.30
1	1A	774	A	O5'-P-OP1	-5.98	100.32	105.70
1	1A	886	U	N3-C4-C5	5.98	118.19	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1087	C	OP2-P-O3'	5.98	118.36	105.20
1	1A	2081	A	C5-C6-N6	5.98	128.48	123.70
1	1A	670	C	O5'-P-OP2	-5.98	100.32	105.70
1	1A	700	A	N1-C6-N6	5.98	122.19	118.60
1	1A	823	G	C8-N9-C4	-5.98	104.01	106.40
1	1A	1842	G	OP2-P-O3'	5.98	118.35	105.20
1	1A	1710	C	C6-N1-C2	5.98	122.69	120.30
1	1A	2450	U	C2-N3-C4	-5.98	123.41	127.00
1	1A	2858	G	OP1-P-OP2	-5.98	110.64	119.60
1	1A	20	C	C4-C5-C6	5.97	120.39	117.40
1	1A	373	G	O5'-P-OP2	-5.97	100.32	105.70
1	1A	1390	G	C5-C6-N1	-5.97	108.51	111.50
1	1A	1549	U	N1-C2-O2	-5.97	118.62	122.80
1	1A	1702	A	C5-N7-C8	5.97	106.89	103.90
32	1a	702	A	O5'-P-OP2	-5.97	100.32	105.70
32	1a	1530	G	N3-C2-N2	-5.97	115.72	119.90
1	2A	2511	U	C2-N3-C4	-5.97	123.42	127.00
1	2A	2720	U	OP1-P-O3'	5.97	118.34	105.20
1	1A	283	G	OP1-P-O3'	5.97	118.34	105.20
1	1A	737	G	N7-C8-N9	-5.97	110.11	113.10
1	1A	2476	C	N1-C2-O2	-5.97	115.32	118.90
1	1A	2503	U	N1-C2-O2	-5.97	118.62	122.80
1	1A	2867	G	O5'-P-OP1	-5.97	100.33	105.70
1	2A	882	G	C8-N9-C1'	5.97	134.76	127.00
1	1A	554	A	C6-N1-C2	-5.97	115.02	118.60
1	1A	1635	C	C5-C4-N4	-5.97	116.02	120.20
1	1A	1721	G	N3-C4-N9	5.97	129.58	126.00
1	1A	2007	G	OP2-P-O3'	5.97	118.33	105.20
32	2a	354	G	C4-C5-N7	5.97	113.19	110.80
45	2n	44	LEU	CA-CB-CG	5.97	129.03	115.30
1	1A	545	G	C6-C5-N7	5.97	133.98	130.40
1	1A	1841	A	N1-C6-N6	5.97	122.18	118.60
1	1A	1855	G	N9-C4-C5	-5.97	103.01	105.40
1	1A	2100	C	N1-C2-O2	-5.97	115.32	118.90
32	1a	238	G	N1-C6-O6	5.97	123.48	119.90
1	2A	374	A	C5-C6-N1	-5.97	114.72	117.70
1	1A	182	U	N3-C4-O4	5.96	123.58	119.40
1	1A	850	U	C2-N3-C4	-5.96	123.42	127.00
1	1A	2399	U	OP2-P-O3'	5.96	118.32	105.20
11	1P	41	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	2A	790	C	N1-C2-O2	-5.96	115.32	118.90
1	1A	892	G	C8-N9-C4	-5.96	104.02	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1190	G	C5-C6-O6	5.96	132.18	128.60
32	1a	880	C	N3-C4-C5	5.96	124.28	121.90
1	2A	1992	G	O4'-C1'-N9	-5.96	103.43	108.20
1	1A	1475	G	N3-C2-N2	5.96	124.07	119.90
1	1A	2398	C	N1-C2-O2	5.96	122.48	118.90
32	1a	1492	A	N3-C4-C5	-5.96	122.63	126.80
1	2A	1146	C	N1-C2-O2	-5.96	115.32	118.90
1	2A	1966	A	C5-C6-N6	5.96	128.47	123.70
1	1A	622	G	N7-C8-N9	-5.96	110.12	113.10
1	1A	1155	C	N3-C4-N4	5.96	122.17	118.00
1	1A	2687	A	N7-C8-N9	-5.96	110.82	113.80
1	2A	2105	C	C2-N3-C4	5.96	122.88	119.90
1	1A	1889	G	O4'-C1'-N9	5.96	112.97	108.20
1	1A	2193	A	C5-C6-N6	-5.96	118.93	123.70
1	2A	1678	G	C4-N9-C1'	5.96	134.25	126.50
32	2a	662	G	C5-C6-O6	-5.96	125.03	128.60
32	2a	902	G	C5-N7-C8	5.96	107.28	104.30
1	1A	691	G	C5-C6-N1	-5.96	108.52	111.50
32	1a	892	A	N1-C6-N6	5.96	122.17	118.60
1	2A	786	C	N1-C2-O2	-5.96	115.33	118.90
1	2A	1616	A	C5-N7-C8	-5.96	100.92	103.90
1	1A	1193	C	C2-N1-C1'	-5.95	112.25	118.80
1	1A	1426	G	C8-N9-C4	5.95	108.78	106.40
1	1A	2075	G	N3-C4-N9	-5.95	122.43	126.00
1	1A	2717	A	C5-N7-C8	-5.95	100.92	103.90
16	1U	112	ARG	NE-CZ-NH1	5.95	123.28	120.30
32	1a	172	A	N7-C8-N9	5.95	116.78	113.80
32	1a	1285	A	P-O3'-C3'	5.95	126.84	119.70
1	2A	909	A	N1-C6-N6	-5.95	115.03	118.60
1	2A	975	C	O5'-P-OP1	-5.95	100.34	105.70
1	2A	1340	U	C2-N3-C4	-5.95	123.43	127.00
1	2A	2716	U	N3-C2-O2	-5.95	118.03	122.20
1	1A	508	A	N1-C2-N3	5.95	132.28	129.30
1	1A	807	G	C2-N3-C4	-5.95	108.92	111.90
1	1A	958	C	N3-C2-O2	-5.95	117.73	121.90
1	1A	1055	A	C8-N9-C4	5.95	108.18	105.80
1	1A	2100	C	N1-C2-N3	5.95	123.37	119.20
1	1A	1423	G	C6-N1-C2	-5.95	121.53	125.10
1	1A	2607	G	N1-C6-O6	-5.95	116.33	119.90
32	1a	875	C	OP1-P-O3'	5.95	118.29	105.20
32	1a	1054	C	N3-C2-O2	-5.95	117.73	121.90
1	2A	12	U	C2-N1-C1'	5.95	124.84	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1648	C	O5'-P-OP1	5.95	117.84	110.70
1	1A	843	C	C5-C6-N1	-5.95	118.03	121.00
29	17	28	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	2A	2515	C	N1-C2-O2	-5.95	115.33	118.90
1	1A	812	G	C5-C6-O6	5.95	132.17	128.60
13	1R	1	MET	CG-SD-CE	5.95	109.72	100.20
32	1a	399	G	N3-C4-C5	5.95	131.57	128.60
32	1a	1456	G	C8-N9-C4	5.95	108.78	106.40
1	2A	2143	C	C6-N1-C2	-5.95	117.92	120.30
1	1A	501	U	C5-C6-N1	-5.95	119.73	122.70
1	1A	1294	G	N1-C6-O6	5.95	123.47	119.90
1	1A	1456	G	N3-C4-C5	5.95	131.57	128.60
1	1A	2526	U	N3-C4-O4	-5.95	115.24	119.40
32	1a	288	A	C8-N9-C4	5.95	108.18	105.80
1	2A	1462	C	C6-N1-C2	-5.95	117.92	120.30
32	2a	1003	G	N9-C4-C5	5.95	107.78	105.40
1	1A	2043	C	N3-C2-O2	5.94	126.06	121.90
32	2a	1030	C	C2-N1-C1'	5.94	125.34	118.80
1	1A	218	A	N7-C8-N9	5.94	116.77	113.80
1	1A	790	G	N9-C4-C5	5.94	107.78	105.40
1	1A	1455	C	O5'-P-OP1	5.94	117.83	110.70
1	1A	2228	G	C8-N9-C1'	5.94	134.72	127.00
1	1A	2756	C	C6-N1-C2	5.94	122.68	120.30
32	1a	297	G	C8-N9-C4	5.94	108.78	106.40
1	2A	447	A	C8-N9-C4	5.94	108.18	105.80
1	2A	572	A	C5-C6-N6	5.94	128.45	123.70
1	1A	57	G	C5-C6-N1	5.94	114.47	111.50
1	1A	2048	C	C4-C5-C6	5.94	120.37	117.40
1	1A	2764	G	OP1-P-OP2	5.94	128.51	119.60
32	1a	13	U	C6-N1-C2	5.94	124.56	121.00
32	1a	43	C	C6-N1-C2	5.94	122.68	120.30
32	1a	1406	U	O5'-P-OP2	-5.94	100.35	105.70
1	2A	1247	A	C2-N3-C4	-5.94	107.63	110.60
32	2a	893	C	N1-C2-N3	-5.94	115.04	119.20
1	1A	2228	G	N3-C4-N9	-5.94	122.44	126.00
1	2A	1286	A	O5'-P-OP2	-5.94	100.36	105.70
1	1A	1604	C	C6-N1-C2	5.94	122.67	120.30
2	1B	71	C	C4-C5-C6	5.94	120.37	117.40
1	2A	1145	C	C6-N1-C2	-5.94	117.93	120.30
1	2A	2894	G	N9-C4-C5	5.94	107.77	105.40
1	1A	385	G	C5-C6-O6	-5.93	125.04	128.60
1	1A	1524	A	N1-C6-N6	5.93	122.16	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2057	G	C4-C5-N7	5.93	113.17	110.80
1	1A	2512	U	C6-N1-C2	5.93	124.56	121.00
32	1a	770	C	O5'-P-OP1	5.93	117.82	110.70
32	1a	1004	A	P-O3'-C3'	5.93	126.82	119.70
1	2A	1501	C	N3-C4-N4	5.93	122.15	118.00
1	1A	250	G	N1-C6-O6	5.93	123.46	119.90
1	1A	891	C	C5-C6-N1	-5.93	118.03	121.00
1	1A	995	G	N3-C2-N2	5.93	124.05	119.90
1	1A	1670	G	C2-N3-C4	-5.93	108.93	111.90
1	1A	1808	U	C5-C6-N1	-5.93	119.73	122.70
1	1A	1919	G	N1-C6-O6	5.93	123.46	119.90
1	1A	2379	G	C2-N3-C4	-5.93	108.93	111.90
1	2A	6	A	N9-C4-C5	5.93	108.17	105.80
32	2a	341	C	N1-C2-O2	-5.93	115.34	118.90
1	2A	1979	C	C6-N1-C2	-5.93	117.93	120.30
1	1A	2569	G	N9-C4-C5	5.93	107.77	105.40
1	1A	2621	U	C2-N3-C4	-5.93	123.44	127.00
1	1A	2778	A	C4-C5-C6	5.93	119.97	117.00
1	2A	702	G	C4-C5-N7	-5.93	108.43	110.80
1	2A	1416	G	C4-N9-C1'	-5.93	118.79	126.50
1	2A	1647	G	N1-C6-O6	5.93	123.46	119.90
32	2a	766	A	C8-N9-C4	5.93	108.17	105.80
32	2a	1021	G	C4-C5-N7	-5.93	108.43	110.80
32	2a	1530	G	N9-C4-C5	-5.93	103.03	105.40
1	1A	238	C	C5-C6-N1	-5.93	118.04	121.00
1	1A	773	G	C4-C5-N7	5.93	113.17	110.80
1	1A	1211	U	C4-C5-C6	5.93	123.26	119.70
2	2B	71	C	C6-N1-C2	5.93	122.67	120.30
1	1A	20	C	N3-C4-N4	-5.93	113.85	118.00
1	1A	188	A	C5-C6-N6	5.93	128.44	123.70
1	1A	795	G	OP1-P-O3'	5.93	118.24	105.20
1	1A	1051	C	N3-C2-O2	-5.93	117.75	121.90
32	1a	1276	G	N7-C8-N9	5.93	116.06	113.10
1	2A	568	U	C5-C4-O4	-5.93	122.34	125.90
1	2A	1614	A	O5'-P-OP1	-5.93	100.37	105.70
1	2A	2893	G	N9-C4-C5	-5.93	103.03	105.40
1	1A	2725	A	N9-C4-C5	-5.92	103.43	105.80
1	2A	386	G	O5'-P-OP2	5.92	117.81	110.70
1	2A	1439	A	C8-N9-C4	5.92	108.17	105.80
1	2A	2197	U	N3-C4-O4	-5.92	115.25	119.40
32	2a	1219	U	C5-C6-N1	5.92	125.66	122.70
1	1A	635	C	C6-N1-C2	5.92	122.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1130	A	C5-C6-N6	5.92	128.44	123.70
1	1A	1642	A	C2-N3-C4	-5.92	107.64	110.60
1	1A	1832	G	C4-C5-N7	5.92	113.17	110.80
1	1A	2671	G	N1-C6-O6	5.92	123.45	119.90
1	1A	1441	A	N7-C8-N9	-5.92	110.84	113.80
1	1A	1985	U	OP1-P-O3'	5.92	118.23	105.20
1	2A	1231	G	C5-C6-N1	-5.92	108.54	111.50
32	2a	810	C	C6-N1-C2	5.92	122.67	120.30
32	2a	1054	C	O4'-C1'-N1	5.92	112.94	108.20
1	2A	1899	G	OP1-P-OP2	5.92	128.48	119.60
1	1A	129	G	C8-N9-C4	5.92	108.77	106.40
1	1A	787	U	C5-C6-N1	-5.92	119.74	122.70
1	1A	790	G	C6-N1-C2	-5.92	121.55	125.10
1	1A	1310	G	C8-N9-C4	5.92	108.77	106.40
1	1A	1552	C	C6-N1-C2	-5.92	117.93	120.30
32	1a	186	C	OP1-P-O3'	5.92	118.22	105.20
1	2A	445	C	OP1-P-O3'	5.92	118.22	105.20
1	2A	651	G	O5'-P-OP1	-5.92	100.37	105.70
32	2a	649	G	C4-N9-C1'	-5.92	118.81	126.50
1	1A	903	C	C6-N1-C2	-5.92	117.93	120.30
1	1A	1740	U	O4'-C1'-N1	-5.92	103.47	108.20
1	1A	2297	C	N3-C2-O2	-5.92	117.76	121.90
1	2A	686	G	C6-N1-C2	-5.92	121.55	125.10
1	2A	1831	G	C5-C6-N1	-5.92	108.54	111.50
1	2A	2049	G	C2-N3-C4	-5.92	108.94	111.90
1	2A	2144	U	N3-C2-O2	-5.92	118.06	122.20
1	2A	2565	A	O5'-P-OP2	5.92	117.80	110.70
1	1A	2201	C	C5-C6-N1	5.92	123.96	121.00
1	1A	2447	A	O5'-P-OP2	5.92	117.80	110.70
1	1A	822	G	O5'-P-OP1	-5.91	100.38	105.70
32	1a	409	G	O5'-P-OP2	-5.91	100.38	105.70
1	2A	706	A	C8-N9-C4	5.91	108.17	105.80
1	2A	1937	A	OP2-P-O3'	5.91	118.21	105.20
32	2a	1001	A	N1-C6-N6	-5.91	115.05	118.60
1	1A	2096	U	C6-N1-C2	-5.91	117.45	121.00
8	2I	116	LEU	CA-CB-CG	5.91	128.90	115.30
1	1A	855	G	C5-C6-N1	5.91	114.45	111.50
32	1a	15	G	N1-C6-O6	5.91	123.45	119.90
32	1a	653	A	N9-C4-C5	-5.91	103.44	105.80
1	2A	778	G	N3-C2-N2	5.91	124.04	119.90
32	2a	1030(B)	C	N3-C2-O2	-5.91	117.76	121.90
32	2a	1466	C	N1-C2-O2	-5.91	115.35	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	595	A	N9-C4-C5	5.91	108.16	105.80
1	1A	1213	U	C5-C4-O4	-5.91	122.35	125.90
1	1A	2242	G	N1-C2-N2	5.91	121.52	116.20
1	1A	2545	A	C6-N1-C2	-5.91	115.06	118.60
32	1a	528	C	C6-N1-C2	-5.91	117.94	120.30
1	2A	2612	C	C5-C6-N1	-5.91	118.05	121.00
1	1A	1675	U	N3-C2-O2	-5.91	118.06	122.20
1	1A	1985	U	OP1-P-OP2	5.91	128.46	119.60
1	1A	2501	G	N3-C4-N9	5.91	129.54	126.00
1	1A	1094	A	C8-N9-C4	-5.91	103.44	105.80
1	1A	1304	C	C5-C6-N1	-5.91	118.05	121.00
32	1a	1531	A	C4-C5-C6	-5.91	114.05	117.00
1	2A	1268	A	N7-C8-N9	-5.91	110.85	113.80
1	2A	2695	C	C6-N1-C2	5.91	122.66	120.30
1	2A	2699	C	C2-N1-C1'	-5.91	112.30	118.80
32	2a	411	A	O5'-P-OP1	5.91	117.79	110.70
32	2a	1260	C	C6-N1-C2	-5.91	117.94	120.30
1	1A	1922	A	N3-C4-C5	-5.90	122.67	126.80
1	1A	2767	U	OP2-P-O3'	5.90	118.19	105.20
32	2a	533	A	OP1-P-OP2	-5.90	110.74	119.60
1	1A	551	A	C5-N7-C8	-5.90	100.95	103.90
1	1A	1130	A	C4-C5-N7	-5.90	107.75	110.70
1	1A	1686	U	C2-N1-C1'	-5.90	110.62	117.70
32	1a	254	G	O5'-P-OP2	5.90	117.78	110.70
1	2A	635	C	C6-N1-C2	-5.90	117.94	120.30
1	2A	1076	C	C2-N1-C1'	5.90	125.29	118.80
32	2a	1205	U	C6-N1-C2	-5.90	117.46	121.00
1	1A	1340	U	C5-C6-N1	-5.90	119.75	122.70
1	1A	1481	G	C8-N9-C4	-5.90	104.04	106.40
1	1A	2355	C	C5-C6-N1	-5.90	118.05	121.00
1	1A	2610	A	C5-N7-C8	5.90	106.85	103.90
2	1B	46	A	O5'-P-OP1	-5.90	100.39	105.70
1	2A	308	G	N1-C6-O6	5.90	123.44	119.90
32	2a	665	A	O5'-P-OP2	-5.90	100.39	105.70
1	2A	620	G	O5'-P-OP2	-5.90	100.39	105.70
1	2A	776	G	C6-C5-N7	-5.90	126.86	130.40
1	2A	1079	C	C4-C5-C6	5.90	120.35	117.40
32	2a	1422	G	O5'-P-OP2	-5.90	100.39	105.70
1	1A	1083	G	C5-C6-O6	-5.90	125.06	128.60
1	1A	1093	G	C4-N9-C1'	5.90	134.17	126.50
1	1A	1178	A	N1-C2-N3	5.90	132.25	129.30
1	1A	2215	G	C8-N9-C4	5.90	108.76	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1841	U	N3-C2-O2	-5.90	118.07	122.20
1	2A	2269	A	C8-N9-C4	5.90	108.16	105.80
1	1A	1388	A	C6-N1-C2	-5.90	115.06	118.60
1	1A	1713	G	N1-C6-O6	-5.90	116.36	119.90
32	1a	903	G	O5'-P-OP1	5.90	117.78	110.70
1	1A	855	G	N7-C8-N9	-5.89	110.15	113.10
1	1A	1379	C	C5-C4-N4	-5.89	116.07	120.20
32	2a	533	A	C6-N1-C2	-5.89	115.06	118.60
1	1A	508	A	N9-C4-C5	-5.89	103.44	105.80
1	1A	2662	U	C5-C6-N1	-5.89	119.75	122.70
1	1A	2822	G	N1-C6-O6	-5.89	116.36	119.90
1	2A	937	U	N1-C2-O2	-5.89	118.68	122.80
1	1A	706	C	C6-N1-C2	5.89	122.66	120.30
1	1A	2419	G	C8-N9-C1'	-5.89	119.34	127.00
1	1A	2297	C	OP2-P-O3'	5.89	118.16	105.20
32	1a	183	G	N7-C8-N9	5.89	116.05	113.10
32	1a	903	G	N1-C2-N2	-5.89	110.90	116.20
32	1a	1113	C	C6-N1-C2	-5.89	117.94	120.30
1	2A	695	G	N1-C6-O6	-5.89	116.37	119.90
1	2A	1311	G	OP1-P-O3'	5.89	118.16	105.20
1	1A	661	G	N1-C6-O6	5.89	123.43	119.90
1	1A	616	G	O5'-P-OP2	-5.89	100.40	105.70
1	1A	1319	U	OP1-P-OP2	5.89	128.43	119.60
32	1a	104	G	O5'-P-OP1	-5.89	100.40	105.70
1	2A	2057	A	N1-C6-N6	5.89	122.13	118.60
1	1A	595	A	C8-N9-C4	-5.88	103.45	105.80
1	1A	2234	G	N1-C6-O6	5.88	123.43	119.90
1	1A	2271	G	N1-C2-N2	5.88	121.50	116.20
1	1A	2524	C	C5-C4-N4	-5.88	116.08	120.20
32	1a	266	G	O4'-C1'-N9	-5.88	103.49	108.20
1	2A	331	A	C5-C6-N6	5.88	128.41	123.70
1	2A	1795	C	C2-N3-C4	-5.88	116.96	119.90
32	2a	1507	A	O5'-P-OP1	-5.88	100.41	105.70
1	2A	1899	G	OP1-P-O3'	5.88	118.14	105.20
1	2A	2022	U	N3-C4-O4	5.88	123.52	119.40
1	1A	184	A	C8-N9-C4	-5.88	103.45	105.80
1	1A	1666	G	N7-C8-N9	-5.88	110.16	113.10
1	1A	2699	U	C4-C5-C6	5.88	123.23	119.70
1	1A	2758	C	OP1-P-OP2	-5.88	110.78	119.60
1	2A	584	C	N3-C2-O2	5.88	126.02	121.90
1	2A	1985	G	N3-C4-N9	-5.88	122.47	126.00
1	2A	2639	A	C8-N9-C4	5.88	108.15	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1378	G	OP1-P-O3'	5.88	118.14	105.20
1	2A	2440	C	N1-C2-O2	-5.88	115.37	118.90
1	1A	745	C	N1-C2-O2	-5.88	115.37	118.90
1	1A	797	A	N1-C2-N3	5.88	132.24	129.30
1	1A	2343	G	N7-C8-N9	-5.88	110.16	113.10
32	1a	689	C	O5'-P-OP1	-5.88	100.41	105.70
1	2A	331	A	N1-C6-N6	-5.88	115.07	118.60
1	2A	761	A	N7-C8-N9	-5.88	110.86	113.80
1	2A	2451	A	C8-N9-C4	-5.88	103.45	105.80
1	2A	2708	G	N9-C4-C5	-5.88	103.05	105.40
1	1A	180	A	C4-C5-N7	-5.88	107.76	110.70
1	1A	483	A	C5-C6-N1	-5.88	114.76	117.70
1	1A	486	A	C8-N9-C4	-5.88	103.45	105.80
1	1A	519	G	C5-N7-C8	-5.88	101.36	104.30
1	1A	1694	G	C5-N7-C8	5.88	107.24	104.30
32	1a	354	G	O5'-P-OP2	-5.88	100.41	105.70
1	2A	186	G	N1-C6-O6	5.88	123.43	119.90
1	2A	1802	A	N7-C8-N9	-5.88	110.86	113.80
1	2A	2421	G	O5'-P-OP1	-5.88	100.41	105.70
32	2a	904	C	N3-C2-O2	5.88	126.01	121.90
1	1A	490	U	C2-N3-C4	-5.88	123.47	127.00
1	1A	1097	G	O5'-P-OP2	5.88	117.75	110.70
1	1A	1420	G	O5'-P-OP2	5.88	117.75	110.70
1	2A	254	G	C2-N3-C4	-5.88	108.96	111.90
1	2A	1997	G	OP1-P-OP2	-5.88	110.79	119.60
2	2B	33	G	N3-C4-C5	5.88	131.54	128.60
1	1A	215	G	N3-C2-N2	-5.87	115.79	119.90
1	1A	648	G	N1-C6-O6	-5.87	116.38	119.90
1	1A	1859	G	C2-N3-C4	-5.87	108.96	111.90
1	1A	2064	A	N7-C8-N9	-5.87	110.86	113.80
32	1a	262	A	OP1-P-O3'	5.87	118.12	105.20
32	1a	1505	G	OP1-P-OP2	-5.87	110.79	119.60
32	2a	93	G	O4'-C1'-N9	5.87	112.90	108.20
1	1A	2273	C	C5-C4-N4	5.87	124.31	120.20
1	1A	2497	G	N1-C2-N2	-5.87	110.92	116.20
1	1A	2888	U	C5-C6-N1	5.87	125.64	122.70
32	1a	569	C	N3-C4-C5	5.87	124.25	121.90
32	2a	525	C	C5-C6-N1	5.87	123.94	121.00
1	1A	1862	G	C6-N1-C2	5.87	128.62	125.10
1	2A	2511	U	N1-C2-O2	-5.87	118.69	122.80
1	2A	1130	U	O5'-P-OP1	-5.87	100.42	105.70
1	2A	1913	A	N7-C8-N9	5.87	116.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	105	G	N3-C2-N2	-5.87	115.79	119.90
32	2a	880	C	C6-N1-C2	5.87	122.65	120.30
1	1A	831	A	O4'-C1'-N9	5.87	112.89	108.20
1	1A	841	G	N3-C2-N2	5.87	124.01	119.90
1	1A	2429	C	O5'-P-OP2	-5.87	100.42	105.70
1	1A	2565	G	O5'-P-OP1	-5.87	100.42	105.70
1	2A	695	G	OP1-P-OP2	-5.87	110.80	119.60
32	2a	802	A	N1-C6-N6	5.87	122.12	118.60
1	1A	1725	G	N7-C8-N9	5.87	116.03	113.10
32	1a	171	A	OP1-P-O3'	5.87	118.10	105.20
32	1a	557	G	N1-C6-O6	-5.87	116.38	119.90
32	1a	1530	G	N9-C4-C5	-5.87	103.05	105.40
1	2A	220	G	C5-C6-O6	-5.87	125.08	128.60
1	2A	1092	C	C6-N1-C2	-5.87	117.95	120.30
1	1A	1769	G	C4-C5-N7	-5.86	108.45	110.80
1	1A	2064	A	N3-C4-C5	5.86	130.90	126.80
32	1a	1358	U	N3-C2-O2	-5.86	118.10	122.20
1	2A	1702	G	N1-C6-O6	-5.86	116.38	119.90
1	1A	94	G	N1-C6-O6	-5.86	116.38	119.90
1	1A	495	G	N1-C2-N2	5.86	121.48	116.20
1	1A	1383	G	C4-C5-N7	-5.86	108.45	110.80
29	27	21	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	1A	292	G	N3-C4-C5	5.86	131.53	128.60
1	1A	474	U	C4-C5-C6	5.86	123.22	119.70
1	1A	2005	C	C2-N3-C4	-5.86	116.97	119.90
1	1A	2459	G	OP1-P-O3'	-5.86	92.31	105.20
1	2A	41	C	O5'-P-OP2	-5.86	100.43	105.70
1	2A	116	C	N3-C4-C5	-5.86	119.56	121.90
1	2A	250	G	N3-C2-N2	-5.86	115.80	119.90
1	2A	1610	A	O5'-P-OP2	-5.86	100.42	105.70
1	2A	2140	C	C2-N3-C4	5.86	122.83	119.90
1	2A	2516	G	N1-C2-N3	5.86	127.42	123.90
1	1A	1455	C	N1-C2-O2	-5.86	115.39	118.90
1	1A	747	G	N1-C2-N2	-5.86	110.93	116.20
1	1A	1769	G	N1-C6-O6	-5.86	116.39	119.90
32	1a	576	G	C8-N9-C1'	-5.86	119.39	127.00
32	1a	1511	G	OP1-P-O3'	-5.86	92.31	105.20
1	1A	117	A	N9-C4-C5	5.86	108.14	105.80
1	1A	427	G	C5-C6-O6	-5.86	125.09	128.60
1	1A	1229	G	OP2-P-O3'	5.86	118.08	105.20
1	1A	1320	A	N9-C4-C5	-5.86	103.46	105.80
1	1A	1811	A	N9-C4-C5	5.86	108.14	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2626	A	N1-C2-N3	-5.86	126.37	129.30
32	1a	890	G	O4'-C1'-N9	5.86	112.88	108.20
1	2A	1632	A	C8-N9-C4	5.86	108.14	105.80
1	2A	2385	C	N1-C2-O2	-5.86	115.39	118.90
32	2a	18	C	O5'-P-OP1	-5.86	100.43	105.70
32	2a	1375	A	C8-N9-C4	-5.86	103.46	105.80
2	1B	57	A	C6-C5-N7	-5.85	128.20	132.30
32	1a	300	A	C6-C5-N7	-5.85	128.20	132.30
1	1A	16	G	C4-C5-N7	-5.85	108.46	110.80
1	1A	2227	G	O4'-C1'-N9	5.85	112.88	108.20
1	1A	2772	G	N3-C2-N2	-5.85	115.80	119.90
1	1A	2780	C	N1-C2-N3	5.85	123.30	119.20
1	1A	2786	C	O5'-P-OP2	-5.85	100.43	105.70
32	1a	483	C	C5-C6-N1	-5.85	118.07	121.00
1	2A	2055	C	N1-C2-O2	-5.85	115.39	118.90
1	2A	2390	U	C5-C6-N1	5.85	125.63	122.70
32	2a	578	C	C6-N1-C2	-5.85	117.96	120.30
32	2a	1258	G	O4'-C1'-N9	5.85	112.88	108.20
1	1A	504	A	N7-C8-N9	5.85	116.72	113.80
1	1A	721	G	N7-C8-N9	5.85	116.03	113.10
1	1A	1829	U	OP1-P-OP2	5.85	128.38	119.60
1	1A	1717	C	N1-C2-O2	-5.85	115.39	118.90
1	1A	2129	C	C5-C6-N1	5.85	123.92	121.00
1	1A	2762	A	O5'-P-OP1	-5.85	100.44	105.70
29	17	34	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	2A	936	C	N3-C4-C5	5.85	124.24	121.90
1	2A	1430	C	OP1-P-OP2	5.85	128.37	119.60
32	2a	866	C	C6-N1-C2	-5.85	117.96	120.30
1	1A	745	C	N3-C4-N4	5.85	122.09	118.00
1	1A	2014	G	N7-C8-N9	-5.85	110.18	113.10
1	1A	2087	C	C5-C6-N1	-5.85	118.08	121.00
1	1A	2590	G	N9-C4-C5	5.85	107.74	105.40
1	2A	1702	G	N7-C8-N9	-5.85	110.18	113.10
26	24	18	CYS	CB-CA-C	-5.85	98.70	110.40
1	1A	1721	G	OP1-P-O3'	5.85	118.06	105.20
1	1A	2184	G	N3-C4-C5	-5.85	125.68	128.60
1	2A	1051	G	N1-C6-O6	5.85	123.41	119.90
1	1A	602	G	N1-C6-O6	-5.84	116.39	119.90
1	1A	697	C	C2-N1-C1'	5.84	125.23	118.80
1	1A	1696	G	N9-C4-C5	5.84	107.74	105.40
1	1A	2277	U	N1-C2-O2	-5.84	118.71	122.80
1	1A	2442	A	OP1-P-OP2	5.84	128.37	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1075	C	C6-N1-C2	5.84	122.64	120.30
1	2A	1493	C	N3-C2-O2	-5.84	117.81	121.90
1	2A	1937	A	C5-N7-C8	5.84	106.82	103.90
1	2A	2142	C	O4'-C1'-N1	5.84	112.88	108.20
32	2a	819	A	C5-C6-N6	-5.84	119.02	123.70
32	2a	1163	C	C6-N1-C2	-5.84	117.96	120.30
32	2a	971	G	O5'-P-OP1	5.84	117.71	110.70
32	2a	1078	U	N1-C2-O2	5.84	126.89	122.80
1	1A	1098	C	C5-C6-N1	5.84	123.92	121.00
1	1A	1419	A	O5'-P-OP1	5.84	117.71	110.70
1	1A	1421	C	N3-C4-N4	5.84	122.09	118.00
1	1A	2138	G	N7-C8-N9	5.84	116.02	113.10
32	1a	186	C	C5-C6-N1	5.84	123.92	121.00
32	1a	1428	A	O5'-P-OP2	-5.84	100.44	105.70
1	2A	769	G	C5-C6-O6	-5.84	125.09	128.60
1	2A	1509	C	O4'-C1'-N1	5.84	112.87	108.20
1	2A	2425	A	OP1-P-OP2	-5.84	110.84	119.60
32	2a	1003	G	N3-C4-N9	5.84	129.50	126.00
1	1A	2251	G	C5-N7-C8	5.84	107.22	104.30
1	2A	1402	C	O5'-P-OP1	-5.84	100.44	105.70
32	2a	269	C	C2-N1-C1'	-5.84	112.38	118.80
1	2A	2097	C	O5'-P-OP2	-5.84	100.45	105.70
32	2a	266	G	C4-C5-C6	5.84	122.30	118.80
1	1A	1748	A	N1-C6-N6	5.84	122.10	118.60
1	1A	2379	G	N9-C4-C5	-5.84	103.06	105.40
1	2A	349	G	N3-C4-C5	-5.84	125.68	128.60
32	2a	1079	G	C8-N9-C4	-5.84	104.06	106.40
1	1A	848	G	OP2-P-O3'	5.83	118.04	105.20
1	1A	2415	C	C5-C6-N1	-5.83	118.08	121.00
1	1A	2501	G	C8-N9-C1'	-5.83	119.41	127.00
1	2A	1331	A	OP1-P-O3'	5.83	118.04	105.20
1	1A	737	G	O5'-P-OP1	-5.83	100.45	105.70
1	1A	1962	U	C5-C6-N1	-5.83	119.78	122.70
1	1A	2082	A	N3-C4-N9	-5.83	122.73	127.40
1	1A	2265	G	N1-C2-N2	5.83	121.45	116.20
1	1A	2756	C	C2-N3-C4	-5.83	116.98	119.90
32	1a	288	A	OP2-P-O3'	-5.83	92.37	105.20
1	2A	1998	G	C4-C5-N7	-5.83	108.47	110.80
1	1A	339	G	C5-C6-N1	-5.83	108.58	111.50
1	1A	1000	C	C5-C4-N4	5.83	124.28	120.20
1	1A	1054	C	N3-C4-C5	-5.83	119.57	121.90
1	1A	1622	C	O5'-P-OP2	5.83	117.70	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	786	C	O5'-P-OP2	-5.83	100.45	105.70
32	2a	134	A	N9-C4-C5	-5.83	103.47	105.80
32	1a	740	U	C2-N1-C1'	-5.83	110.71	117.70
32	1a	836	G	N9-C4-C5	-5.83	103.07	105.40
1	2A	669	G	N1-C2-N2	5.83	121.44	116.20
1	2A	1251	C	OP1-P-OP2	5.83	128.34	119.60
1	2A	2597	G	OP2-P-O3'	5.83	118.02	105.20
1	1A	13	A	N1-C6-N6	-5.83	115.10	118.60
1	1A	352	U	N1-C2-O2	5.83	126.88	122.80
1	1A	996	C	C6-N1-C2	5.83	122.63	120.30
1	1A	1026	A	C4-C5-C6	-5.83	114.09	117.00
1	1A	700	A	C5-C6-N6	-5.83	119.04	123.70
1	1A	1520	G	N1-C2-N2	-5.83	110.96	116.20
1	1A	2807	C	C5-C6-N1	5.83	123.91	121.00
1	1A	2825	C	OP1-P-OP2	5.83	128.34	119.60
2	1B	113	G	N3-C4-N9	5.83	129.50	126.00
32	1a	68	G	C8-N9-C4	5.83	108.73	106.40
32	1a	105	G	N1-C6-O6	5.83	123.39	119.90
1	2A	1460	A	N9-C1'-C2'	5.83	121.57	114.00
1	2A	2394	C	C2-N3-C4	-5.83	116.99	119.90
1	1A	1813	C	C4-C5-C6	5.82	120.31	117.40
32	1a	1345	U	O4'-C1'-N1	5.82	112.86	108.20
1	2A	1666	G	N1-C2-N2	-5.82	110.96	116.20
32	2a	858	G	C4-N9-C1'	5.82	134.07	126.50
1	1A	2709	G	O5'-P-OP1	-5.82	100.46	105.70
32	1a	399	G	C5-C6-O6	-5.82	125.11	128.60
32	2a	890	G	O4'-C1'-N9	5.82	112.86	108.20
1	1A	322	G	O5'-P-OP2	-5.82	100.46	105.70
1	1A	1256	U	O5'-P-OP1	-5.82	100.46	105.70
1	1A	1621	C	C6-N1-C2	5.82	122.63	120.30
1	1A	1656	A	C4-C5-N7	5.82	113.61	110.70
1	1A	2047	C	N3-C4-N4	5.82	122.08	118.00
1	1A	2869	G	N3-C2-N2	-5.82	115.83	119.90
2	1B	97	G	N9-C4-C5	5.82	107.73	105.40
1	1A	2451	A	N9-C4-C5	-5.82	103.47	105.80
1	2A	2614	A	N1-C6-N6	-5.82	115.11	118.60
1	1A	55	A	N9-C4-C5	-5.82	103.47	105.80
1	1A	1783	C	N3-C2-O2	5.82	125.97	121.90
32	1a	583	A	N1-C2-N3	5.82	132.21	129.30
1	2A	2828	C	C2-N3-C4	-5.82	116.99	119.90
1	1A	634	C	C6-N1-C2	5.82	122.63	120.30
1	1A	2546	A	N1-C6-N6	5.82	122.09	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2595	G	C5-N7-C8	5.82	107.21	104.30
1	1A	2697	G	OP1-P-OP2	5.82	128.32	119.60
1	2A	610	G	O5'-P-OP2	-5.82	100.47	105.70
32	2a	200	G	N7-C8-N9	-5.82	110.19	113.10
1	1A	1848	G	C4-C5-N7	-5.81	108.47	110.80
1	1A	841	G	C8-N9-C4	5.81	108.72	106.40
1	1A	1007	G	C2-N3-C4	5.81	114.81	111.90
1	1A	2238	C	C5-C6-N1	-5.81	118.09	121.00
1	1A	2526	U	C5-C4-O4	5.81	129.39	125.90
1	1A	2620	G	OP1-P-O3'	5.81	117.99	105.20
32	1a	133	U	N3-C2-O2	5.81	126.27	122.20
1	2A	799	G	N1-C6-O6	-5.81	116.41	119.90
1	2A	1409	C	O5'-P-OP2	-5.81	100.47	105.70
32	2a	44	G	C5-C6-N1	-5.81	108.59	111.50
1	1A	2897	U	O5'-P-OP1	-5.81	100.47	105.70
1	1A	120	G	OP2-P-O3'	5.81	117.98	105.20
1	1A	294	C	O5'-P-OP1	5.81	117.67	110.70
1	1A	672	G	N3-C2-N2	-5.81	115.83	119.90
1	1A	881	C	OP1-P-OP2	5.81	128.31	119.60
1	1A	1135	G	N9-C1'-C2'	5.81	121.55	114.00
1	1A	1790	A	C5-C6-N6	-5.81	119.05	123.70
1	1A	1826	C	OP1-P-OP2	5.81	128.31	119.60
1	1A	2565	G	N3-C4-N9	5.81	129.49	126.00
32	1a	971	G	N3-C4-N9	-5.81	122.51	126.00
1	2A	1186	G	N1-C6-O6	5.81	123.39	119.90
32	2a	819	A	N1-C6-N6	5.81	122.09	118.60
1	1A	719	C	C2-N3-C4	-5.81	117.00	119.90
1	2A	1179	C	C6-N1-C2	5.81	122.62	120.30
1	2A	2053	G	C5-C6-O6	-5.81	125.12	128.60
32	2a	297	G	C2-N3-C4	-5.81	109.00	111.90
1	1A	122	G	C4-C5-N7	5.81	113.12	110.80
1	1A	1132	A	C2-N3-C4	5.81	113.50	110.60
1	2A	989	G	C4-C5-N7	5.81	113.12	110.80
1	2A	1979	C	N3-C2-O2	-5.81	117.84	121.90
1	2A	2659	G	N3-C4-C5	5.81	131.50	128.60
32	2a	1139	G	C4-C5-N7	-5.81	108.48	110.80
1	1A	89	U	N1-C2-N3	5.80	118.38	114.90
1	1A	110	U	C5-C4-O4	-5.80	122.42	125.90
1	1A	354	A	C5-C6-N1	-5.80	114.80	117.70
1	1A	1665	G	O5'-P-OP2	-5.80	100.48	105.70
1	1A	2624	C	C6-N1-C2	5.80	122.62	120.30
32	1a	1417	G	C6-N1-C2	-5.80	121.62	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1513	A	C2-N3-C4	5.80	113.50	110.60
1	2A	1170	G	N7-C8-N9	5.80	116.00	113.10
1	2A	2129	C	N1-C2-O2	5.80	122.38	118.90
1	2A	2388	A	O5'-P-OP1	5.80	117.67	110.70
1	1A	359	C	N3-C2-O2	5.80	125.96	121.90
1	1A	1322	A	OP1-P-OP2	-5.80	110.90	119.60
1	1A	2076	A	N1-C2-N3	5.80	132.20	129.30
1	2A	1778	U	C5-C4-O4	-5.80	122.42	125.90
2	2B	115	G	N7-C8-N9	-5.80	110.20	113.10
1	1A	241	G	N9-C4-C5	5.80	107.72	105.40
1	1A	590	A	C8-N9-C4	-5.80	103.48	105.80
1	1A	1025	G	C5-N7-C8	5.80	107.20	104.30
1	1A	1125	C	N1-C2-O2	5.80	122.38	118.90
1	1A	1193	C	O5'-P-OP2	-5.80	100.48	105.70
1	1A	2726	A	N9-C4-C5	5.80	108.12	105.80
32	1a	122	G	O5'-P-OP1	-5.80	100.48	105.70
1	2A	888	C	C6-N1-C2	-5.80	117.98	120.30
1	2A	1086	A	C2-N3-C4	5.80	113.50	110.60
1	2A	1597	A	N1-C6-N6	-5.80	115.12	118.60
1	2A	1635	G	C8-N9-C4	5.80	108.72	106.40
1	1A	130	G	N1-C6-O6	-5.80	116.42	119.90
1	2A	1125	G	N1-C6-O6	5.80	123.38	119.90
32	2a	893	C	N1-C2-O2	5.80	122.38	118.90
32	1a	1112	C	OP2-P-O3'	5.80	117.96	105.20
1	2A	2755	C	C2-N3-C4	5.80	122.80	119.90
32	2a	1499	A	N9-C4-C5	-5.80	103.48	105.80
1	1A	1209	G	N1-C6-O6	5.80	123.38	119.90
1	1A	1956	C	C6-N1-C2	5.80	122.62	120.30
32	1a	173	U	N3-C2-O2	-5.80	118.14	122.20
32	1a	757	U	C2-N3-C4	-5.80	123.52	127.00
32	1a	1411	C	C6-N1-C2	5.80	122.62	120.30
32	2a	354	G	C4-N9-C1'	5.80	134.04	126.50
1	1A	2577	A	C5-C6-N6	-5.79	119.06	123.70
1	2A	2549	G	OP2-P-O3'	5.79	117.95	105.20
1	2A	2598	A	OP2-P-O3'	5.79	117.95	105.20
1	2A	2867	G	C5-C6-O6	-5.79	125.12	128.60
1	1A	107	G	C6-C5-N7	5.79	133.88	130.40
1	1A	1007	G	N9-C4-C5	5.79	107.72	105.40
2	1B	26	A	C8-N9-C4	5.79	108.12	105.80
32	2a	802	A	N7-C8-N9	5.79	116.70	113.80
1	1A	2094	G	C8-N9-C4	-5.79	104.08	106.40
1	1A	2265	G	N7-C8-N9	-5.79	110.20	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	781	A	C4-C5-N7	5.79	113.59	110.70
1	2A	363(B)	G	C8-N9-C1'	-5.79	119.47	127.00
1	2A	845	G	C4-N9-C1'	5.79	134.03	126.50
1	1A	566	C	O5'-P-OP2	-5.79	100.49	105.70
1	1A	1245	C	N1-C2-O2	-5.79	115.43	118.90
1	1A	1355	G	C4-C5-N7	-5.79	108.48	110.80
1	2A	1760	A	C8-N9-C4	5.79	108.11	105.80
32	2a	887	G	C4-C5-N7	5.79	113.11	110.80
1	1A	2476	C	N3-C2-O2	5.79	125.95	121.90
32	1a	1475	G	N7-C8-N9	5.79	115.99	113.10
1	2A	2261	C	N1-C2-O2	-5.79	115.43	118.90
1	1A	256	C	N3-C4-C5	5.79	124.21	121.90
1	1A	813	C	C5-C6-N1	-5.79	118.11	121.00
1	1A	1505	C	N3-C2-O2	-5.79	117.85	121.90
1	1A	1513	G	N1-C2-N2	5.79	121.41	116.20
1	1A	1653	C	OP1-P-O3'	5.79	117.93	105.20
1	1A	2049	G	C4-C5-N7	-5.79	108.48	110.80
1	1A	2630	G	N9-C4-C5	5.79	107.71	105.40
32	1a	520	A	C8-N9-C4	-5.79	103.49	105.80
1	2A	1650	G	C8-N9-C4	-5.79	104.09	106.40
1	1A	899	G	C5-C6-O6	5.78	132.07	128.60
1	1A	1028	C	O4'-C1'-N1	-5.78	103.57	108.20
1	1A	1099	C	N1-C2-N3	-5.78	115.15	119.20
1	1A	1277	G	C5-C6-O6	-5.78	125.13	128.60
1	1A	1369	U	N1-C2-N3	5.78	118.37	114.90
1	1A	2455	C	N3-C4-N4	5.78	122.05	118.00
32	1a	14	U	C5-C6-N1	5.78	125.59	122.70
32	1a	1384	C	C6-N1-C2	-5.78	117.99	120.30
1	2A	1347	G	C5-C6-N1	-5.78	108.61	111.50
1	1A	586	G	O5'-P-OP2	-5.78	100.50	105.70
1	1A	1559	C	O5'-P-OP1	-5.78	100.50	105.70
1	2A	647	G	C8-N9-C4	-5.78	104.09	106.40
32	2a	1043	C	O4'-C1'-N1	5.78	112.83	108.20
1	1A	1080	G	C5-C6-N1	5.78	114.39	111.50
1	1A	1415	G	C5-C6-N1	-5.78	108.61	111.50
1	1A	2129	C	C2-N3-C4	5.78	122.79	119.90
11	1P	55	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	2A	415	A	O5'-P-OP2	-5.78	100.50	105.70
1	2A	529	A	O4'-C1'-N9	5.78	112.82	108.20
1	2A	2300	G	C8-N9-C4	-5.78	104.09	106.40
1	2A	114	U	C2-N1-C1'	5.78	124.64	117.70
1	2A	2282	G	O5'-P-OP1	-5.78	100.50	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2228	G	C4-N9-C1'	-5.78	118.99	126.50
1	1A	2707	C	C2-N3-C4	-5.78	117.01	119.90
2	1B	32	C	N3-C4-C5	5.78	124.21	121.90
1	2A	1740	G	C5-C6-N1	5.78	114.39	111.50
1	2A	2105	C	C2-N1-C1'	5.78	125.16	118.80
1	1A	1950	A	N1-C2-N3	-5.78	126.41	129.30
1	1A	2883	A	C5-C6-N1	-5.78	114.81	117.70
5	1F	53	THR	N-CA-CB	-5.78	99.33	110.30
32	1a	1021	G	N3-C4-N9	5.78	129.47	126.00
1	2A	282	A	C8-N9-C4	-5.78	103.49	105.80
1	2A	568	U	C2-N3-C4	-5.78	123.53	127.00
1	2A	1336	A	N1-C6-N6	-5.78	115.14	118.60
32	2a	142	G	N1-C6-O6	-5.78	116.44	119.90
32	2a	851	G	N7-C8-N9	5.78	115.99	113.10
1	1A	1662	A	N9-C4-C5	-5.77	103.49	105.80
1	1A	2638	C	C6-N1-C2	5.77	122.61	120.30
1	1A	1370	G	OP1-P-OP2	-5.77	110.94	119.60
1	1A	1727	U	N3-C4-C5	5.77	118.06	114.60
1	1A	2298	A	N1-C2-N3	5.77	132.19	129.30
32	2a	993	G	C4-N9-C1'	5.77	134.00	126.50
1	1A	215	G	N1-C2-N2	5.77	121.39	116.20
1	2A	2126	A	P-O3'-C3'	5.77	126.62	119.70
1	1A	72	A	N1-C2-N3	5.77	132.19	129.30
1	1A	601	A	C8-N9-C4	-5.77	103.49	105.80
1	1A	728	G	C2-N3-C4	-5.77	109.02	111.90
1	2A	645	C	N1-C2-O2	5.77	122.36	118.90
1	2A	1928	A	N1-C2-N3	-5.77	126.42	129.30
1	2A	2033	A	C6-N1-C2	-5.77	115.14	118.60
1	1A	393	A	C5-C6-N6	5.77	128.31	123.70
1	1A	788	G	N3-C2-N2	-5.77	115.86	119.90
1	1A	828	A	C5-C6-N1	5.77	120.58	117.70
1	1A	1863	C	C6-N1-C2	-5.77	117.99	120.30
1	1A	2443	U	C4-C5-C6	5.77	123.16	119.70
16	1U	50	ARG	CB-CA-C	5.77	121.93	110.40
1	2A	704	G	N3-C4-C5	-5.77	125.72	128.60
1	2A	1076	C	N1-C1'-C2'	5.77	121.50	114.00
1	2A	1235	G	C8-N9-C4	-5.77	104.09	106.40
32	2a	854	G	N7-C8-N9	5.77	115.98	113.10
32	2a	1077	G	N7-C8-N9	-5.77	110.22	113.10
32	2a	1371	G	O5'-P-OP2	5.77	117.62	110.70
1	2A	994	C	C4-C5-C6	5.77	120.28	117.40
1	1A	126	C	C6-N1-C2	5.76	122.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1347	A	N7-C8-N9	5.76	116.68	113.80
1	1A	1548	C	C6-N1-C2	-5.76	117.99	120.30
1	1A	1911	A	N7-C8-N9	-5.76	110.92	113.80
13	1R	64	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	2A	117	G	OP1-P-OP2	-5.76	110.95	119.60
1	2A	458	G	N3-C2-N2	5.76	123.94	119.90
1	2A	989	G	OP2-P-O3'	5.76	117.88	105.20
1	2A	1109	C	C2-N1-C1'	5.76	125.14	118.80
1	2A	1180	C	C6-N1-C2	5.76	122.61	120.30
1	2A	1350	C	C5-C6-N1	5.76	123.88	121.00
1	2A	2433	A	C5-C6-N6	-5.76	119.09	123.70
2	2B	41	U	C6-N1-C2	-5.76	117.54	121.00
1	1A	423	G	C5-C6-N1	5.76	114.38	111.50
1	1A	1177	G	N1-C2-N2	-5.76	111.01	116.20
1	2A	2023	G	N3-C4-N9	5.76	129.46	126.00
1	1A	2497	G	C6-N1-C2	5.76	128.56	125.10
1	2A	1628	G	N3-C2-N2	5.76	123.93	119.90
1	2A	2270	G	C5-N7-C8	-5.76	101.42	104.30
1	2A	2763	G	N3-C4-N9	5.76	129.46	126.00
1	1A	996	C	N3-C4-C5	5.76	124.20	121.90
1	2A	272(E)	G	N9-C4-C5	-5.76	103.10	105.40
1	2A	1305	C	C6-N1-C2	-5.76	118.00	120.30
1	2A	1913	A	N9-C4-C5	5.76	108.10	105.80
1	2A	2053	G	N3-C2-N2	-5.76	115.87	119.90
1	2A	784	A	O4'-C1'-N9	5.76	112.81	108.20
1	2A	807	U	C2-N1-C1'	5.76	124.61	117.70
1	2A	2013	A	N1-C2-N3	5.76	132.18	129.30
1	1A	776	G	C4-C5-N7	5.76	113.10	110.80
1	1A	881	C	N3-C4-C5	5.76	124.20	121.90
1	1A	884	C	N3-C4-N4	-5.76	113.97	118.00
15	1T	53	ARG	CB-CA-C	-5.76	98.89	110.40
32	1a	1053	G	C8-N9-C4	5.76	108.70	106.40
1	2A	1303	G	O5'-P-OP2	-5.76	100.52	105.70
1	2A	1799	G	C5-C6-N1	5.76	114.38	111.50
32	2a	1138	G	C8-N9-C4	-5.76	104.10	106.40
1	1A	1630	A	C4-C5-C6	-5.75	114.12	117.00
1	2A	2394	C	C6-N1-C2	5.75	122.60	120.30
1	1A	980	C	C5-C6-N1	-5.75	118.12	121.00
1	1A	1419	A	C6-N1-C2	-5.75	115.15	118.60
1	1A	2403	G	OP1-P-OP2	5.75	128.23	119.60
32	1a	204	U	C6-N1-C2	-5.75	117.55	121.00
1	2A	698	C	C2-N3-C4	-5.75	117.02	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	180	A	OP2-P-O3'	5.75	117.86	105.20
1	1A	311	C	C6-N1-C2	5.75	122.60	120.30
1	1A	903	C	C5-C6-N1	5.75	123.88	121.00
1	1A	2052	A	C5-N7-C8	-5.75	101.02	103.90
32	1a	576	G	N3-C4-N9	5.75	129.45	126.00
32	1a	1260	C	O5'-P-OP1	-5.75	100.52	105.70
32	2a	230	G	N1-C2-N3	5.75	127.35	123.90
1	1A	295	C	O5'-P-OP1	5.75	117.60	110.70
1	1A	1640	G	N7-C8-N9	5.75	115.97	113.10
1	1A	1921	G	C5-N7-C8	-5.75	101.42	104.30
32	1a	801	U	N1-C2-O2	5.75	126.83	122.80
1	2A	1063	G	C4-N9-C1'	5.75	133.97	126.50
1	1A	71	U	N3-C2-O2	5.75	126.22	122.20
1	1A	702	A	O4'-C1'-N9	5.75	112.80	108.20
1	1A	757	G	C8-N9-C4	5.75	108.70	106.40
1	1A	2392	C	C5-C6-N1	-5.75	118.12	121.00
32	1a	657	G	O5'-P-OP2	-5.75	100.53	105.70
32	1a	1403	C	C6-N1-C2	-5.75	118.00	120.30
1	2A	1191	G	N3-C2-N2	5.75	123.92	119.90
32	2a	1510	U	C5-C4-O4	-5.75	122.45	125.90
1	1A	1035	G	N3-C4-C5	-5.75	125.73	128.60
1	1A	2460	A	C8-N9-C4	5.75	108.10	105.80
1	2A	1154	G	O5'-P-OP2	-5.75	100.53	105.70
1	2A	2895	U	C6-N1-C2	-5.75	117.55	121.00
1	1A	1694	G	C4-C5-N7	-5.75	108.50	110.80
20	1Y	34	LYS	CD-CE-NZ	5.75	124.91	111.70
1	2A	1780	A	N7-C8-N9	5.75	116.67	113.80
32	2a	839	U	C2-N1-C1'	5.75	124.59	117.70
32	2a	1108	G	N3-C4-N9	5.75	129.45	126.00
1	1A	867	A	OP2-P-O3'	5.74	117.84	105.20
1	1A	1652	G	N1-C2-N3	5.74	127.35	123.90
1	1A	2187	G	C5-C6-O6	5.74	132.05	128.60
32	1a	670	G	C4-C5-N7	-5.74	108.50	110.80
32	1a	1140	C	C6-N1-C2	-5.74	118.00	120.30
1	2A	6	A	N1-C6-N6	-5.74	115.15	118.60
1	1A	875	U	OP2-P-O3'	5.74	117.83	105.20
32	2a	893	C	C5-C4-N4	-5.74	116.18	120.20
1	1A	757	G	N1-C6-O6	5.74	123.34	119.90
1	2A	1989	G	N1-C2-N2	-5.74	111.03	116.20
1	2A	2429	G	C8-N9-C4	-5.74	104.10	106.40
1	2A	2821	A	C2-N3-C4	-5.74	107.73	110.60
32	2a	945	G	N1-C6-O6	5.74	123.34	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1075	A	O5'-P-OP1	5.74	117.59	110.70
1	1A	1880	G	C5-C6-N1	-5.74	108.63	111.50
1	1A	2392	C	N3-C4-C5	5.74	124.19	121.90
1	1A	2818	U	C5-C4-O4	-5.74	122.46	125.90
32	1a	284	G	N1-C6-O6	5.74	123.34	119.90
1	2A	983	A	C5-C6-N1	-5.74	114.83	117.70
1	2A	1277	G	C8-N9-C4	5.74	108.70	106.40
1	1A	1678	A	C4-C5-C6	5.74	119.87	117.00
1	2A	1257	C	O5'-P-OP1	-5.74	100.54	105.70
1	1A	348	A	N9-C4-C5	-5.74	103.51	105.80
1	1A	1661	C	N1-C2-N3	5.74	123.22	119.20
1	1A	2066	C	N1-C2-N3	5.74	123.21	119.20
2	1B	106	G	N1-C2-N2	5.74	121.36	116.20
1	2A	41	C	O5'-P-OP1	5.74	117.58	110.70
1	1A	1268	C	C6-N1-C2	5.73	122.59	120.30
1	1A	1513	G	OP2-P-O3'	5.73	117.81	105.20
4	1E	144	ARG	NE-CZ-NH1	5.73	123.17	120.30
32	1a	831	U	C5-C6-N1	5.73	125.57	122.70
1	2A	130	C	N3-C4-C5	5.73	124.19	121.90
1	2A	1045	A	N1-C6-N6	5.73	122.04	118.60
1	1A	424	G	C2-N3-C4	-5.73	109.03	111.90
1	1A	818	G	N3-C2-N2	5.73	123.91	119.90
1	1A	1788	U	C5-C4-O4	-5.73	122.46	125.90
1	1A	2283	G	N3-C4-C5	-5.73	125.73	128.60
32	1a	220	G	N7-C8-N9	5.73	115.97	113.10
32	1a	340	U	C5-C6-N1	-5.73	119.83	122.70
32	1a	442	C	C5-C6-N1	5.73	123.87	121.00
1	2A	234	C	C6-N1-C2	-5.73	118.01	120.30
1	2A	829	A	OP1-P-OP2	5.73	128.20	119.60
1	2A	2344	U	OP1-P-O3'	5.73	117.81	105.20
1	1A	2529	C	N3-C2-O2	5.73	125.91	121.90
1	2A	2444	G	N9-C4-C5	5.73	107.69	105.40
32	2a	297	G	C8-N9-C4	5.73	108.69	106.40
1	1A	2051	G	N3-C2-N2	-5.73	115.89	119.90
1	1A	2069	U	OP2-P-O3'	5.73	117.80	105.20
1	1A	2330	G	C2-N3-C4	-5.73	109.03	111.90
1	2A	271(X)	G	N3-C4-N9	-5.73	122.56	126.00
1	2A	1998	G	C5-N7-C8	5.73	107.17	104.30
1	1A	1768	U	C2-N1-C1'	5.73	124.57	117.70
1	1A	2030	C	C2-N3-C4	-5.73	117.04	119.90
1	1A	2304	C	C6-N1-C2	5.73	122.59	120.30
1	1A	2632	C	OP1-P-OP2	5.73	128.19	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	366	C	OP1-P-OP2	5.73	128.19	119.60
1	2A	1071	G	C5-C6-N1	-5.73	108.64	111.50
1	2A	1671	U	C6-N1-C2	5.73	124.44	121.00
1	1A	673	G	C2-N3-C4	-5.73	109.04	111.90
22	10	25	ARG	NE-CZ-NH1	-5.73	117.44	120.30
32	1a	1008	C	O4'-C1'-N1	5.73	112.78	108.20
1	1A	200	A	C2-N3-C4	5.72	113.46	110.60
1	1A	1466	U	P-O3'-C3'	5.72	126.57	119.70
32	1a	1000	U	O4'-C1'-N1	5.72	112.78	108.20
32	1a	1046	A	O5'-P-OP1	-5.72	100.55	105.70
1	2A	668	G	OP2-P-O3'	5.72	117.80	105.20
1	1A	2608	U	C5-C4-O4	-5.72	122.47	125.90
32	1a	189(G)	G	N3-C4-N9	-5.72	122.57	126.00
1	2A	1162	G	N3-C4-N9	-5.72	122.57	126.00
1	2A	1269	A	N1-C2-N3	5.72	132.16	129.30
1	2A	2201	C	OP2-P-O3'	5.72	117.79	105.20
1	2A	2585	U	C5-C6-N1	-5.72	119.84	122.70
1	1A	12	U	C2-N1-C1'	5.72	124.56	117.70
32	1a	1279	A	C8-N9-C4	-5.72	103.51	105.80
1	2A	363(B)	G	N3-C4-N9	5.72	129.43	126.00
1	2A	992	C	C6-N1-C2	-5.72	118.01	120.30
1	1A	10	G	N3-C2-N2	5.72	123.90	119.90
1	1A	122	G	C6-C5-N7	-5.72	126.97	130.40
1	1A	489	G	OP1-P-O3'	5.72	117.78	105.20
1	1A	1826	C	N3-C4-C5	5.72	124.19	121.90
1	1A	1835	C	OP1-P-OP2	-5.72	111.02	119.60
1	1A	2706	G	C5-C6-O6	-5.72	125.17	128.60
1	1A	2719	G	N7-C8-N9	-5.72	110.24	113.10
32	1a	105	G	C5-C6-O6	-5.72	125.17	128.60
32	1a	1010	G	N3-C4-C5	5.72	131.46	128.60
32	2a	397	A	OP2-P-O3'	5.72	117.78	105.20
32	2a	487	A	N7-C8-N9	-5.72	110.94	113.80
32	2a	785	G	C4-N9-C1'	-5.72	119.07	126.50
32	1a	803	G	C5-C6-N1	-5.72	108.64	111.50
1	2A	314	A	N9-C4-C5	5.72	108.09	105.80
1	1A	284	G	N1-C6-O6	5.72	123.33	119.90
1	1A	2111	U	C6-N1-C2	5.72	124.43	121.00
1	1A	2227	G	C2-N3-C4	-5.72	109.04	111.90
32	1a	73	G	C6-C5-N7	5.72	133.83	130.40
32	1a	163	C	C5-C4-N4	5.72	124.20	120.20
32	1a	578	C	O5'-P-OP1	-5.72	100.56	105.70
1	2A	698	C	N3-C4-C5	5.72	124.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2198	A	N1-C6-N6	5.72	122.03	118.60
1	2A	2629	A	C5'-C4'-O4'	5.72	115.96	109.10
1	1A	502	G	C8-N9-C4	5.71	108.69	106.40
1	1A	553	A	C4-N9-C1'	5.71	136.59	126.30
1	1A	569	G	N9-C4-C5	5.71	107.69	105.40
1	1A	781	A	C6-C5-N7	-5.71	128.30	132.30
1	1A	990	A	N9-C4-C5	-5.71	103.51	105.80
1	1A	1295	U	C5-C6-N1	-5.71	119.84	122.70
1	1A	1494	G	C8-N9-C4	-5.71	104.11	106.40
1	1A	1855	G	OP2-P-O3'	5.71	117.77	105.20
1	1A	2136	A	O4'-C1'-N9	5.71	112.77	108.20
1	1A	2534	U	C5-C6-N1	-5.71	119.84	122.70
1	1A	2742	G	C8-N9-C4	-5.71	104.11	106.40
1	2A	927	G	O5'-P-OP1	-5.71	100.56	105.70
1	2A	1616	A	C8-N9-C4	-5.71	103.51	105.80
1	2A	1781	C	N1-C2-O2	-5.71	115.47	118.90
32	2a	380	G	N9-C4-C5	5.71	107.69	105.40
1	1A	124	A	OP2-P-O3'	5.71	117.77	105.20
1	1A	1281	G	OP2-P-O3'	5.71	117.77	105.20
32	1a	664	G	N9-C4-C5	5.71	107.69	105.40
1	1A	879	G	C5-C6-N1	-5.71	108.64	111.50
1	1A	962	G	C8-N9-C4	5.71	108.69	106.40
1	1A	1838	G	OP1-P-O3'	5.71	117.76	105.20
1	1A	1867	C	N3-C4-C5	-5.71	119.62	121.90
1	1A	2255	U	N1-C2-O2	-5.71	118.80	122.80
1	1A	2456	G	N9-C4-C5	5.71	107.68	105.40
1	2A	1678	G	N1-C2-N3	5.71	127.33	123.90
1	1A	1700	G	C4-N9-C1'	5.71	133.92	126.50
1	1A	2136	A	N9-C4-C5	5.71	108.08	105.80
1	1A	150	C	OP1-P-OP2	5.71	128.16	119.60
1	1A	2262	G	O5'-P-OP2	-5.71	100.56	105.70
1	2A	1597	A	N3-C4-N9	-5.71	122.83	127.40
1	2A	2274	A	OP2-P-O3'	5.71	117.76	105.20
2	2B	108	U	C5-C4-O4	5.71	129.32	125.90
32	2a	399	G	N1-C6-O6	5.71	123.33	119.90
32	2a	748	C	P-O3'-C3'	5.71	126.55	119.70
1	1A	634	C	N3-C4-C5	5.71	124.18	121.90
1	1A	869	U	N1-C2-N3	5.71	118.32	114.90
1	1A	1412	A	N1-C6-N6	5.71	122.02	118.60
1	1A	1657	C	C6-N1-C2	-5.71	118.02	120.30
1	1A	1755	C	C5-C6-N1	-5.71	118.15	121.00
1	1A	2551	C	C4-C5-C6	5.71	120.25	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2900	G	C5-C6-O6	-5.71	125.18	128.60
1	1A	1347	A	C2-N3-C4	-5.71	107.75	110.60
2	1B	79	C	N3-C2-O2	-5.71	117.91	121.90
32	1a	1168	A	N7-C8-N9	5.71	116.65	113.80
1	2A	602	G	O5'-P-OP2	-5.71	100.57	105.70
1	2A	2130	U	C5-C6-N1	5.71	125.55	122.70
32	2a	15	G	C8-N9-C4	-5.71	104.12	106.40
1	1A	1145	G	C2-N3-C4	5.70	114.75	111.90
1	1A	2356	U	O4'-C1'-N1	-5.70	103.64	108.20
1	1A	2401	G	OP1-P-O3'	5.70	117.75	105.20
1	1A	2598	C	C5-C4-N4	-5.70	116.21	120.20
1	2A	272(A)	U	O5'-P-OP2	-5.70	100.57	105.70
1	2A	779	U	N1-C2-O2	-5.70	118.81	122.80
1	2A	1133	U	N1-C2-O2	-5.70	118.81	122.80
1	2A	2629	A	C2-N3-C4	-5.70	107.75	110.60
1	1A	200	A	C8-N9-C4	5.70	108.08	105.80
1	1A	1117	G	C4-C5-N7	-5.70	108.52	110.80
1	1A	1668	G	N3-C2-N2	-5.70	115.91	119.90
1	2A	1774	C	N3-C4-N4	5.70	121.99	118.00
1	1A	131	C	O5'-P-OP1	5.70	117.54	110.70
1	1A	619	G	N7-C8-N9	-5.70	110.25	113.10
1	1A	1075	A	C5-C6-N6	-5.70	119.14	123.70
1	1A	1320	A	C5-N7-C8	-5.70	101.05	103.90
1	1A	2499	G	N1-C6-O6	5.70	123.32	119.90
1	2A	1466	G	N7-C8-N9	-5.70	110.25	113.10
1	2A	1493	C	C4-C5-C6	5.70	120.25	117.40
1	2A	2468	G	O4'-C1'-N9	5.70	112.76	108.20
32	2a	1002	G	C8-N9-C4	-5.70	104.12	106.40
1	1A	953	U	OP2-P-O3'	5.70	117.74	105.20
32	1a	975	A	C5-N7-C8	-5.70	101.05	103.90
32	1a	1376	U	C5-C4-O4	5.70	129.32	125.90
1	2A	705	A	N9-C4-C5	-5.70	103.52	105.80
1	2A	1779	U	O4'-C1'-N1	5.70	112.76	108.20
32	2a	618	C	C2-N3-C4	5.70	122.75	119.90
32	2a	885	G	N3-C2-N2	5.70	123.89	119.90
1	1A	788	G	N1-C2-N2	5.70	121.33	116.20
1	1A	710	G	C4-C5-N7	-5.70	108.52	110.80
1	1A	742	G	N1-C6-O6	-5.70	116.48	119.90
1	1A	2603	C	C5-C6-N1	5.70	123.85	121.00
32	2a	110	C	N1-C2-O2	5.70	122.32	118.90
1	1A	149	A	O5'-P-OP1	-5.69	100.58	105.70
1	1A	1812	C	C6-N1-C1'	-5.69	113.97	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	331	A	N9-C4-C5	5.69	108.08	105.80
1	2A	1998	G	N7-C8-N9	-5.69	110.25	113.10
32	2a	378	G	N9-C4-C5	-5.69	103.12	105.40
32	1a	340	U	C6-N1-C2	5.69	124.42	121.00
32	1a	572	A	C8-N9-C4	5.69	108.08	105.80
1	2A	878	A	C5-C6-N1	-5.69	114.85	117.70
1	2A	1100	C	N3-C4-C5	-5.69	119.62	121.90
1	2A	1658	C	C5-C6-N1	5.69	123.85	121.00
1	2A	1681	G	N7-C8-N9	5.69	115.95	113.10
1	2A	1966	A	N9-C4-C5	5.69	108.08	105.80
1	2A	2256	G	OP2-P-O3'	5.69	117.72	105.20
1	2A	2697	G	N1-C6-O6	-5.69	116.48	119.90
32	2a	970	C	N1-C2-O2	5.69	122.32	118.90
1	1A	975	U	C2-N3-C4	-5.69	123.58	127.00
1	1A	1132	A	O4'-C1'-N9	5.69	112.75	108.20
1	1A	1525	G	C8-N9-C4	-5.69	104.12	106.40
1	1A	1637	G	C5-C6-O6	5.69	132.01	128.60
1	1A	2562	G	C8-N9-C4	-5.69	104.12	106.40
32	1a	1423	G	O5'-P-OP2	-5.69	100.58	105.70
1	2A	2725	A	C2-N3-C4	-5.69	107.75	110.60
32	2a	1427	U	N1-C2-O2	-5.69	118.82	122.80
1	1A	2513	C	C2-N1-C1'	-5.69	112.54	118.80
1	1A	2892	A	O5'-P-OP2	-5.69	100.58	105.70
1	1A	500	G	N1-C2-N2	-5.69	111.08	116.20
1	1A	1079	U	C6-N1-C2	5.69	124.41	121.00
1	2A	567	A	C4-C5-N7	5.69	113.54	110.70
1	2A	954	G	C4-C5-N7	-5.69	108.53	110.80
1	2A	2177	C	C2-N1-C1'	5.69	125.06	118.80
32	2a	244	U	C6-N1-C2	5.69	124.41	121.00
1	1A	200	A	OP2-P-O3'	5.69	117.71	105.20
1	1A	575	G	N1-C2-N2	-5.69	111.08	116.20
1	1A	654	G	C5-C6-O6	5.69	132.01	128.60
1	1A	1024	G	N7-C8-N9	-5.69	110.26	113.10
32	1a	123	C	C6-N1-C2	5.69	122.57	120.30
32	1a	396	G	N3-C4-N9	-5.69	122.59	126.00
1	2A	622	G	C8-N9-C4	5.69	108.67	106.40
1	2A	885	C	C5-C6-N1	5.69	123.84	121.00
1	2A	1148	A	N9-C4-C5	5.69	108.07	105.80
1	2A	2551	C	N1-C2-O2	-5.69	115.49	118.90
1	1A	744	C	O5'-P-OP2	-5.68	100.58	105.70
1	1A	976	G	N3-C4-N9	5.68	129.41	126.00
1	1A	1301	U	C4-C5-C6	5.68	123.11	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1361	C	O5'-P-OP1	5.68	117.52	110.70
1	1A	1379	C	N3-C4-C5	5.68	124.17	121.90
1	1A	1514	C	C6-N1-C2	-5.68	118.03	120.30
1	1A	1892	G	C4-N9-C1'	-5.68	119.11	126.50
32	2a	400	C	OP1-P-OP2	-5.68	111.07	119.60
32	2a	1058	G	O5'-P-OP1	5.68	117.52	110.70
1	1A	588	C	C5-C6-N1	5.68	123.84	121.00
32	1a	250	A	N3-C4-C5	-5.68	122.82	126.80
32	1a	635	G	N1-C6-O6	5.68	123.31	119.90
1	2A	365	C	C4-C5-C6	5.68	120.24	117.40
1	2A	1607	C	N1-C2-O2	5.68	122.31	118.90
1	1A	424	G	C5-C6-O6	5.68	132.01	128.60
1	1A	1857	G	C8-N9-C4	-5.68	104.13	106.40
1	2A	1574	C	C4-C5-C6	-5.68	114.56	117.40
1	1A	9	U	N1-C2-N3	-5.68	111.49	114.90
1	1A	2635	G	C8-N9-C4	-5.68	104.13	106.40
32	1a	708	C	N1-C2-O2	5.68	122.31	118.90
1	2A	870	A	O5'-P-OP2	-5.68	100.59	105.70
32	2a	168	G	N3-C4-N9	5.68	129.41	126.00
1	1A	851	A	N1-C2-N3	-5.68	126.46	129.30
1	1A	1475	G	N1-C6-O6	-5.68	116.49	119.90
1	2A	734	A	C2-N3-C4	-5.68	107.76	110.60
1	2A	1309	G	N9-C4-C5	-5.68	103.13	105.40
1	2A	1721	G	C4-C5-N7	5.68	113.07	110.80
1	2A	2585	U	C6-N1-C2	5.68	124.41	121.00
32	2a	884	U	N3-C2-O2	-5.68	118.22	122.20
1	1A	657	A	O5'-P-OP2	5.68	117.51	110.70
1	1A	776	G	C5-N7-C8	-5.68	101.46	104.30
1	1A	1456	G	N1-C6-O6	5.68	123.31	119.90
1	1A	1757	C	C2-N1-C1'	-5.68	112.56	118.80
1	1A	1956	C	C5-C6-N1	-5.68	118.16	121.00
32	1a	760	G	N3-C2-N2	-5.68	115.93	119.90
32	2a	771	G	N3-C2-N2	-5.68	115.93	119.90
1	1A	417	A	N9-C4-C5	-5.67	103.53	105.80
1	1A	977	G	N3-C4-C5	-5.67	125.76	128.60
1	1A	1485	A	C5-C6-N1	-5.67	114.86	117.70
1	1A	1816	A	O5'-P-OP2	-5.67	100.59	105.70
1	1A	2107	C	C2-N3-C4	-5.67	117.06	119.90
1	1A	2236	G	N1-C6-O6	-5.67	116.50	119.90
2	1B	100	A	N9-C4-C5	5.67	108.07	105.80
32	1a	536	C	O5'-P-OP2	-5.67	100.59	105.70
2	2B	59	A	C2-N3-C4	5.67	113.44	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	878	G	C8-N9-C4	5.67	108.67	106.40
1	1A	2545	A	N1-C2-N3	5.67	132.14	129.30
32	1a	905	U	N1-C2-O2	-5.67	118.83	122.80
1	1A	69	G	N1-C2-N2	-5.67	111.10	116.20
1	1A	593	G	C2-N3-C4	5.67	114.74	111.90
1	1A	1264	G	OP2-P-O3'	5.67	117.68	105.20
32	1a	726	C	N1-C2-O2	-5.67	115.50	118.90
1	2A	250	G	C4-C5-N7	-5.67	108.53	110.80
1	2A	271(S)	G	N1-C6-O6	5.67	123.30	119.90
1	2A	1614	A	N9-C4-C5	5.67	108.07	105.80
1	2A	2033	A	O4'-C1'-N9	5.67	112.74	108.20
1	2A	2180	U	N3-C4-O4	5.67	123.37	119.40
1	2A	2306	C	N3-C4-C5	5.67	124.17	121.90
1	2A	2378	A	C4-N9-C1'	5.67	136.51	126.30
1	2A	2622	C	C6-N1-C2	5.67	122.57	120.30
1	2A	2726	U	N3-C2-O2	5.67	126.17	122.20
1	1A	255	G	C5-C6-O6	-5.67	125.20	128.60
1	1A	1256	U	OP1-P-OP2	-5.67	111.09	119.60
1	1A	1457	C	O5'-P-OP2	-5.67	100.60	105.70
1	1A	1714	G	N1-C6-O6	-5.67	116.50	119.90
1	1A	2759	U	C5-C6-N1	-5.67	119.87	122.70
1	2A	639	U	C5-C6-N1	-5.67	119.87	122.70
1	2A	878	A	C2-N3-C4	-5.67	107.77	110.60
1	2A	976	C	N3-C2-O2	-5.67	117.93	121.90
1	1A	352	U	N1-C2-N3	5.67	118.30	114.90
1	1A	2439	C	O5'-P-OP2	5.67	117.50	110.70
1	1A	2698	G	N3-C2-N2	5.67	123.87	119.90
5	1F	188	ARG	NE-CZ-NH1	-5.67	117.47	120.30
32	2a	1030	C	N3-C2-O2	-5.67	117.93	121.90
32	2a	1152	A	C8-N9-C4	-5.67	103.53	105.80
1	1A	1511	C	N3-C4-C5	-5.67	119.63	121.90
1	1A	2085	C	O5'-P-OP2	-5.67	100.60	105.70
1	1A	2663	C	N3-C4-N4	5.67	121.97	118.00
32	1a	168	G	C8-N9-C4	5.67	108.67	106.40
32	1a	1287	A	C5-C6-N1	-5.67	114.87	117.70
1	2A	2144	U	C6-N1-C2	-5.67	117.60	121.00
1	1A	918	U	C2-N3-C4	-5.66	123.60	127.00
1	1A	2386	C	C5-C4-N4	-5.66	116.24	120.20
1	1A	2443	U	N3-C4-O4	-5.66	115.44	119.40
1	1A	2450	U	C6-N1-C2	5.66	124.40	121.00
1	1A	1104	G	C4-C5-N7	5.66	113.06	110.80
1	2A	2455	G	N3-C2-N2	-5.66	115.94	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	352	C	OP2-P-O3'	5.66	117.66	105.20
32	2a	1299	A	C8-N9-C4	-5.66	103.53	105.80
1	1A	418	G	N7-C8-N9	-5.66	110.27	113.10
1	1A	752	A	C5-N7-C8	-5.66	101.07	103.90
32	1a	142	G	N3-C4-N9	-5.66	122.60	126.00
32	1a	1409	C	O5'-P-OP1	5.66	117.49	110.70
1	2A	271(M)	G	OP1-P-O3'	5.66	117.65	105.20
1	2A	1040	C	C6-N1-C2	5.66	122.56	120.30
32	2a	872	A	C8-N9-C4	-5.66	103.54	105.80
1	1A	612	C	C5-C6-N1	-5.66	118.17	121.00
1	1A	2386	C	N3-C4-C5	5.66	124.16	121.90
1	2A	1024	G	C8-N9-C4	-5.66	104.14	106.40
1	2A	2457	U	C5-C4-O4	5.66	129.30	125.90
32	2a	1087	G	C8-N9-C4	-5.66	104.14	106.40
1	1A	1264	G	C5-N7-C8	-5.66	101.47	104.30
1	1A	1903	C	C6-N1-C2	-5.66	118.04	120.30
1	1A	2423	A	O5'-P-OP1	-5.66	100.61	105.70
1	1A	2663	C	N1-C2-O2	-5.66	115.51	118.90
2	2B	61	G	O5'-P-OP1	-5.66	100.61	105.70
32	2a	854	G	C8-N9-C4	-5.66	104.14	106.40
1	1A	274	U	C5-C4-O4	-5.66	122.51	125.90
1	1A	735	U	N1-C2-O2	-5.66	118.84	122.80
1	1A	1264	G	C2-N3-C4	-5.66	109.07	111.90
1	1A	1600	A	OP2-P-O3'	5.66	117.64	105.20
1	2A	1269	A	N1-C6-N6	5.66	121.99	118.60
1	2A	2667	C	C6-N1-C2	-5.66	118.04	120.30
1	1A	1345	G	OP2-P-O3'	5.65	117.64	105.20
1	2A	518	G	O5'-P-OP2	-5.65	100.61	105.70
1	2A	2002	G	C5-N7-C8	5.65	107.13	104.30
32	2a	299	G	C8-N9-C4	5.65	108.66	106.40
1	1A	1066	A	N1-C2-N3	5.65	132.13	129.30
1	1A	1310	G	N1-C2-N2	-5.65	111.11	116.20
1	1A	2301	G	OP1-P-O3'	5.65	117.64	105.20
1	1A	2312	G	O5'-P-OP2	5.65	117.48	110.70
2	1B	18	G	N1-C6-O6	5.65	123.29	119.90
32	1a	49	U	N1-C2-O2	5.65	126.76	122.80
32	2a	243	A	O5'-P-OP2	-5.65	100.61	105.70
1	1A	200	A	N7-C8-N9	-5.65	110.97	113.80
1	1A	800	C	C4-C5-C6	5.65	120.23	117.40
1	1A	1323	G	OP2-P-O3'	5.65	117.63	105.20
1	1A	1766	G	C5-C6-N1	5.65	114.33	111.50
1	1A	2215	G	N7-C8-N9	-5.65	110.27	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2332	A	C8-N9-C4	-5.65	103.54	105.80
1	2A	774	A	OP1-P-OP2	5.65	128.08	119.60
32	1a	606	G	N3-C4-C5	-5.65	125.78	128.60
32	2a	1001	A	C4-C5-N7	-5.65	107.88	110.70
1	1A	692	C	N1-C2-O2	5.65	122.29	118.90
1	1A	2359	C	O5'-P-OP2	-5.65	100.62	105.70
1	1A	2728	C	C6-N1-C2	5.65	122.56	120.30
1	2A	272(C)	G	N1-C6-O6	5.65	123.29	119.90
1	2A	1135	C	N3-C4-C5	5.65	124.16	121.90
1	2A	1378	A	OP1-P-OP2	5.65	128.07	119.60
1	1A	1683	C	C4-C5-C6	5.65	120.22	117.40
1	2A	778	G	OP1-P-O3'	5.65	117.62	105.20
1	2A	988	A	C6-C5-N7	-5.65	128.35	132.30
1	2A	1283	G	N1-C2-N3	-5.65	120.51	123.90
1	2A	1477	A	O5'-P-OP2	-5.65	100.62	105.70
1	1A	722	A	C8-N9-C4	5.64	108.06	105.80
1	1A	1292	A	C5-N7-C8	5.64	106.72	103.90
1	1A	2524	C	C6-N1-C2	5.64	122.56	120.30
1	1A	2598	C	OP1-P-OP2	-5.64	111.14	119.60
1	1A	2619	G	N1-C2-N2	-5.64	111.12	116.20
1	1A	2814	C	C6-N1-C2	-5.64	118.04	120.30
32	1a	1492	A	N1-C6-N6	-5.64	115.21	118.60
1	2A	527	C	N1-C2-O2	-5.64	115.51	118.90
1	2A	779	U	C5-C4-O4	-5.64	122.51	125.90
32	2a	517	G	N3-C4-C5	-5.64	125.78	128.60
1	1A	1216	G	C6-C5-N7	-5.64	127.01	130.40
1	1A	1470	G	C2-N3-C4	-5.64	109.08	111.90
1	1A	2421	G	N3-C4-C5	-5.64	125.78	128.60
1	2A	887	A	N1-C2-N3	-5.64	126.48	129.30
1	2A	1440	G	C4-C5-N7	-5.64	108.54	110.80
1	2A	1595	G	O5'-P-OP1	-5.64	100.62	105.70
1	1A	580	U	C2-N3-C4	-5.64	123.61	127.00
1	1A	720	C	N1-C2-N3	5.64	123.15	119.20
1	1A	1006	C	OP1-P-O3'	5.64	117.61	105.20
1	1A	1624	C	O5'-P-OP2	-5.64	100.62	105.70
1	1A	997	G	C8-N9-C4	-5.64	104.14	106.40
1	1A	2703	C	OP1-P-OP2	-5.64	111.14	119.60
32	1a	293	G	N7-C8-N9	5.64	115.92	113.10
1	2A	271(X)	G	C5-C6-O6	5.64	131.98	128.60
1	2A	685	A	O5'-P-OP1	-5.64	100.62	105.70
1	2A	1989	G	OP2-P-O3'	5.64	117.61	105.20
1	2A	2321	G	C8-N9-C4	-5.64	104.14	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	948	C	C2-N1-C1'	-5.64	112.60	118.80
1	1A	2748	G	N9-C4-C5	5.64	107.66	105.40
42	2k	118	GLY	N-CA-C	5.64	127.19	113.10
1	1A	399	G	O5'-P-OP2	-5.64	100.63	105.70
1	1A	585	U	OP1-P-OP2	5.64	128.05	119.60
1	1A	1397	C	N3-C4-C5	5.64	124.15	121.90
1	1A	1622	C	C6-N1-C2	-5.64	118.05	120.30
1	1A	1857	G	N1-C6-O6	-5.64	116.52	119.90
1	1A	2009	G	N3-C2-N2	-5.64	115.95	119.90
1	1A	2443	U	C5-C4-O4	5.64	129.28	125.90
1	1A	2593	G	C5-N7-C8	-5.64	101.48	104.30
32	1a	78	G	N3-C2-N2	-5.64	115.95	119.90
32	1a	831	U	N3-C4-O4	5.64	123.34	119.40
1	2A	1904	G	O5'-P-OP2	-5.64	100.63	105.70
32	2a	1052	U	N1-C2-O2	5.64	126.75	122.80
32	2a	1442(A)	G	N1-C6-O6	5.64	123.28	119.90
1	1A	1071	G	C4-C5-N7	-5.63	108.55	110.80
1	1A	1193	C	C5-C6-N1	-5.63	118.18	121.00
1	1A	1579	C	C6-N1-C2	-5.63	118.05	120.30
1	1A	1669	G	N7-C8-N9	-5.63	110.28	113.10
1	1A	1996	C	C4-C5-C6	5.63	120.22	117.40
1	2A	2589	A	C8-N9-C4	5.63	108.05	105.80
1	2A	2708	G	N3-C2-N2	5.63	123.84	119.90
1	2A	2789	C	O5'-P-OP2	-5.63	100.63	105.70
32	2a	504	C	C5-C6-N1	5.63	123.82	121.00
32	2a	670	G	C5-C6-O6	5.63	131.98	128.60
1	1A	1809	U	C5-C4-O4	-5.63	122.52	125.90
1	1A	2319	G	C4-C5-N7	5.63	113.05	110.80
32	1a	899	C	N3-C2-O2	5.63	125.84	121.90
32	2a	246	A	O5'-P-OP2	-5.63	100.63	105.70
1	1A	2250	G	OP1-P-OP2	5.63	128.05	119.60
1	1A	2609	G	N3-C4-N9	-5.63	122.62	126.00
32	1a	383	A	O4'-C1'-N9	5.63	112.70	108.20
32	1a	1200	C	OP1-P-O3'	5.63	117.59	105.20
1	2A	1345	C	C6-N1-C2	5.63	122.55	120.30
1	2A	1660	C	C4-C5-C6	5.63	120.22	117.40
1	2A	1863	G	C2-N3-C4	-5.63	109.08	111.90
1	2A	1963	U	O5'-P-OP1	-5.63	100.63	105.70
32	2a	1137	C	N3-C4-C5	-5.63	119.65	121.90
1	1A	2553	A	OP1-P-OP2	5.63	128.04	119.60
2	1B	19	G	O5'-P-OP2	-5.63	100.63	105.70
32	1a	266	G	C4-C5-N7	5.63	113.05	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2506	U	O4'-C1'-N1	5.63	112.70	108.20
1	1A	369	A	N1-C6-N6	5.63	121.98	118.60
1	1A	1701	A	C8-N9-C4	5.63	108.05	105.80
1	1A	2423	A	C5-N7-C8	-5.63	101.08	103.90
1	2A	1926	U	C6-N1-C1'	5.63	129.08	121.20
32	2a	357	G	N9-C4-C5	5.63	107.65	105.40
32	2a	926	G	OP1-P-OP2	5.63	128.04	119.60
32	2a	1027	C	C6-N1-C2	-5.63	118.05	120.30
1	1A	69	G	N1-C6-O6	-5.63	116.52	119.90
1	1A	733	G	O5'-P-OP1	-5.63	100.64	105.70
1	1A	840	A	C2-N3-C4	-5.63	107.79	110.60
1	1A	1181	G	N9-C4-C5	-5.63	103.15	105.40
1	1A	1249	A	C5-N7-C8	-5.63	101.09	103.90
1	1A	1853	G	N1-C6-O6	-5.63	116.52	119.90
1	2A	906	G	C8-N9-C4	-5.63	104.15	106.40
1	1A	1057	G	OP2-P-O3'	5.62	117.58	105.20
32	1a	860	A	N7-C8-N9	5.62	116.61	113.80
1	2A	1207	C	N3-C2-O2	5.62	125.84	121.90
1	1A	115	G	N1-C2-N2	-5.62	111.14	116.20
1	1A	789	G	OP2-P-O3'	5.62	117.57	105.20
1	1A	2573	A	N1-C2-N3	5.62	132.11	129.30
2	1B	90	A	C8-N9-C4	5.62	108.05	105.80
1	1A	985	G	N3-C4-N9	5.62	129.37	126.00
1	1A	2071	G	C4-C5-N7	5.62	113.05	110.80
32	1a	903	G	C5-N7-C8	5.62	107.11	104.30
32	1a	1030(C)	G	N3-C4-C5	-5.62	125.79	128.60
1	2A	90	U	N3-C2-O2	-5.62	118.27	122.20
1	2A	600	G	O5'-P-OP2	5.62	117.45	110.70
1	2A	1074	G	C8-N9-C1'	5.62	134.31	127.00
1	2A	2057	A	N9-C4-C5	-5.62	103.55	105.80
32	2a	334	C	C6-N1-C2	5.62	122.55	120.30
32	2a	819	A	N9-C4-C5	-5.62	103.55	105.80
1	1A	1966	U	N1-C2-O2	5.62	126.73	122.80
12	1Q	42	ILE	CG1-CB-CG2	-5.62	99.04	111.40
1	2A	2002	G	C8-N9-C4	5.62	108.65	106.40
1	2A	2035	G	N3-C2-N2	-5.62	115.97	119.90
1	1A	201	G	N3-C4-C5	5.62	131.41	128.60
1	1A	533	G	OP1-P-O3'	5.62	117.56	105.20
1	1A	1010	C	N1-C2-O2	-5.62	115.53	118.90
1	1A	1356	G	O4'-C1'-N9	5.62	112.69	108.20
1	1A	2091	G	C5-N7-C8	5.62	107.11	104.30
1	1A	2383	G	C4-C5-N7	5.62	113.05	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	106	G	C5-C6-O6	-5.62	125.23	128.60
1	2A	1287	A	OP1-P-OP2	-5.62	111.17	119.60
1	2A	2032	G	N7-C8-N9	-5.62	110.29	113.10
1	2A	860	U	C5-C4-O4	5.62	129.27	125.90
32	1a	769	G	OP1-P-OP2	-5.62	111.18	119.60
1	2A	2008	C	C5-C6-N1	-5.62	118.19	121.00
11	2P	148	LEU	CA-CB-CG	5.62	128.21	115.30
32	2a	32	A	N3-C4-C5	-5.62	122.87	126.80
1	1A	56	C	O5'-P-OP2	-5.61	100.65	105.70
1	1A	400	U	N3-C4-O4	-5.61	115.47	119.40
1	1A	578	U	OP1-P-OP2	5.61	128.02	119.60
1	1A	760	G	C6-C5-N7	-5.61	127.03	130.40
1	1A	2587	C	O5'-P-OP1	5.61	117.44	110.70
1	1A	2649	U	N3-C2-O2	-5.61	118.27	122.20
2	1B	104	U	OP2-P-O3'	5.61	117.55	105.20
1	2A	353	G	C6-C5-N7	-5.61	127.03	130.40
1	1A	2093	A	C6-C5-N7	-5.61	128.37	132.30
1	2A	1045	A	C4-C5-N7	5.61	113.51	110.70
1	2A	2502	G	N1-C6-O6	-5.61	116.53	119.90
1	2A	2708	G	O5'-P-OP2	-5.61	100.65	105.70
1	1A	1310	G	N1-C6-O6	-5.61	116.53	119.90
1	1A	1679	A	C4-C5-C6	5.61	119.81	117.00
1	1A	2116	G	C5-C6-O6	5.61	131.97	128.60
1	1A	2294	G	O4'-C1'-N9	5.61	112.69	108.20
32	1a	369	C	C6-N1-C2	-5.61	118.06	120.30
32	1a	1184	G	C4-C5-N7	5.61	113.04	110.80
1	2A	1953	A	C2-N3-C4	-5.61	107.80	110.60
32	2a	240	C	N3-C4-C5	5.61	124.14	121.90
1	1A	1720	U	C2-N1-C1'	-5.61	110.97	117.70
1	2A	2476	A	N1-C6-N6	-5.61	115.23	118.60
1	1A	68	C	OP2-P-O3'	5.61	117.54	105.20
1	1A	422	U	N1-C2-O2	5.61	126.72	122.80
1	1A	1425	A	O4'-C1'-N9	-5.61	103.71	108.20
1	1A	2759	U	OP2-P-O3'	5.61	117.54	105.20
2	1B	36	C	N3-C2-O2	5.61	125.83	121.90
32	1a	474	G	C6-C5-N7	5.61	133.76	130.40
32	1a	1348	U	N3-C2-O2	-5.61	118.28	122.20
1	1A	181	C	N3-C2-O2	5.61	125.82	121.90
1	1A	315	C	N1-C2-O2	-5.61	115.54	118.90
1	1A	494	G	C4-C5-C6	5.61	122.16	118.80
1	1A	1784	G	C5-N7-C8	-5.61	101.50	104.30
1	1A	2505	U	OP2-P-O3'	5.61	117.53	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2624	C	N1-C2-O2	5.61	122.26	118.90
1	1A	2769	U	OP1-P-O3'	5.61	117.53	105.20
32	1a	170	U	OP1-P-O3'	5.61	117.53	105.20
1	2A	108	U	O5'-P-OP2	-5.61	100.66	105.70
32	2a	375	U	O5'-P-OP2	5.61	117.43	110.70
1	1A	592	U	C5-C6-N1	-5.60	119.90	122.70
1	1A	2474	U	C5-C6-N1	-5.60	119.90	122.70
32	1a	354	G	C4-N9-C1'	5.60	133.79	126.50
1	1A	23	G	N1-C6-O6	5.60	123.26	119.90
1	1A	101	A	C8-N9-C1'	-5.60	117.61	127.70
1	1A	2240	G	C5-C6-O6	5.60	131.96	128.60
2	1B	51	G	OP1-P-OP2	-5.60	111.20	119.60
1	2A	672	C	N3-C4-N4	-5.60	114.08	118.00
1	2A	1804	C	C4-C5-C6	-5.60	114.60	117.40
1	2A	2057	A	O5'-P-OP1	5.60	117.42	110.70
1	2A	2778	A	O5'-P-OP2	-5.60	100.66	105.70
32	2a	1515	C	C5-C6-N1	-5.60	118.20	121.00
1	1A	2561	G	N3-C4-C5	-5.60	125.80	128.60
32	1a	369	C	C5-C6-N1	5.60	123.80	121.00
1	1A	1325	G	C5-C6-O6	5.60	131.96	128.60
1	1A	1325	G	N3-C4-C5	-5.60	125.80	128.60
2	1B	118	G	N3-C4-C5	5.60	131.40	128.60
32	1a	830	G	O5'-P-OP2	5.60	117.42	110.70
1	2A	2388	A	O4'-C1'-N9	5.60	112.68	108.20
32	2a	1035	A	P-O3'-C3'	5.60	126.42	119.70
1	1A	182	U	N1-C2-N3	5.60	118.26	114.90
1	1A	621	G	OP2-P-O3'	5.60	117.51	105.20
1	1A	1234	A	C5-C6-N6	-5.60	119.22	123.70
1	1A	1755	C	C6-N1-C2	5.60	122.54	120.30
1	1A	2243	C	N1-C2-O2	-5.60	115.54	118.90
1	2A	2444	G	N1-C2-N3	5.60	127.26	123.90
32	2a	993	G	C2-N3-C4	5.60	114.70	111.90
32	2a	1024	G	N3-C2-N2	-5.60	115.98	119.90
1	1A	1255	A	OP2-P-O3'	5.60	117.51	105.20
1	1A	1622	C	N1-C2-O2	-5.60	115.54	118.90
32	1a	280	C	N1-C2-N3	-5.60	115.28	119.20
1	2A	1404	C	O5'-P-OP2	-5.60	100.66	105.70
32	2a	372	C	C5-C4-N4	-5.60	116.28	120.20
1	1A	1343	C	O5'-P-OP2	-5.59	100.67	105.70
1	1A	2062	C	C2-N3-C4	5.59	122.70	119.90
1	1A	2249	G	O5'-P-OP2	-5.59	100.67	105.70
1	1A	2529	C	N3-C4-N4	5.59	121.92	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2701	U	N3-C2-O2	-5.59	118.28	122.20
1	1A	2886	G	C5-C6-O6	-5.59	125.24	128.60
1	2A	1285	G	OP2-P-O3'	5.59	117.51	105.20
1	1A	1523	C	C6-N1-C2	-5.59	118.06	120.30
1	1A	1610	G	OP2-P-O3'	5.59	117.51	105.20
1	2A	1509(A)	A	C8-N9-C4	-5.59	103.56	105.80
1	2A	2564	A	N3-C4-N9	5.59	131.87	127.40
1	1A	786	G	OP1-P-O3'	5.59	117.50	105.20
1	1A	1662	A	OP1-P-O3'	5.59	117.50	105.20
1	1A	1824	C	C5-C6-N1	-5.59	118.20	121.00
1	1A	2240	G	N9-C4-C5	5.59	107.64	105.40
32	1a	1524	C	OP1-P-OP2	5.59	127.99	119.60
1	2A	2346	A	C6-N1-C2	-5.59	115.25	118.60
32	2a	1123	A	N1-C6-N6	-5.59	115.25	118.60
32	2a	1391	U	N3-C4-O4	-5.59	115.49	119.40
1	1A	543	G	OP1-P-OP2	5.59	127.98	119.60
1	1A	657	A	C5-N7-C8	-5.59	101.11	103.90
1	1A	1707	C	N3-C4-N4	-5.59	114.09	118.00
32	1a	773	G	N9-C4-C5	5.59	107.64	105.40
32	2a	402	G	C2-N3-C4	-5.59	109.11	111.90
32	2a	1023	G	N7-C8-N9	5.59	115.89	113.10
1	1A	293	C	OP2-P-O3'	5.59	117.49	105.20
1	1A	313	A	C5-C6-N1	-5.59	114.91	117.70
1	1A	1681	A	OP1-P-OP2	-5.59	111.22	119.60
1	1A	2612	A	O5'-P-OP2	-5.59	100.67	105.70
1	1A	2639	G	N7-C8-N9	-5.59	110.31	113.10
1	2A	113	G	C8-N9-C1'	5.59	134.26	127.00
1	2A	386	G	N1-C6-O6	-5.59	116.55	119.90
1	2A	2207	G	C5-N7-C8	-5.59	101.51	104.30
1	1A	2063	U	N1-C2-N3	5.59	118.25	114.90
1	1A	2832	G	OP1-P-OP2	-5.59	111.22	119.60
2	1B	75	G	C5-C6-N1	5.59	114.29	111.50
32	1a	174	C	N3-C2-O2	-5.59	117.99	121.90
1	2A	1064	C	C6-N1-C2	-5.59	118.07	120.30
1	1A	1378	G	C2-N3-C4	-5.58	109.11	111.90
1	1A	1425	A	C4-C5-C6	-5.58	114.21	117.00
2	1B	1	U	N1-C2-N3	-5.58	111.55	114.90
1	2A	1091	G	O3'-P-O5'	5.58	114.61	104.00
1	2A	2560	C	O5'-P-OP1	-5.58	100.67	105.70
1	1A	596	G	C6-N1-C2	-5.58	121.75	125.10
1	1A	618	C	C5-C4-N4	-5.58	116.29	120.20
1	1A	2310	A	C8-N9-C4	5.58	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	144	G	C8-N9-C4	-5.58	104.17	106.40
32	1a	1030(D)	A	N7-C8-N9	5.58	116.59	113.80
1	2A	1802	A	N9-C4-C5	-5.58	103.57	105.80
32	2a	1442	G	N3-C4-C5	-5.58	125.81	128.60
1	1A	709	G	N1-C6-O6	-5.58	116.55	119.90
32	1a	550	G	N3-C2-N2	-5.58	115.99	119.90
1	2A	323	G	N1-C6-O6	5.58	123.25	119.90
1	2A	1076	C	OP1-P-O3'	5.58	117.48	105.20
1	2A	1123	C	C6-N1-C2	5.58	122.53	120.30
1	2A	2223	G	OP2-P-O3'	5.58	117.48	105.20
32	2a	1261	A	N1-C6-N6	5.58	121.95	118.60
1	1A	533	G	N9-C4-C5	5.58	107.63	105.40
1	1A	1809	U	C6-N1-C2	5.58	124.35	121.00
1	1A	2111	U	C2-N3-C4	-5.58	123.65	127.00
1	1A	2633	A	C8-N9-C4	-5.58	103.57	105.80
32	1a	113	G	C5-C6-O6	5.58	131.95	128.60
32	1a	722	A	C2-N3-C4	-5.58	107.81	110.60
32	1a	1452	C	C2-N1-C1'	-5.58	112.66	118.80
1	2A	645	C	C2-N1-C1'	5.58	124.94	118.80
1	1A	461	U	C2-N3-C4	-5.58	123.65	127.00
1	1A	566	C	N3-C4-C5	5.58	124.13	121.90
1	1A	1043	G	N1-C2-N2	-5.58	111.18	116.20
1	1A	1095	C	O5'-P-OP2	-5.58	100.68	105.70
1	1A	1392	G	C5-N7-C8	5.58	107.09	104.30
1	1A	2438	A	N1-C2-N3	5.58	132.09	129.30
1	1A	2784	C	C2-N3-C4	-5.58	117.11	119.90
1	1A	2797	C	C5-C4-N4	-5.58	116.30	120.20
1	1A	702	A	N3-C4-N9	-5.58	122.94	127.40
1	1A	872	C	OP2-P-O3'	5.58	117.47	105.20
1	1A	1814	A	N1-C6-N6	-5.58	115.25	118.60
1	1A	11	G	C4-N9-C1'	-5.58	119.25	126.50
1	1A	608	G	N1-C6-O6	5.58	123.25	119.90
1	1A	781	A	C5-C6-N1	-5.58	114.91	117.70
1	1A	1018	A	C2-N3-C4	-5.58	107.81	110.60
1	1A	1307	C	N3-C4-C5	5.58	124.13	121.90
1	1A	1621	C	N3-C4-C5	5.58	124.13	121.90
1	1A	1715	A	O5'-P-OP2	-5.58	100.68	105.70
1	1A	2611	G	N3-C2-N2	5.58	123.80	119.90
1	2A	1573	G	N3-C4-N9	-5.58	122.66	126.00
1	2A	2502	G	C4'-C3'-O3'	5.58	124.15	113.00
1	1A	358	C	N1-C2-O2	-5.57	115.56	118.90
1	1A	968	U	O5'-P-OP2	-5.57	100.68	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1198	C	OP1-P-OP2	-5.57	111.24	119.60
1	1A	2125	C	C5-C6-N1	5.57	123.79	121.00
1	1A	2523	U	C4-C5-C6	5.57	123.05	119.70
2	1B	31	C	OP2-P-O3'	5.57	117.46	105.20
1	2A	1320	C	OP1-P-OP2	5.57	127.96	119.60
1	2A	1757	U	C6-N1-C2	5.57	124.34	121.00
1	2A	1929	G	O5'-P-OP2	-5.57	100.68	105.70
1	2A	2810	A	N1-C6-N6	5.57	121.94	118.60
32	2a	305	G	O5'-P-OP2	-5.57	100.68	105.70
32	2a	898	G	N7-C8-N9	-5.57	110.31	113.10
1	1A	38	A	N1-C6-N6	-5.57	115.26	118.60
1	1A	494	G	C4-C5-N7	-5.57	108.57	110.80
1	1A	1365	G	OP2-P-O3'	5.57	117.46	105.20
1	1A	1566	U	O5'-P-OP2	-5.57	100.69	105.70
1	1A	2264	G	C6-C5-N7	-5.57	127.06	130.40
1	1A	366	G	O5'-P-OP2	-5.57	100.69	105.70
1	1A	1981	G	N7-C8-N9	-5.57	110.31	113.10
1	1A	2054	G	O4'-C1'-N9	-5.57	103.74	108.20
32	1a	575	G	C4-C5-N7	-5.57	108.57	110.80
32	1a	1467	G	N9-C4-C5	5.57	107.63	105.40
1	2A	2301	C	C6-N1-C2	-5.57	118.07	120.30
1	2A	2476	A	N9-C4-C5	5.57	108.03	105.80
32	2a	353	A	OP2-P-O3'	5.57	117.45	105.20
32	2a	795	C	N3-C2-O2	-5.57	118.00	121.90
2	1B	113	G	N1-C6-O6	5.57	123.24	119.90
32	1a	1424	C	O5'-P-OP2	-5.57	100.69	105.70
1	2A	517	C	C5-C4-N4	-5.57	116.30	120.20
1	2A	1787	A	O5'-P-OP1	-5.57	100.69	105.70
1	2A	2427	C	N1-C2-O2	-5.57	115.56	118.90
1	2A	2508	G	N3-C4-N9	5.57	129.34	126.00
1	1A	189	U	C2-N3-C4	-5.57	123.66	127.00
1	1A	220	C	C4-C5-C6	5.57	120.18	117.40
1	1A	1051	C	N1-C2-O2	5.57	122.24	118.90
1	1A	1310	G	N3-C2-N2	5.57	123.80	119.90
1	1A	1543	U	C5-C6-N1	-5.57	119.92	122.70
1	1A	2033	U	C4-C5-C6	5.57	123.04	119.70
1	1A	2837	C	N1-C2-O2	-5.57	115.56	118.90
32	1a	615	C	C5-C6-N1	5.57	123.78	121.00
1	2A	216	A	O5'-P-OP1	-5.57	100.69	105.70
1	2A	951	C	OP1-P-OP2	-5.57	111.25	119.60
1	2A	1586	A	O5'-P-OP2	5.57	117.38	110.70
1	2A	2347	C	N3-C2-O2	-5.57	118.00	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	271	C	C6-N1-C2	-5.57	118.07	120.30
1	1A	331	G	O5'-P-OP2	-5.57	100.69	105.70
1	1A	846	G	OP2-P-O3'	5.57	117.44	105.20
32	1a	1527	C	C4-C5-C6	5.57	120.18	117.40
1	2A	482	A	OP1-P-OP2	-5.57	111.25	119.60
1	2A	950	G	OP2-P-O3'	5.57	117.44	105.20
1	2A	1934	C	C5-C6-N1	-5.57	118.22	121.00
32	2a	1394	A	N1-C6-N6	5.57	121.94	118.60
1	1A	234	G	N1-C6-O6	5.56	123.24	119.90
1	1A	2834	C	C2-N3-C4	5.56	122.68	119.90
32	1a	906	G	OP1-P-OP2	5.56	127.95	119.60
1	1A	1813	C	N1-C2-O2	-5.56	115.56	118.90
1	1A	2176	G	C8-N9-C1'	5.56	134.23	127.00
1	1A	2507	G	C2-N3-C4	-5.56	109.12	111.90
1	1A	2695	C	O5'-P-OP1	5.56	117.37	110.70
1	1A	2774	G	N3-C2-N2	-5.56	116.01	119.90
32	1a	774	G	OP2-P-O3'	5.56	117.44	105.20
32	1a	817	C	C6-N1-C2	5.56	122.53	120.30
1	2A	1602	U	C6-N1-C2	5.56	124.34	121.00
1	2A	2555	U	C5-C6-N1	-5.56	119.92	122.70
1	1A	82	G	N3-C4-C5	5.56	131.38	128.60
1	1A	537	G	OP2-P-O3'	5.56	117.43	105.20
1	1A	1814	A	C6-C5-N7	5.56	136.19	132.30
32	1a	346	G	C4-C5-N7	-5.56	108.58	110.80
1	1A	624	C	C4-C5-C6	5.56	120.18	117.40
1	1A	2626	A	C2-N3-C4	5.56	113.38	110.60
14	1S	59	LYS	N-CA-C	5.56	126.01	111.00
32	1a	168	G	N3-C2-N2	5.56	123.79	119.90
1	2A	958	U	C4-C5-C6	5.56	123.03	119.70
1	2A	1934	C	N3-C4-C5	5.56	124.12	121.90
1	2A	2073	C	N3-C2-O2	5.56	125.79	121.90
1	2A	2576	G	O5'-P-OP2	5.56	117.37	110.70
1	1A	535	C	C6-N1-C2	-5.56	118.08	120.30
1	1A	993	G	O5'-P-OP1	-5.56	100.70	105.70
1	1A	1377	A	N9-C4-C5	5.56	108.02	105.80
1	1A	1683	C	C6-N1-C2	5.56	122.52	120.30
1	1A	2295	C	N3-C4-C5	5.56	124.12	121.90
1	1A	2467	G	N1-C2-N2	-5.56	111.20	116.20
32	1a	913	A	N9-C4-C5	5.56	108.02	105.80
32	1a	984	C	C6-N1-C2	5.56	122.52	120.30
1	2A	459	U	N1-C2-O2	5.56	126.69	122.80
1	2A	1087	G	N9-C4-C5	5.56	107.62	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1776	G	C4-C5-N7	5.56	113.02	110.80
1	2A	1835	G	N3-C4-N9	5.56	129.33	126.00
1	2A	2252	G	N3-C2-N2	5.56	123.79	119.90
32	2a	914	A	C4-C5-N7	-5.56	107.92	110.70
1	1A	765	A	C2-N3-C4	-5.56	107.82	110.60
1	1A	964	A	OP2-P-O3'	5.56	117.42	105.20
1	1A	1070	G	C8-N9-C4	5.56	108.62	106.40
1	1A	1282	G	C4-C5-C6	-5.56	115.47	118.80
1	1A	2375	C	N3-C4-C5	5.56	124.12	121.90
1	1A	2852	G	C4-C5-N7	-5.56	108.58	110.80
1	2A	26	G	C5-C6-O6	-5.56	125.27	128.60
1	1A	115	G	C8-N9-C4	5.55	108.62	106.40
1	1A	1019	G	C8-N9-C4	-5.55	104.18	106.40
1	1A	1063	G	C8-N9-C4	-5.55	104.18	106.40
1	1A	2580	C	OP2-P-O3'	5.55	117.42	105.20
32	1a	360	A	OP1-P-O3'	5.55	117.42	105.20
32	1a	1521	G	C5-C6-O6	-5.55	125.27	128.60
1	2A	386	G	C5-C6-N1	5.55	114.28	111.50
1	2A	671	C	C2-N1-C1'	-5.55	112.69	118.80
1	1A	426	G	C8-N9-C4	5.55	108.62	106.40
1	1A	1453	C	N1-C2-O2	-5.55	115.57	118.90
1	1A	198	C	C5-C4-N4	-5.55	116.31	120.20
1	1A	601	A	N1-C2-N3	5.55	132.08	129.30
1	1A	1456	G	C8-N9-C4	5.55	108.62	106.40
1	1A	1837	C	C2-N1-C1'	-5.55	112.69	118.80
1	1A	2051	G	N1-C6-O6	5.55	123.23	119.90
1	1A	2069	U	C2-N1-C1'	5.55	124.36	117.70
32	1a	781	A	OP2-P-O3'	5.55	117.41	105.20
1	2A	743	G	N1-C6-O6	-5.55	116.57	119.90
1	2A	745	G	OP1-P-OP2	-5.55	111.27	119.60
1	2A	2410	G	OP1-P-O3'	5.55	117.41	105.20
32	2a	306	G	OP2-P-O3'	5.55	117.41	105.20
1	1A	197	C	O5'-P-OP2	5.55	117.36	110.70
1	1A	414	U	N3-C4-O4	5.55	123.28	119.40
1	1A	490	U	C5-C6-N1	-5.55	119.92	122.70
1	1A	903	C	O5'-P-OP1	-5.55	100.70	105.70
1	1A	1014	U	C5-C4-O4	-5.55	122.57	125.90
1	1A	1543	U	C2-N3-C4	-5.55	123.67	127.00
1	1A	2520	G	C6-N1-C2	-5.55	121.77	125.10
1	1A	2897	U	OP1-P-OP2	5.55	127.92	119.60
2	1B	47	C	C6-N1-C2	5.55	122.52	120.30
1	2A	15	G	N9-C1'-C2'	-5.55	105.90	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	271(X)	G	C2-N3-C4	-5.55	109.13	111.90
1	2A	1644	C	C6-N1-C2	-5.55	118.08	120.30
1	1A	705	C	C6-N1-C1'	-5.55	114.14	120.80
1	1A	1358	U	C5-C6-N1	-5.55	119.93	122.70
1	1A	2388	A	C8-N9-C4	5.55	108.02	105.80
32	1a	852	G	OP2-P-O3'	5.55	117.40	105.20
1	2A	2334	G	N3-C4-N9	5.55	129.33	126.00
32	2a	691	G	N9-C4-C5	-5.55	103.18	105.40
32	2a	824	C	C4-C5-C6	5.55	120.17	117.40
1	1A	1821	C	P-O3'-C3'	5.54	126.35	119.70
1	1A	1876	G	N1-C2-N3	5.54	127.23	123.90
1	2A	149	A	N9-C4-C5	-5.54	103.58	105.80
1	2A	2629	A	C6-N1-C2	5.54	121.93	118.60
32	2a	1033	G	N3-C4-C5	5.54	131.37	128.60
1	1A	1463	C	C6-N1-C2	5.54	122.52	120.30
1	1A	2341	G	C5-C6-O6	-5.54	125.27	128.60
1	1A	2585	C	N3-C2-O2	5.54	125.78	121.90
1	1A	2835	C	N1-C2-O2	-5.54	115.57	118.90
2	1B	80	U	N3-C4-C5	5.54	117.93	114.60
32	1a	1021	G	N3-C2-N2	5.54	123.78	119.90
1	2A	1493	C	C5-C6-N1	-5.54	118.23	121.00
1	2A	2652	C	O5'-P-OP2	-5.54	100.71	105.70
32	2a	174	C	N3-C2-O2	-5.54	118.02	121.90
1	1A	356	A	O5'-P-OP1	-5.54	100.71	105.70
1	1A	1075	A	C6-C5-N7	-5.54	128.42	132.30
1	1A	1708	G	N3-C2-N2	-5.54	116.02	119.90
1	1A	2574	U	N3-C2-O2	-5.54	118.32	122.20
32	1a	46	G	O5'-P-OP2	5.54	117.35	110.70
1	2A	1017	G	N3-C2-N2	-5.54	116.02	119.90
1	2A	2206	G	C8-N9-C4	5.54	108.62	106.40
1	2A	2807	G	C5-C6-O6	5.54	131.93	128.60
1	2A	2082	A	C5-C6-N6	-5.54	119.27	123.70
1	2A	2168	G	C8-N9-C4	-5.54	104.18	106.40
2	2B	73	A	C8-N9-C4	5.54	108.02	105.80
1	1A	424	G	N1-C2-N2	-5.54	111.22	116.20
1	1A	1104	G	C8-N9-C4	5.54	108.61	106.40
1	1A	1343	C	N1-C2-O2	-5.54	115.58	118.90
1	1A	2073	A	N1-C2-N3	5.54	132.07	129.30
1	1A	2241	C	C5-C6-N1	5.54	123.77	121.00
1	2A	314	A	N1-C6-N6	-5.54	115.28	118.60
1	2A	754	C	N3-C2-O2	5.54	125.78	121.90
1	1A	1652	G	N3-C2-N2	-5.54	116.02	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2346	G	N1-C2-N2	-5.54	111.22	116.20
1	1A	2656	G	OP1-P-OP2	-5.54	111.29	119.60
32	1a	1096	C	C6-N1-C2	-5.54	118.08	120.30
1	2A	1903	G	N3-C2-N2	-5.54	116.02	119.90
1	2A	2596	U	C2-N3-C4	-5.54	123.68	127.00
6	2G	3	LEU	CA-CB-CG	5.54	128.03	115.30
1	1A	89	U	N3-C4-O4	-5.54	115.53	119.40
1	1A	1079	U	N3-C4-C5	5.54	117.92	114.60
1	1A	1247	C	N1-C2-O2	-5.54	115.58	118.90
1	1A	1270	C	C2-N1-C1'	-5.54	112.71	118.80
1	1A	1995	G	C6-C5-N7	5.54	133.72	130.40
1	1A	2044	U	O5'-P-OP1	-5.54	100.72	105.70
32	1a	740	U	OP1-P-OP2	5.54	127.90	119.60
1	1A	2376	C	C2-N1-C1'	-5.53	112.71	118.80
1	1A	2434	A	C5-C6-N1	-5.53	114.93	117.70
2	1B	39	A	N1-C6-N6	-5.53	115.28	118.60
1	2A	2140	C	C6-N1-C2	-5.53	118.09	120.30
1	2A	2685	G	C5-C6-O6	5.53	131.92	128.60
32	2a	397	A	C4-C5-C6	5.53	119.77	117.00
1	1A	415	G	N3-C2-N2	5.53	123.77	119.90
1	2A	1051	G	O5'-P-OP1	-5.53	100.72	105.70
32	2a	848	C	C6-N1-C2	-5.53	118.09	120.30
1	1A	448	U	N1-C2-O2	-5.53	118.93	122.80
1	1A	969	C	O5'-P-OP1	-5.53	100.72	105.70
1	1A	1958	A	C5-N7-C8	-5.53	101.14	103.90
1	1A	2155	G	C6-C5-N7	5.53	133.72	130.40
1	1A	2258	G	C5-C6-O6	-5.53	125.28	128.60
1	1A	2395	G	N3-C4-N9	-5.53	122.68	126.00
1	1A	2633	A	OP2-P-O3'	5.53	117.37	105.20
2	1B	23	G	O5'-P-OP1	-5.53	100.72	105.70
32	1a	756	C	C6-N1-C2	5.53	122.51	120.30
1	2A	1597	A	N9-C4-C5	5.53	108.01	105.80
32	2a	38	G	C8-N9-C4	5.53	108.61	106.40
1	1A	514	G	N9-C4-C5	5.53	107.61	105.40
1	1A	739	C	OP2-P-O3'	5.53	117.36	105.20
1	1A	1434	G	N1-C2-N2	-5.53	111.22	116.20
1	1A	2480	G	N3-C4-C5	-5.53	125.83	128.60
32	1a	577	G	C5-C6-O6	5.53	131.92	128.60
32	1a	804	U	C6-N1-C2	-5.53	117.68	121.00
1	2A	383	U	N3-C4-C5	-5.53	111.28	114.60
1	2A	2094	G	OP2-P-O3'	5.53	117.36	105.20
1	1A	234	G	OP1-P-O3'	5.53	117.36	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	285	U	OP1-P-O3'	5.53	117.36	105.20
1	1A	1792	C	OP2-P-O3'	5.53	117.36	105.20
1	1A	2652	G	C5-N7-C8	5.53	107.06	104.30
32	1a	1521	G	N1-C6-O6	5.53	123.22	119.90
1	2A	1640	C	O4'-C1'-N1	-5.53	103.78	108.20
1	2A	2012	G	C2-N3-C4	-5.53	109.14	111.90
32	2a	19	C	N1-C2-O2	-5.53	115.58	118.90
32	2a	1502	A	O5'-P-OP2	-5.53	100.72	105.70
1	1A	189	U	N1-C2-N3	5.53	118.22	114.90
1	1A	1179	U	N1-C2-O2	-5.53	118.93	122.80
1	1A	2203	G	C4-N9-C1'	-5.53	119.32	126.50
1	1A	2561	G	N1-C6-O6	5.53	123.22	119.90
1	1A	2568	C	C5-C4-N4	-5.53	116.33	120.20
1	1A	2642	G	N1-C6-O6	5.53	123.22	119.90
32	1a	1041	A	O4'-C1'-N9	5.53	112.62	108.20
1	1A	309	C	C5-C6-N1	-5.52	118.24	121.00
1	1A	505	A	O4'-C1'-N9	5.52	112.62	108.20
1	1A	1079	U	C2-N3-C4	-5.52	123.69	127.00
32	1a	949	A	C8-N9-C4	-5.52	103.59	105.80
1	2A	271(L)	U	C5-C6-N1	5.52	125.46	122.70
1	2A	1597	A	C2-N3-C4	-5.52	107.84	110.60
1	2A	2499	C	N3-C4-N4	5.52	121.86	118.00
32	2a	1082	G	N3-C4-C5	5.52	131.36	128.60
32	2a	1149	C	C5-C6-N1	5.52	123.76	121.00
1	1A	715	G	C2-N3-C4	-5.52	109.14	111.90
1	1A	1598	C	C6-N1-C2	-5.52	118.09	120.30
1	1A	2176	G	C6-C5-N7	5.52	133.71	130.40
1	1A	2598	C	N3-C4-N4	5.52	121.86	118.00
2	1B	6	C	O5'-P-OP2	-5.52	100.73	105.70
32	1a	78	G	N1-C2-N2	5.52	121.17	116.20
1	2A	788	A	C6-C5-N7	-5.52	128.44	132.30
1	2A	1393	A	C5-C6-N1	5.52	120.46	117.70
1	2A	1501	C	N1-C2-O2	-5.52	115.59	118.90
1	2A	1826	G	N3-C4-C5	-5.52	125.84	128.60
32	2a	1401	G	C8-N9-C4	5.52	108.61	106.40
1	1A	116	A	N9-C4-C5	5.52	108.01	105.80
1	1A	1850	A	C5-C6-N6	5.52	128.12	123.70
1	1A	2073	A	C4-C5-N7	-5.52	107.94	110.70
32	1a	134	A	C8-N9-C4	5.52	108.01	105.80
32	1a	552	U	C5-C6-N1	-5.52	119.94	122.70
32	1a	1505	G	C8-N9-C4	-5.52	104.19	106.40
1	2A	186	G	N1-C2-N2	5.52	121.17	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	798	G	C5-C6-O6	5.52	131.91	128.60
1	2A	1692	U	OP1-P-OP2	5.52	127.88	119.60
1	1A	1070	G	N1-C6-O6	5.52	123.21	119.90
1	2A	794	G	C2-N3-C4	-5.52	109.14	111.90
1	2A	1660	C	C5-C6-N1	-5.52	118.24	121.00
1	2A	1804	C	OP1-P-O3'	5.52	117.34	105.20
32	2a	353	A	C5-N7-C8	-5.52	101.14	103.90
32	2a	357	G	C4-C5-N7	-5.52	108.59	110.80
32	2a	1501	C	C5-C6-N1	-5.52	118.24	121.00
1	2A	622	G	N7-C8-N9	-5.52	110.34	113.10
1	2A	1473	G	N3-C4-N9	5.52	129.31	126.00
1	2A	1913	A	C4-C5-C6	5.52	119.76	117.00
1	1A	1372	U	N3-C2-O2	-5.51	118.34	122.20
32	1a	577	G	C2-N3-C4	-5.51	109.14	111.90
1	1A	1514	C	O5'-P-OP1	-5.51	100.74	105.70
1	1A	1629	C	C5-C6-N1	-5.51	118.24	121.00
1	2A	331	A	C4-C5-N7	-5.51	107.94	110.70
32	2a	395	C	OP1-P-OP2	5.51	127.87	119.60
1	1A	359	C	C2-N3-C4	5.51	122.66	119.90
1	1A	2078	G	C5-N7-C8	-5.51	101.54	104.30
1	1A	2565	G	N1-C6-O6	-5.51	116.59	119.90
1	1A	2584	A	C6-N1-C2	-5.51	115.29	118.60
1	1A	2671	G	N3-C2-N2	-5.51	116.04	119.90
1	1A	2832	G	C5-C6-O6	-5.51	125.29	128.60
32	1a	92	C	O4'-C1'-N1	5.51	112.61	108.20
32	1a	809	G	C2-N3-C4	-5.51	109.14	111.90
1	2A	297	C	N1-C2-O2	5.51	122.21	118.90
1	2A	852	G	N1-C6-O6	-5.51	116.59	119.90
1	2A	1416	G	C8-N9-C4	5.51	108.61	106.40
32	2a	869	G	C2-N3-C4	-5.51	109.14	111.90
32	2a	948	C	C6-N1-C2	5.51	122.50	120.30
1	1A	2017	U	C5-C6-N1	-5.51	119.95	122.70
32	1a	926	G	N9-C4-C5	5.51	107.60	105.40
1	2A	97	C	N3-C4-N4	-5.51	114.14	118.00
1	2A	697	C	N3-C4-C5	-5.51	119.70	121.90
1	2A	1119	C	C5-C4-N4	5.51	124.06	120.20
32	2a	189(I)	G	N1-C6-O6	-5.51	116.59	119.90
32	2a	498	U	C5-C4-O4	5.51	129.21	125.90
1	1A	1816	A	N1-C6-N6	5.51	121.91	118.60
1	1A	2685	G	C5-C6-O6	5.51	131.91	128.60
1	1A	2840	G	O5'-P-OP2	-5.51	100.74	105.70
1	2A	2037	G	C5-C6-O6	5.51	131.91	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	15	G	C5-C6-O6	-5.51	125.30	128.60
1	2A	271(H)	G	O5'-P-OP2	-5.51	100.74	105.70
1	2A	1159	U	O5'-P-OP2	-5.51	100.74	105.70
1	1A	1959	A	N9-C4-C5	5.50	108.00	105.80
1	2A	1557	C	O5'-P-OP2	-5.50	100.75	105.70
1	2A	2042	A	N7-C8-N9	-5.50	111.05	113.80
1	2A	2463	C	O5'-P-OP2	-5.50	100.75	105.70
32	2a	7	G	C2-N3-C4	-5.50	109.15	111.90
1	1A	38	A	N7-C8-N9	-5.50	111.05	113.80
1	1A	258	U	C6-N1-C2	5.50	124.30	121.00
1	1A	2073	A	C4-C5-C6	5.50	119.75	117.00
2	1B	36	C	C6-N1-C2	5.50	122.50	120.30
2	1B	41	U	N3-C2-O2	-5.50	118.35	122.20
32	1a	1287	A	C6-N1-C2	5.50	121.90	118.60
1	2A	1274	A	OP1-P-OP2	5.50	127.85	119.60
32	2a	697	U	C6-N1-C2	5.50	124.30	121.00
1	1A	177	G	N1-C6-O6	-5.50	116.60	119.90
1	1A	1148	C	C5-C6-N1	5.50	123.75	121.00
1	1A	1294	G	C5-C6-N1	-5.50	108.75	111.50
1	1A	1549	U	O5'-P-OP2	-5.50	100.75	105.70
1	2A	450	G	O5'-P-OP2	-5.50	100.75	105.70
1	2A	1638	C	C6-N1-C2	5.50	122.50	120.30
1	2A	1905	C	O5'-P-OP2	-5.50	100.75	105.70
1	2A	2866	U	C5-C4-O4	5.50	129.20	125.90
1	1A	554	A	C5-C6-N1	5.50	120.45	117.70
1	1A	1823	G	N7-C8-N9	-5.50	110.35	113.10
1	1A	2383	G	N1-C2-N3	-5.50	120.60	123.90
1	2A	2579	C	C5-C6-N1	5.50	123.75	121.00
1	1A	241	G	C8-N9-C4	-5.50	104.20	106.40
1	1A	727	G	N7-C8-N9	5.50	115.85	113.10
1	1A	1830	G	C5-N7-C8	5.50	107.05	104.30
2	1B	65	C	C6-N1-C2	5.50	122.50	120.30
32	1a	697	U	C5-C6-N1	-5.50	119.95	122.70
1	2A	1577	C	O5'-P-OP2	-5.50	100.75	105.70
1	1A	1242	G	C8-N9-C1'	5.50	134.15	127.00
1	1A	2027	A	N7-C8-N9	-5.50	111.05	113.80
1	2A	123	G	C5-C6-O6	-5.50	125.30	128.60
1	2A	1063	G	C2-N3-C4	5.50	114.65	111.90
1	2A	2522	U	OP1-P-OP2	5.50	127.85	119.60
2	2B	54	G	C8-N9-C4	-5.50	104.20	106.40
1	1A	740	C	C5-C6-N1	-5.50	118.25	121.00
1	1A	1256	U	O5'-P-OP2	5.50	117.29	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1828	C	C2-N3-C4	-5.50	117.15	119.90
1	2A	718	A	C5-C6-N6	-5.50	119.30	123.70
1	2A	1551	C	OP2-P-O3'	5.50	117.29	105.20
1	1A	82	G	N3-C4-N9	5.49	129.30	126.00
1	1A	102	U	C2-N3-C4	-5.49	123.70	127.00
1	1A	952	G	C8-N9-C1'	5.49	134.14	127.00
1	1A	1221	G	OP1-P-O3'	5.49	117.29	105.20
1	1A	2075	G	N3-C2-N2	-5.49	116.05	119.90
32	1a	669	U	OP2-P-O3'	5.49	117.29	105.20
32	1a	1210	C	C6-N1-C2	5.49	122.50	120.30
1	2A	12	U	N1-C2-O2	5.49	126.65	122.80
1	2A	1610	A	N9-C4-C5	-5.49	103.60	105.80
1	2A	1904	G	C6-C5-N7	5.49	133.70	130.40
2	2B	24	G	C6-N1-C2	-5.49	121.80	125.10
1	1A	2134	G	C8-N9-C4	-5.49	104.20	106.40
1	1A	2540	U	N3-C4-O4	5.49	123.24	119.40
1	1A	2818	U	N3-C4-O4	5.49	123.25	119.40
1	2A	448	U	OP1-P-O3'	-5.49	93.12	105.20
1	2A	695	G	C4-C5-C6	-5.49	115.50	118.80
1	2A	1778	U	C2-N3-C4	-5.49	123.70	127.00
1	1A	136	G	N3-C4-C5	-5.49	125.86	128.60
1	1A	348	A	N7-C8-N9	-5.49	111.06	113.80
1	1A	424	G	C5-C6-N1	-5.49	108.75	111.50
1	1A	486	A	N1-C6-N6	-5.49	115.31	118.60
1	1A	722	A	C4-C5-N7	5.49	113.45	110.70
3	1D	52	ARG	NE-CZ-NH2	5.49	123.05	120.30
32	1a	665	A	N1-C6-N6	-5.49	115.31	118.60
1	2A	2569	G	O5'-P-OP1	-5.49	100.76	105.70
1	1A	216	A	C5-N7-C8	5.49	106.64	103.90
1	1A	284	G	C2-N3-C4	-5.49	109.16	111.90
1	1A	495	G	N3-C2-N2	-5.49	116.06	119.90
1	1A	2529	C	C5-C4-N4	-5.49	116.36	120.20
32	1a	266	G	C5-C6-O6	-5.49	125.31	128.60
38	1g	59	LEU	CA-CB-CG	5.49	127.92	115.30
1	2A	312	G	C5-C6-O6	-5.49	125.31	128.60
1	2A	966	G	C5-N7-C8	-5.49	101.56	104.30
32	2a	948	C	N3-C4-N4	-5.49	114.16	118.00
1	2A	998	C	OP1-P-O3'	5.49	117.27	105.20
1	2A	1045	A	C8-N9-C4	-5.49	103.61	105.80
1	2A	2561	A	N9-C4-C5	5.49	108.00	105.80
1	1A	834	U	N1-C2-N3	5.49	118.19	114.90
1	1A	1070	G	C5-C6-O6	-5.49	125.31	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1320	A	C4-C5-N7	5.49	113.44	110.70
1	1A	1912	A	OP2-P-O3'	5.49	117.27	105.20
1	1A	2510	C	N1-C2-O2	-5.49	115.61	118.90
1	1A	2788	A	C8-N9-C4	5.49	107.99	105.80
32	1a	848	C	C5-C6-N1	5.49	123.74	121.00
32	1a	1046	A	C5-C6-N6	-5.49	119.31	123.70
1	2A	332	A	C8-N9-C4	5.49	108.00	105.80
1	2A	1846	G	O5'-P-OP2	-5.49	100.76	105.70
32	2a	132	C	C6-N1-C2	5.49	122.49	120.30
32	2a	299	G	C5-N7-C8	-5.49	101.56	104.30
1	1A	1382	A	C4-C5-N7	-5.48	107.96	110.70
1	1A	2479	C	OP2-P-O3'	5.48	117.27	105.20
18	1W	82	LEU	CB-CG-CD2	-5.48	101.68	111.00
32	1a	1076	C	N1-C2-O2	-5.48	115.61	118.90
1	2A	2064	C	O5'-P-OP2	-5.48	100.76	105.70
1	1A	1109	G	C8-N9-C4	-5.48	104.21	106.40
1	1A	1235	G	N1-C2-N2	-5.48	111.27	116.20
1	1A	1439	A	C6-N1-C2	-5.48	115.31	118.60
1	1A	1687	C	O4'-C1'-N1	5.48	112.59	108.20
1	1A	1742	G	OP1-P-OP2	5.48	127.82	119.60
1	1A	1814	A	C4-C5-C6	-5.48	114.26	117.00
1	1A	1986	G	C2-N3-C4	-5.48	109.16	111.90
32	1a	148	G	C8-N9-C4	-5.48	104.21	106.40
32	1a	686	U	N3-C2-O2	-5.48	118.36	122.20
1	2A	380	U	C5-C6-N1	5.48	125.44	122.70
1	1A	46	C	C6-N1-C2	-5.48	118.11	120.30
1	1A	587	C	N3-C4-C5	-5.48	119.71	121.90
1	1A	1383	G	C2-N3-C4	5.48	114.64	111.90
32	1a	737	A	O5'-P-OP1	-5.48	100.77	105.70
1	2A	61	G	C6-C5-N7	-5.48	127.11	130.40
1	2A	747	U	N1-C2-O2	-5.48	118.96	122.80
32	2a	138	G	N3-C4-N9	-5.48	122.71	126.00
1	1A	2056	U	N3-C4-O4	-5.48	115.56	119.40
1	2A	958	U	N1-C2-N3	5.48	118.19	114.90
1	2A	2416	C	C6-N1-C2	-5.48	118.11	120.30
1	1A	137	G	O5'-P-OP1	-5.48	100.77	105.70
1	1A	486	A	N9-C4-C5	5.48	107.99	105.80
1	1A	505	A	C4-C5-N7	-5.48	107.96	110.70
1	1A	2508	C	C5-C6-N1	-5.48	118.26	121.00
1	1A	2621	U	N1-C2-O2	-5.48	118.97	122.80
32	1a	481	G	N3-C4-N9	5.48	129.29	126.00
1	2A	1281	G	O5'-P-OP1	-5.48	100.77	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1890	A	N1-C6-N6	-5.48	115.31	118.60
1	2A	2109	U	C5-C6-N1	5.48	125.44	122.70
32	2a	831	U	C5-C6-N1	5.48	125.44	122.70
1	1A	1750	G	OP1-P-OP2	5.48	127.81	119.60
1	1A	2055	A	C6-N1-C2	-5.48	115.31	118.60
1	1A	2251	G	O5'-P-OP2	-5.48	100.77	105.70
32	1a	722	A	C5-C6-N1	-5.48	114.96	117.70
1	2A	681	G	N1-C2-N3	5.48	127.19	123.90
32	2a	522	C	N1-C2-O2	5.48	122.19	118.90
32	2a	1043	C	C6-N1-C1'	5.48	127.37	120.80
1	1A	95	G	N7-C8-N9	-5.47	110.36	113.10
1	1A	597	C	OP1-P-O3'	5.47	117.24	105.20
1	1A	1863	C	OP1-P-OP2	5.47	127.81	119.60
1	1A	2092	G	C5'-C4'-O4'	5.47	115.67	109.10
1	1A	2271	G	C2-N3-C4	5.47	114.64	111.90
1	1A	2387	G	O5'-P-OP1	5.47	117.27	110.70
1	2A	752	A	N9-C4-C5	5.47	107.99	105.80
1	2A	1497	U	O4'-C1'-N1	5.47	112.58	108.20
1	2A	1667	G	C8-N9-C4	5.47	108.59	106.40
1	2A	1831	G	C5-C6-O6	5.47	131.88	128.60
32	2a	400	C	O5'-P-OP2	5.47	117.27	110.70
32	2a	917	G	N3-C2-N2	-5.47	116.07	119.90
1	1A	101	A	C6-C5-N7	-5.47	128.47	132.30
1	1A	1135	G	N3-C4-N9	5.47	129.28	126.00
1	1A	1425	A	C5-C6-N6	-5.47	119.32	123.70
1	1A	1916	C	O5'-P-OP1	5.47	117.27	110.70
1	1A	2289	G	N3-C2-N2	-5.47	116.07	119.90
1	1A	2879	G	N3-C4-N9	-5.47	122.72	126.00
32	1a	823	G	O5'-P-OP2	5.47	117.27	110.70
1	2A	1062	G	C8-N9-C4	-5.47	104.21	106.40
1	2A	1813	G	C8-N9-C4	5.47	108.59	106.40
1	2A	2486	G	C8-N9-C4	5.47	108.59	106.40
32	2a	705	U	N1-C2-O2	-5.47	118.97	122.80
1	1A	1320	A	N7-C8-N9	5.47	116.53	113.80
1	1A	1856	A	N9-C4-C5	5.47	107.99	105.80
1	1A	2863	C	C5-C6-N1	-5.47	118.26	121.00
1	2A	1956	U	N1-C2-O2	-5.47	118.97	122.80
32	2a	1426	C	N1-C2-O2	-5.47	115.62	118.90
1	1A	201	G	OP2-P-O3'	5.47	117.23	105.20
1	1A	872	C	C5-C6-N1	-5.47	118.27	121.00
1	1A	1966	U	C2-N3-C4	-5.47	123.72	127.00
1	1A	2641	A	C2-N3-C4	-5.47	107.86	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	14	U	C6-N1-C2	-5.47	117.72	121.00
32	1a	1010	G	N3-C4-N9	-5.47	122.72	126.00
32	1a	1523	G	C2-N3-C4	5.47	114.64	111.90
1	2A	350	U	N3-C2-O2	-5.47	118.37	122.20
1	2A	1330	C	C6-N1-C2	5.47	122.49	120.30
1	2A	2220	G	N3-C2-N2	-5.47	116.07	119.90
1	1A	61	C	OP1-P-OP2	5.47	127.80	119.60
1	1A	101	A	C8-N9-C4	5.47	107.99	105.80
1	1A	316	C	O5'-P-OP1	-5.47	100.78	105.70
1	1A	606	G	N7-C8-N9	-5.47	110.37	113.10
1	1A	1177	G	C4-C5-N7	-5.47	108.61	110.80
1	1A	1885	A	C8-N9-C4	5.47	107.99	105.80
1	1A	1919	G	C5-C6-O6	-5.47	125.32	128.60
1	2A	601	C	C6-N1-C2	-5.47	118.11	120.30
1	2A	1003	G	O5'-P-OP1	-5.47	100.78	105.70
1	2A	2751	G	N3-C4-N9	-5.47	122.72	126.00
1	2A	2773	C	C5-C6-N1	-5.47	118.27	121.00
1	1A	504	A	C5-N7-C8	-5.47	101.17	103.90
1	1A	549	U	OP2-P-O3'	5.47	117.23	105.20
1	1A	816	G	OP2-P-O3'	5.47	117.23	105.20
1	1A	1062	G	OP2-P-O3'	5.47	117.23	105.20
1	1A	1216	G	C5-N7-C8	-5.47	101.57	104.30
1	1A	1804	A	N9-C1'-C2'	-5.47	105.99	112.00
1	1A	2501	G	OP2-P-O3'	5.47	117.23	105.20
32	1a	204	U	N3-C2-O2	-5.47	118.37	122.20
32	1a	981	U	N3-C2-O2	5.47	126.03	122.20
1	2A	1085	A	C8-N9-C4	5.47	107.99	105.80
1	2A	1954	G	OP1-P-OP2	5.47	127.80	119.60
1	1A	566	C	OP2-P-O3'	5.46	117.22	105.20
1	1A	1006	C	C6-N1-C1'	5.46	127.36	120.80
1	1A	2530	A	OP1-P-OP2	-5.46	111.40	119.60
32	1a	1495	U	N3-C4-O4	5.46	123.22	119.40
1	2A	1601	G	OP1-P-O3'	5.46	117.22	105.20
1	2A	2033	A	OP2-P-O3'	5.46	117.22	105.20
32	2a	912	C	C2-N1-C1'	-5.46	112.79	118.80
32	1a	337	C	C6-N1-C2	-5.46	118.11	120.30
1	2A	566	U	C6-N1-C2	5.46	124.28	121.00
1	2A	887	A	N1-C6-N6	5.46	121.88	118.60
1	2A	1799	G	N3-C4-C5	-5.46	125.87	128.60
1	1A	1261	G	OP1-P-OP2	-5.46	111.41	119.60
1	1A	1766	G	N7-C8-N9	5.46	115.83	113.10
1	1A	2242	G	C5-C6-O6	-5.46	125.32	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	56	G	C5-C6-O6	5.46	131.88	128.60
32	2a	38	G	N3-C4-C5	5.46	131.33	128.60
1	1A	1076	G	C2-N3-C4	-5.46	109.17	111.90
1	1A	1809	U	N3-C4-C5	5.46	117.88	114.60
32	1a	738	C	C5-C6-N1	5.46	123.73	121.00
32	2a	7	G	C5-C6-O6	-5.46	125.32	128.60
32	2a	581	G	N1-C6-O6	5.46	123.18	119.90
1	1A	508	A	C2-N3-C4	-5.46	107.87	110.60
1	1A	2368	C	N1-C2-O2	-5.46	115.62	118.90
1	1A	2612	A	N9-C4-C5	5.46	107.98	105.80
32	1a	630	G	C2-N3-C4	5.46	114.63	111.90
1	2A	752	A	C2'-C3'-O3'	5.46	122.43	113.70
1	2A	1771	C	C2-N1-C1'	5.46	124.80	118.80
1	2A	2714	G	O5'-P-OP2	-5.46	100.79	105.70
1	1A	130	G	N9-C4-C5	5.46	107.58	105.40
1	1A	1237	G	N9-C1'-C2'	-5.46	106.00	112.00
1	1A	1824	C	C2-N3-C4	-5.46	117.17	119.90
5	1F	46	ARG	NE-CZ-NH1	-5.46	117.57	120.30
32	1a	533	A	N1-C2-N3	5.46	132.03	129.30
32	1a	670	G	N1-C6-O6	-5.46	116.63	119.90
1	2A	1201	C	C6-N1-C2	5.46	122.48	120.30
1	2A	2386	C	C5-C6-N1	-5.46	118.27	121.00
32	2a	472	A	C8-N9-C4	-5.46	103.62	105.80
32	1a	811	C	N3-C4-C5	5.46	124.08	121.90
32	2a	573	A	O5'-P-OP1	5.46	117.25	110.70
32	2a	1042	G	C8-N9-C4	5.46	108.58	106.40
1	1A	1725	G	C8-N9-C4	-5.45	104.22	106.40
1	1A	2005	C	OP2-P-O3'	5.45	117.20	105.20
1	1A	2260	C	OP2-P-O3'	5.45	117.20	105.20
1	1A	2316	G	N1-C6-O6	5.45	123.17	119.90
1	1A	2597	U	OP1-P-O3'	5.45	117.20	105.20
2	1B	108	U	N3-C4-O4	-5.45	115.58	119.40
32	1a	394	G	C8-N9-C4	-5.45	104.22	106.40
32	2a	893	C	C6-N1-C1'	-5.45	114.26	120.80
1	2A	303	U	N1-C2-O2	5.45	126.62	122.80
32	2a	1510	U	N3-C4-O4	5.45	123.22	119.40
1	1A	1950	A	O5'-P-OP1	-5.45	100.79	105.70
1	2A	1498	C	C6-N1-C2	5.45	122.48	120.30
1	2A	2602	A	OP2-P-O3'	5.45	117.19	105.20
2	2B	41	U	N1-C2-O2	5.45	126.61	122.80
32	2a	548	G	N1-C6-O6	5.45	123.17	119.90
32	2a	663	A	C2-N3-C4	-5.45	107.88	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	10	G	C2-N3-C4	5.45	114.62	111.90
1	1A	563	G	N1-C6-O6	-5.45	116.63	119.90
1	1A	1995	G	N7-C8-N9	-5.45	110.38	113.10
1	1A	2245	U	N1-C2-N3	5.45	118.17	114.90
1	1A	2441	G	OP1-P-O3'	5.45	117.19	105.20
1	1A	2698	G	C5-N7-C8	-5.45	101.58	104.30
32	1a	807	A	C8-N9-C4	-5.45	103.62	105.80
32	1a	1082	G	C4-C5-N7	5.45	112.98	110.80
1	2A	981	A	C5-C6-N6	5.45	128.06	123.70
1	2A	1533	G	N7-C8-N9	5.45	115.82	113.10
1	1A	512	C	C5-C6-N1	-5.45	118.28	121.00
1	1A	2612	A	C4-C5-N7	-5.45	107.98	110.70
1	1A	500	G	N7-C8-N9	5.45	115.82	113.10
1	1A	1012	C	C5-C6-N1	-5.45	118.28	121.00
1	1A	2285	A	C5-C6-N6	-5.45	119.34	123.70
1	1A	2292	G	N1-C6-O6	-5.45	116.63	119.90
27	15	20	ARG	NE-CZ-NH1	5.45	123.02	120.30
32	1a	1473	A	N1-C6-N6	-5.45	115.33	118.60
1	2A	383	U	C2-N3-C4	5.45	130.27	127.00
1	2A	1702	G	C5-N7-C8	5.45	107.02	104.30
1	2A	2743	C	N1-C2-O2	-5.45	115.63	118.90
1	1A	1024	G	C5-N7-C8	5.44	107.02	104.30
1	1A	1199	C	N3-C4-N4	5.44	121.81	118.00
1	1A	1575	A	OP2-P-O3'	5.44	117.18	105.20
1	1A	2214	G	C8-N9-C4	-5.44	104.22	106.40
1	1A	614	C	C2-N3-C4	-5.44	117.18	119.90
1	1A	958	C	N3-C4-C5	-5.44	119.72	121.90
1	1A	1118	C	N3-C4-C5	-5.44	119.72	121.90
1	1A	1197	G	N7-C8-N9	-5.44	110.38	113.10
1	1A	1533	G	OP1-P-O3'	5.44	117.18	105.20
1	1A	2509	A	C5-N7-C8	5.44	106.62	103.90
32	1a	438	G	C5-C6-O6	5.44	131.87	128.60
32	1a	1530	G	C5-N7-C8	-5.44	101.58	104.30
1	2A	936	C	C2-N1-C1'	-5.44	112.81	118.80
1	2A	1975	G	O5'-P-OP2	-5.44	100.80	105.70
32	2a	691	G	C8-N9-C4	5.44	108.58	106.40
1	1A	1199	C	N3-C2-O2	5.44	125.71	121.90
1	1A	1365	G	C5-N7-C8	-5.44	101.58	104.30
1	1A	1854	G	OP2-P-O3'	5.44	117.17	105.20
1	1A	2091	G	N3-C2-N2	-5.44	116.09	119.90
1	1A	2176	G	C4-N9-C1'	-5.44	119.43	126.50
1	1A	2279	A	C8-N9-C4	5.44	107.98	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	6	C	C6-N1-C2	5.44	122.48	120.30
32	1a	1528	U	O5'-P-OP2	-5.44	100.80	105.70
1	2A	195	A	C5-N7-C8	-5.44	101.18	103.90
1	2A	843	G	O5'-P-OP1	5.44	117.23	110.70
1	2A	2132	U	O4'-C1'-N1	5.44	112.55	108.20
1	2A	2893	G	C5-C6-N1	5.44	114.22	111.50
32	2a	79	G	N3-C4-C5	5.44	131.32	128.60
32	2a	517	G	C8-N9-C4	-5.44	104.22	106.40
1	1A	185	A	C5-N7-C8	-5.44	101.18	103.90
1	1A	765	A	C6-C5-N7	-5.44	128.49	132.30
1	1A	906	G	N7-C8-N9	-5.44	110.38	113.10
1	1A	1169	C	C2-N3-C4	-5.44	117.18	119.90
1	1A	1614	A	C4-C5-N7	-5.44	107.98	110.70
1	1A	2397	C	OP1-P-OP2	5.44	127.76	119.60
1	2A	335	C	OP1-P-O3'	5.44	117.16	105.20
1	2A	763	G	O5'-P-OP1	-5.44	100.81	105.70
1	2A	896	A	O5'-P-OP2	-5.44	100.81	105.70
1	2A	2041	U	N3-C2-O2	5.44	126.01	122.20
1	2A	2093	G	C4-C5-N7	5.44	112.97	110.80
32	2a	1125	U	N3-C2-O2	-5.44	118.39	122.20
1	1A	545	G	C4-C5-N7	-5.44	108.63	110.80
1	1A	1269	G	C6-N1-C2	5.44	128.36	125.10
32	1a	1232	U	N3-C4-O4	5.44	123.20	119.40
32	2a	1427	U	N3-C2-O2	5.44	126.00	122.20
1	1A	623	G	C4-C5-N7	-5.43	108.63	110.80
1	1A	762	G	N1-C6-O6	5.43	123.16	119.90
1	1A	2058	C	C2-N3-C4	-5.43	117.18	119.90
1	1A	2294	G	C6-N1-C2	5.43	128.36	125.10
1	1A	2511	C	C4-C5-C6	5.43	120.12	117.40
32	1a	404	U	C2-N1-C1'	5.43	124.22	117.70
32	1a	1523	G	N9-C4-C5	5.43	107.57	105.40
1	2A	1202	C	C2-N1-C1'	-5.43	112.82	118.80
32	2a	265	G	OP2-P-O3'	5.43	117.15	105.20
32	2a	1301	U	C5-C6-N1	-5.43	119.98	122.70
1	1A	65	C	OP2-P-O3'	5.43	117.15	105.20
1	1A	237	G	N1-C6-O6	-5.43	116.64	119.90
1	1A	1445	C	N3-C2-O2	5.43	125.70	121.90
1	1A	2204	G	C4-C5-N7	-5.43	108.63	110.80
1	2A	1071	G	C4-N9-C1'	5.43	133.56	126.50
1	1A	2250	G	N9-C4-C5	-5.43	103.23	105.40
1	1A	2725	A	C6-N1-C2	5.43	121.86	118.60
1	2A	1052	C	C2-N1-C1'	5.43	124.77	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	84	G	C5-N7-C8	5.43	107.02	104.30
1	1A	1290	G	C5-N7-C8	5.43	107.02	104.30
1	1A	1663	C	N3-C4-C5	5.43	124.07	121.90
1	1A	1723	A	N1-C2-N3	-5.43	126.58	129.30
1	1A	2652	G	N7-C8-N9	-5.43	110.39	113.10
32	1a	583	A	C6-N1-C2	-5.43	115.34	118.60
1	2A	785	G	O5'-P-OP2	-5.43	100.81	105.70
1	2A	1999	C	C6-N1-C2	5.43	122.47	120.30
1	2A	2755	C	C2-N1-C1'	5.43	124.77	118.80
32	2a	27	G	C4-C5-N7	5.43	112.97	110.80
32	2a	902	G	C2-N3-C4	5.43	114.61	111.90
32	2a	1505	G	OP1-P-OP2	-5.43	111.46	119.60
32	1a	841	U	C5-C6-N1	5.43	125.41	122.70
1	2A	1280	G	OP2-P-O3'	5.43	117.14	105.20
1	2A	2501	C	C6-N1-C2	5.43	122.47	120.30
32	2a	316	G	C6-C5-N7	-5.43	127.14	130.40
1	1A	339	G	O5'-P-OP2	-5.43	100.82	105.70
1	1A	1057	G	C6-C5-N7	-5.43	127.14	130.40
1	1A	2608	U	N3-C4-C5	5.43	117.86	114.60
1	1A	2609	G	N3-C4-C5	5.43	131.31	128.60
1	2A	866	A	O4'-C1'-N9	-5.43	103.86	108.20
32	2a	1502	A	N1-C6-N6	-5.43	115.34	118.60
1	1A	2465	A	O5'-P-OP2	-5.42	100.82	105.70
1	2A	482	A	C4-C5-C6	5.42	119.71	117.00
1	2A	2253	G	C8-N9-C1'	-5.42	119.95	127.00
1	2A	2555	U	C6-N1-C2	5.42	124.25	121.00
1	2A	2608	G	O5'-P-OP1	5.42	117.21	110.70
1	1A	1559	C	O5'-P-OP2	5.42	117.21	110.70
1	1A	1922	A	N1-C6-N6	-5.42	115.35	118.60
1	1A	2416	C	N3-C2-O2	5.42	125.70	121.90
32	1a	607	A	N1-C6-N6	5.42	121.85	118.60
1	2A	858	U	N1-C2-O2	5.42	126.60	122.80
1	2A	2894	G	C8-N9-C1'	5.42	134.05	127.00
32	2a	587	G	C8-N9-C4	-5.42	104.23	106.40
32	2a	1378	C	C5-C6-N1	5.42	123.71	121.00
1	1A	543	G	C8-N9-C4	-5.42	104.23	106.40
1	1A	1690	G	N9-C4-C5	5.42	107.57	105.40
1	1A	2565	G	N3-C4-C5	-5.42	125.89	128.60
1	2A	15	G	N1-C6-O6	5.42	123.15	119.90
1	2A	860	U	N3-C2-O2	-5.42	118.41	122.20
1	2A	1206	G	O5'-P-OP2	5.42	117.21	110.70
1	2A	2008	C	C6-N1-C2	5.42	122.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	859	C	O5'-P-OP1	-5.42	100.82	105.70
1	1A	1616	A	N1-C2-N3	-5.42	126.59	129.30
1	1A	2737	C	O5'-P-OP2	-5.42	100.82	105.70
1	2A	517	C	N1-C2-O2	-5.42	115.65	118.90
1	2A	1768	U	C5-C4-O4	-5.42	122.65	125.90
32	2a	410	G	C8-N9-C4	-5.42	104.23	106.40
1	1A	822	G	C8-N9-C4	5.42	108.57	106.40
1	1A	1294	G	O5'-P-OP2	-5.42	100.82	105.70
1	1A	1628	G	O4'-C1'-N9	-5.42	103.87	108.20
1	1A	1993	A	OP2-P-O3'	5.42	117.12	105.20
1	1A	2371	C	N1-C2-O2	-5.42	115.65	118.90
17	1V	66	ARG	NE-CZ-NH1	-5.42	117.59	120.30
32	1a	728	A	O5'-P-OP2	-5.42	100.82	105.70
1	2A	1445(A)	C	N3-C2-O2	-5.42	118.11	121.90
1	2A	2352	A	N1-C2-N3	5.42	132.01	129.30
2	2B	62	C	N3-C4-C5	-5.42	119.73	121.90
32	2a	1374	A	O5'-P-OP2	-5.42	100.82	105.70
32	1a	863	U	C2-N1-C1'	-5.42	111.20	117.70
32	2a	442	C	C6-N1-C2	-5.42	118.13	120.30
1	1A	1138	C	N3-C4-C5	5.42	124.07	121.90
1	1A	2453	C	N3-C4-N4	-5.42	114.21	118.00
32	1a	915	A	O5'-P-OP2	-5.42	100.83	105.70
1	2A	1170	G	C4-C5-N7	5.42	112.97	110.80
32	2a	112	G	O5'-P-OP1	-5.42	100.83	105.70
32	2a	401	C	OP2-P-O3'	5.42	117.11	105.20
32	2a	1480	G	N3-C4-C5	5.42	131.31	128.60
1	1A	115	G	O5'-P-OP1	5.41	117.20	110.70
1	1A	2261	U	C5-C4-O4	5.41	129.15	125.90
32	1a	899	C	C6-N1-C2	5.41	122.47	120.30
1	2A	2113	U	C2-N1-C1'	5.41	124.20	117.70
1	2A	2501	C	C6-N1-C1'	5.41	127.30	120.80
1	1A	2239	A	C2-N3-C4	5.41	113.31	110.60
3	1D	71	ASP	N-CA-CB	-5.41	100.86	110.60
1	2A	316	C	C5-C4-N4	-5.41	116.41	120.20
1	1A	114	C	C5-C6-N1	-5.41	118.29	121.00
1	1A	2588	G	C5-C6-N1	5.41	114.20	111.50
32	1a	158	G	O4'-C1'-N9	5.41	112.53	108.20
32	1a	1287	A	N1-C6-N6	-5.41	115.35	118.60
32	1a	1505	G	C4-C5-N7	-5.41	108.64	110.80
1	2A	837	C	N1-C2-O2	-5.41	115.65	118.90
1	2A	1692	U	C5-C6-N1	-5.41	120.00	122.70
1	2A	1776	G	N7-C8-N9	5.41	115.81	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2342	C	O5'-P-OP2	5.41	117.19	110.70
32	2a	242	C	N3-C4-C5	-5.41	119.74	121.90
1	1A	1794	G	C4-C5-N7	-5.41	108.64	110.80
4	1E	111	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	2A	1623	G	C8-N9-C4	-5.41	104.24	106.40
1	2A	1751	C	OP2-P-O3'	5.41	117.10	105.20
1	2A	1897	G	C2-N3-C4	-5.41	109.20	111.90
1	2A	2170	A	N7-C8-N9	5.41	116.50	113.80
1	2A	2729	G	C5-C6-O6	5.41	131.84	128.60
1	2A	2886	G	N9-C4-C5	5.41	107.56	105.40
32	2a	1486	G	OP2-P-O3'	5.41	117.10	105.20
1	1A	546	G	OP1-P-OP2	-5.41	111.49	119.60
1	1A	829	A	O5'-P-OP1	-5.41	100.83	105.70
1	1A	972	A	O5'-P-OP1	5.41	117.19	110.70
1	1A	1320	A	C2-N3-C4	-5.41	107.90	110.60
1	1A	2525	G	C6-C5-N7	-5.41	127.16	130.40
1	1A	268	G	OP1-P-OP2	5.41	127.71	119.60
1	1A	360	C	N3-C4-C5	-5.41	119.74	121.90
1	1A	879	G	C2-N3-C4	-5.41	109.20	111.90
1	1A	980	C	C2-N3-C4	-5.41	117.20	119.90
1	1A	982	U	N3-C4-O4	5.41	123.18	119.40
1	1A	1245	C	N3-C4-C5	5.41	124.06	121.90
1	1A	1378	G	O5'-P-OP1	-5.41	100.83	105.70
1	1A	1700	G	OP2-P-O3'	-5.41	93.31	105.20
23	11	61	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	2A	661	C	N3-C4-C5	5.41	124.06	121.90
1	2A	1427	A	C6-N1-C2	-5.41	115.36	118.60
32	2a	296	U	N3-C4-C5	-5.41	111.36	114.60
32	2a	1183	A	OP1-P-O3'	5.41	117.09	105.20
1	1A	507	G	N9-C4-C5	5.40	107.56	105.40
1	1A	1033	G	O5'-P-OP2	5.40	117.19	110.70
1	1A	1068	G	C6-N1-C2	5.40	128.34	125.10
1	1A	67	G	N3-C4-C5	-5.40	125.90	128.60
1	1A	206	G	N1-C2-N3	5.40	127.14	123.90
1	1A	285	U	C2-N3-C4	-5.40	123.76	127.00
1	1A	1236	G	N1-C6-O6	-5.40	116.66	119.90
1	1A	1510	C	O5'-P-OP2	5.40	117.18	110.70
1	1A	2139	A	C8-N9-C4	-5.40	103.64	105.80
1	1A	2241	C	C6-N1-C2	-5.40	118.14	120.30
1	1A	2259	A	N7-C8-N9	-5.40	111.10	113.80
2	1B	57	A	OP2-P-O3'	5.40	117.09	105.20
32	1a	191	G	C8-N9-C4	-5.40	104.24	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	179	G	C8-N9-C4	5.40	108.56	106.40
1	2A	374	A	C2-N3-C4	-5.40	107.90	110.60
1	2A	1089	G	O4'-C1'-N9	5.40	112.52	108.20
1	2A	2136	C	C6-N1-C2	-5.40	118.14	120.30
2	2B	63	G	C8-N9-C4	5.40	108.56	106.40
32	2a	912	C	C5-C6-N1	-5.40	118.30	121.00
32	2a	1086	U	N1-C2-O2	5.40	126.58	122.80
1	1A	353	G	O4'-C1'-N9	-5.40	103.88	108.20
1	1A	538	A	C2-N3-C4	-5.40	107.90	110.60
1	1A	751	G	O4'-C1'-N9	5.40	112.52	108.20
1	1A	1364	C	C6-N1-C2	5.40	122.46	120.30
1	1A	1626	A	C5-C6-N6	-5.40	119.38	123.70
1	1A	2523	U	C5-C6-N1	-5.40	120.00	122.70
1	1A	2562	G	N3-C4-C5	-5.40	125.90	128.60
2	1B	100	A	O5'-P-OP2	-5.40	100.84	105.70
1	2A	1244	G	C2-N3-C4	-5.40	109.20	111.90
1	2A	1973	G	N7-C8-N9	-5.40	110.40	113.10
1	2A	2861	G	N1-C2-N2	5.40	121.06	116.20
32	2a	446	G	N1-C6-O6	5.40	123.14	119.90
1	1A	176	G	C4-C5-N7	-5.40	108.64	110.80
1	1A	595	A	N1-C6-N6	-5.40	115.36	118.60
1	2A	2468	G	N3-C2-N2	-5.40	116.12	119.90
32	2a	237	C	C6-N1-C2	5.40	122.46	120.30
32	2a	1418	A	C2-N3-C4	5.40	113.30	110.60
1	1A	1986	G	OP2-P-O3'	5.40	117.07	105.20
1	1A	2009	G	OP2-P-O3'	5.40	117.08	105.20
1	1A	2381	A	N9-C4-C5	5.40	107.96	105.80
32	1a	698	G	C8-N9-C4	-5.40	104.24	106.40
32	1a	901	A	N1-C2-N3	5.40	132.00	129.30
32	1a	1392	G	N1-C6-O6	5.40	123.14	119.90
1	2A	172	C	C6-N1-C2	5.40	122.46	120.30
32	2a	218	C	C6-N1-C2	-5.40	118.14	120.30
32	2a	569	C	C4-C5-C6	5.40	120.10	117.40
1	1A	421	A	OP1-P-OP2	5.40	127.69	119.60
1	1A	899	G	N1-C6-O6	-5.40	116.66	119.90
1	2A	1936	A	C4-C5-N7	5.40	113.40	110.70
1	1A	968	U	C5-C4-O4	-5.39	122.66	125.90
1	1A	2183	C	C6-N1-C2	-5.39	118.14	120.30
1	1A	2251	G	OP2-P-O3'	5.39	117.07	105.20
1	1A	2336	C	N3-C4-N4	5.39	121.78	118.00
1	1A	2409	G	N1-C2-N2	5.39	121.06	116.20
1	2A	80	G	N1-C6-O6	-5.39	116.66	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	533	A	O5'-P-OP2	5.39	117.17	110.70
1	1A	355	A	C5-C6-N6	-5.39	119.39	123.70
1	1A	533	G	N3-C2-N2	-5.39	116.12	119.90
1	1A	1071	G	C5-N7-C8	5.39	107.00	104.30
1	1A	2623	U	N1-C2-N3	5.39	118.14	114.90
1	1A	2647	C	C5-C6-N1	-5.39	118.30	121.00
2	1B	7	G	C5'-C4'-C3'	-5.39	107.37	116.00
32	1a	152	A	C8-N9-C4	5.39	107.96	105.80
32	1a	455	C	N1-C2-O2	5.39	122.14	118.90
1	2A	2455	G	C5-C6-O6	-5.39	125.36	128.60
1	1A	1505	C	C6-N1-C2	-5.39	118.14	120.30
1	1A	1862	G	C4-C5-N7	-5.39	108.64	110.80
1	1A	2791	A	C5-C6-N1	-5.39	115.00	117.70
32	1a	142	G	C6-C5-N7	5.39	133.63	130.40
1	1A	44	G	OP2-P-O3'	5.39	117.06	105.20
1	1A	313	A	C2-N3-C4	-5.39	107.91	110.60
1	1A	425	G	C2-N3-C4	-5.39	109.21	111.90
1	1A	745	C	OP1-P-OP2	5.39	127.68	119.60
1	1A	1035	G	C2-N3-C4	5.39	114.59	111.90
1	1A	1644	C	C5-C6-N1	-5.39	118.31	121.00
1	1A	2336	C	N1-C2-O2	-5.39	115.67	118.90
32	1a	685	G	N1-C6-O6	5.39	123.13	119.90
1	2A	2612	C	N3-C4-C5	5.39	124.06	121.90
2	2B	1	U	N1-C2-N3	-5.39	111.67	114.90
2	2B	104	U	C6-N1-C2	5.39	124.23	121.00
32	2a	697	U	OP1-P-OP2	5.39	127.68	119.60
32	2a	873	A	OP1-P-OP2	5.39	127.68	119.60
32	2a	1358	U	C5-C6-N1	-5.39	120.00	122.70
32	2a	1436	U	N3-C4-O4	5.39	123.17	119.40
1	1A	107	G	C5-C6-O6	5.39	131.83	128.60
1	1A	651	U	C5-C4-O4	-5.39	122.67	125.90
1	1A	1006	C	O5'-P-OP1	5.39	117.17	110.70
1	1A	2063	U	OP2-P-O3'	5.39	117.05	105.20
32	1a	1487	G	N1-C6-O6	-5.39	116.67	119.90
1	1A	1006	C	C6-N1-C2	-5.39	118.14	120.30
1	1A	1298	G	OP2-P-O3'	5.39	117.05	105.20
1	1A	1345	G	C2-N3-C4	-5.39	109.21	111.90
1	1A	791	G	N1-C2-N2	-5.38	111.36	116.20
1	1A	964	A	C6-N1-C2	5.38	121.83	118.60
1	1A	1685	C	OP2-P-O3'	5.38	117.05	105.20
1	1A	2240	G	C8-N9-C4	-5.38	104.25	106.40
1	1A	2780	C	C4-C5-C6	5.38	120.09	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	163	C	N3-C4-N4	-5.38	114.23	118.00
1	2A	1352	U	N3-C2-O2	-5.38	118.43	122.20
1	2A	2372	G	N1-C6-O6	5.38	123.13	119.90
1	2A	2645	G	N3-C4-C5	5.38	131.29	128.60
32	2a	954	G	O5'-P-OP2	-5.38	100.86	105.70
1	1A	423	G	C4-C5-N7	5.38	112.95	110.80
1	1A	1735	U	C5-C6-N1	-5.38	120.01	122.70
2	1B	9	G	OP2-P-O3'	5.38	117.04	105.20
32	1a	568	G	O5'-P-OP1	-5.38	100.86	105.70
32	1a	1196	U	OP1-P-O3'	5.38	117.04	105.20
1	2A	2726	U	C5-C6-N1	-5.38	120.01	122.70
1	1A	45	C	C2-N3-C4	-5.38	117.21	119.90
1	1A	1382	A	C8-N9-C4	-5.38	103.65	105.80
1	1A	2287	C	C4-C5-C6	5.38	120.09	117.40
1	2A	741	G	C5-C6-N1	-5.38	108.81	111.50
1	2A	871	U	C2-N3-C4	-5.38	123.77	127.00
1	2A	1011	G	N1-C6-O6	5.38	123.13	119.90
1	2A	1685	C	C6-N1-C2	5.38	122.45	120.30
1	2A	2311	A	O5'-P-OP2	-5.38	100.86	105.70
1	2A	2447	G	OP2-P-O3'	5.38	117.04	105.20
32	2a	7	G	N3-C4-C5	5.38	131.29	128.60
1	1A	2635	G	N9-C4-C5	5.38	107.55	105.40
3	1D	242	ARG	CG-CD-NE	5.38	123.10	111.80
32	1a	971	G	O5'-P-OP2	-5.38	100.86	105.70
1	2A	767	U	C5-C4-O4	5.38	129.13	125.90
1	1A	1440	U	OP2-P-O3'	5.38	117.03	105.20
1	1A	2023	A	N1-C2-N3	-5.38	126.61	129.30
32	1a	1445	C	C6-N1-C2	5.38	122.45	120.30
1	2A	762	U	C5-C4-O4	-5.38	122.67	125.90
1	2A	2557	G	C5-C6-O6	5.38	131.83	128.60
32	2a	129	U	C5-C4-O4	5.38	129.13	125.90
1	1A	1977	U	C2-N1-C1'	-5.38	111.25	117.70
1	1A	2033	U	N3-C4-O4	5.38	123.16	119.40
1	1A	2083	G	C5-C6-N1	5.38	114.19	111.50
1	1A	2254	G	C4-C5-N7	-5.38	108.65	110.80
1	2A	192	C	N1-C2-O2	-5.38	115.67	118.90
1	2A	899	A	N1-C2-N3	5.38	131.99	129.30
1	2A	1973	G	N1-C2-N2	-5.38	111.36	116.20
2	2B	11	C	C6-N1-C2	-5.38	118.15	120.30
32	2a	29	G	O5'-P-OP2	-5.38	100.86	105.70
1	1A	977	G	N1-C6-O6	-5.38	116.67	119.90
1	1A	1255	A	C5-N7-C8	-5.38	101.21	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1854	G	N7-C8-N9	-5.38	110.41	113.10
1	1A	2073	A	O5'-P-OP2	-5.38	100.86	105.70
1	2A	2783	G	N1-C6-O6	-5.38	116.67	119.90
1	1A	1018	A	OP2-P-O3'	5.37	117.02	105.20
1	1A	2468	C	C6-N1-C2	5.37	122.45	120.30
1	1A	2690	C	N3-C4-C5	-5.37	119.75	121.90
15	1T	98	LYS	CD-CE-NZ	5.37	124.06	111.70
32	1a	564	C	N3-C4-C5	-5.37	119.75	121.90
1	2A	668	G	C2-N3-C4	-5.37	109.21	111.90
1	2A	961	C	N3-C2-O2	5.37	125.66	121.90
1	2A	1363	C	N3-C4-N4	-5.37	114.24	118.00
1	2A	1934	C	C6-N1-C2	5.37	122.45	120.30
1	2A	2049	G	N3-C4-C5	5.37	131.29	128.60
1	1A	1721	G	C5-N7-C8	5.37	106.98	104.30
1	1A	2025	G	OP2-P-O3'	5.37	117.02	105.20
1	1A	2264	G	C6-N1-C2	-5.37	121.88	125.10
1	1A	2458	G	N1-C2-N3	-5.37	120.68	123.90
1	1A	2711	C	C5-C4-N4	-5.37	116.44	120.20
1	1A	2713	C	OP2-P-O3'	5.37	117.02	105.20
32	1a	1085	U	O5'-P-OP1	-5.37	100.87	105.70
1	2A	33	U	N1-C2-O2	5.37	126.56	122.80
1	2A	678	C	C2-N3-C4	-5.37	117.21	119.90
1	2A	1046	A	C2-N3-C4	5.37	113.28	110.60
1	2A	2140	C	N1-C2-O2	5.37	122.12	118.90
1	2A	2822	G	N7-C8-N9	-5.37	110.42	113.10
1	1A	2711	C	C2-N3-C4	-5.37	117.22	119.90
1	2A	563	G	O5'-P-OP2	-5.37	100.87	105.70
1	2A	678	C	C5-C6-N1	-5.37	118.31	121.00
1	2A	2132	U	C5-C4-O4	5.37	129.12	125.90
1	1A	413	G	O4'-C1'-N9	5.37	112.50	108.20
1	1A	425	G	OP1-P-OP2	5.37	127.65	119.60
1	1A	1304	C	O5'-P-OP1	-5.37	100.87	105.70
1	1A	1361	C	C2-N3-C4	-5.37	117.22	119.90
1	1A	2239	A	N9-C4-C5	5.37	107.95	105.80
32	1a	888	G	C4-C5-N7	5.37	112.95	110.80
1	2A	271(K)	U	C6-N1-C1'	5.37	128.72	121.20
1	2A	1087	G	C8-N9-C1'	5.37	133.98	127.00
1	2A	2196	C	OP1-P-O3'	5.37	117.01	105.20
1	1A	2034	G	N3-C2-N2	5.37	123.66	119.90
1	2A	135	G	OP2-P-O3'	5.37	117.01	105.20
1	2A	222	A	C8-N9-C4	-5.37	103.65	105.80
1	2A	1438	U	N3-C2-O2	-5.37	118.44	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	839	U	C6-N1-C1'	-5.37	113.69	121.20
1	1A	455	A	C5'-C4'-C3'	-5.37	107.42	116.00
1	1A	553	A	N9-C4-C5	5.37	107.95	105.80
1	1A	733	G	O4'-C1'-N9	5.37	112.49	108.20
1	1A	783	C	N1-C2-O2	-5.37	115.68	118.90
1	1A	2025	G	N9-C4-C5	-5.37	103.25	105.40
2	1B	74	U	C2-N3-C4	-5.37	123.78	127.00
1	2A	261	G	N1-C6-O6	5.37	123.12	119.90
1	2A	1003	G	O5'-P-OP2	5.37	117.14	110.70
1	2A	1846	G	C2-N3-C4	-5.37	109.22	111.90
1	2A	2148	G	N3-C4-N9	5.37	129.22	126.00
32	2a	574	A	C8-N9-C4	5.37	107.95	105.80
32	2a	1394	A	C6-N1-C2	5.37	121.82	118.60
1	1A	36	G	OP2-P-O3'	5.36	117.00	105.20
1	1A	1092	A	N7-C8-N9	5.36	116.48	113.80
1	1A	1423	G	O5'-P-OP2	-5.36	100.87	105.70
1	1A	1876	G	C2-N3-C4	-5.36	109.22	111.90
1	1A	2501	G	N1-C2-N3	5.36	127.12	123.90
1	1A	2691	A	C5-C6-N6	-5.36	119.41	123.70
32	1a	792	A	N7-C8-N9	-5.36	111.12	113.80
32	1a	895	G	N9-C4-C5	5.36	107.55	105.40
1	2A	474	G	C8-N9-C4	-5.36	104.25	106.40
1	2A	738	G	C5-C6-O6	5.36	131.82	128.60
1	2A	1690	A	N9-C4-C5	-5.36	103.66	105.80
1	2A	1994	C	C5-C6-N1	-5.36	118.32	121.00
1	2A	2846	G	N7-C8-N9	-5.36	110.42	113.10
2	2B	56	G	N3-C4-C5	-5.36	125.92	128.60
1	1A	578	U	O4'-C1'-N1	5.36	112.49	108.20
1	2A	2063	C	N1-C2-O2	-5.36	115.68	118.90
1	2A	2707	G	OP1-P-OP2	5.36	127.64	119.60
1	2A	2827	C	N3-C2-O2	5.36	125.65	121.90
1	1A	662	A	N9-C4-C5	-5.36	103.66	105.80
1	1A	762	G	N9-C4-C5	-5.36	103.26	105.40
1	1A	1287	A	C8-N9-C4	5.36	107.94	105.80
1	1A	1518	A	N3-C4-C5	-5.36	123.05	126.80
1	1A	2091	G	C6-N1-C2	-5.36	121.88	125.10
1	1A	2427	G	C8-N9-C4	-5.36	104.26	106.40
1	2A	478	A	O5'-P-OP1	-5.36	100.88	105.70
1	2A	2581	G	C5-C6-O6	5.36	131.82	128.60
1	1A	1819	C	OP2-P-O3'	5.36	116.99	105.20
1	1A	2203	G	N3-C4-N9	-5.36	122.78	126.00
1	1A	2481	A	N1-C6-N6	5.36	121.82	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	568	G	N1-C2-N3	-5.36	120.69	123.90
1	2A	1128	A	O5'-P-OP1	-5.36	100.88	105.70
1	2A	1537	G	C4-N9-C1'	5.36	133.47	126.50
1	2A	2388	A	OP1-P-OP2	-5.36	111.56	119.60
32	2a	265	G	C5-C6-O6	-5.36	125.39	128.60
1	1A	11	G	N3-C4-N9	-5.36	122.79	126.00
1	1A	659	C	O5'-P-OP2	-5.36	100.88	105.70
1	1A	1191	C	C6-N1-C2	5.36	122.44	120.30
1	1A	1298	G	C4-N9-C1'	-5.36	119.53	126.50
1	1A	1393	G	N3-C2-N2	5.36	123.65	119.90
1	1A	2665	U	C6-N1-C2	-5.36	117.78	121.00
2	1B	77	U	OP1-P-OP2	-5.36	111.56	119.60
32	1a	618	C	C5-C6-N1	5.36	123.68	121.00
1	2A	741	G	N9-C4-C5	5.36	107.54	105.40
1	2A	1118	C	C6-N1-C2	-5.36	118.16	120.30
1	1A	10	G	O4'-C1'-N9	5.36	112.48	108.20
1	1A	1088	G	OP2-P-O3'	5.36	116.98	105.20
1	1A	2031	G	N3-C4-N9	-5.36	122.79	126.00
1	1A	2517	G	C5-N7-C8	-5.36	101.62	104.30
1	1A	2865	C	N3-C4-C5	5.36	124.04	121.90
32	1a	375	U	O5'-P-OP1	-5.36	100.88	105.70
32	1a	893	C	C2-N1-C1'	5.36	124.69	118.80
32	1a	1019	C	N1-C1'-C2'	-5.36	106.11	112.00
1	2A	1245	G	N1-C6-O6	5.36	123.11	119.90
40	2i	9	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	1A	38	A	C6-N1-C2	-5.35	115.39	118.60
1	1A	501	U	N1-C2-N3	5.35	118.11	114.90
1	1A	1863	C	N1-C2-N3	5.35	122.95	119.20
1	1A	2302	G	C8-N9-C4	5.35	108.54	106.40
1	1A	2441	G	C8-N9-C4	-5.35	104.26	106.40
1	1A	2878	A	C4-C5-C6	5.35	119.68	117.00
3	1D	131	LEU	CB-CG-CD2	-5.35	101.90	111.00
32	1a	751	U	N3-C2-O2	5.35	125.95	122.20
1	2A	675	A	C2-N3-C4	-5.35	107.92	110.60
32	2a	1274	G	C8-N9-C4	-5.35	104.26	106.40
1	1A	180	A	C5-N7-C8	5.35	106.58	103.90
1	1A	1011	G	N3-C2-N2	5.35	123.65	119.90
1	1A	1532	A	C2-N3-C4	5.35	113.28	110.60
1	1A	1819	C	C2-N3-C4	-5.35	117.22	119.90
1	1A	2541	G	C8-N9-C4	-5.35	104.26	106.40
1	1A	2818	U	N1-C2-O2	-5.35	119.05	122.80
1	2A	271(L)	U	C6-N1-C1'	-5.35	113.70	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	507	A	N3-C4-C5	5.35	130.55	126.80
1	2A	1605	C	N3-C4-N4	5.35	121.75	118.00
1	2A	1798	U	O5'-P-OP1	5.35	117.12	110.70
1	2A	1832	C	OP2-P-O3'	5.35	116.97	105.20
1	2A	2608	G	N1-C6-O6	5.35	123.11	119.90
1	1A	117	A	O5'-P-OP2	-5.35	100.88	105.70
1	1A	1366	C	C5-C4-N4	5.35	123.95	120.20
1	1A	2294	G	C8-N9-C4	5.35	108.54	106.40
32	2a	766	A	N1-C2-N3	-5.35	126.62	129.30
1	1A	1314	A	C5-C6-N6	5.35	127.98	123.70
1	1A	2832	G	N3-C4-N9	5.35	129.21	126.00
32	1a	1488	G	OP2-P-O3'	5.35	116.97	105.20
1	2A	927	G	O5'-P-OP2	5.35	117.12	110.70
1	2A	1045	A	C6-C5-N7	-5.35	128.56	132.30
1	2A	2572	A	C8-N9-C4	5.35	107.94	105.80
1	2A	2832	U	C5-C6-N1	-5.35	120.03	122.70
32	2a	1069	C	C6-N1-C2	-5.35	118.16	120.30
1	1A	495	G	C8-N9-C4	-5.35	104.26	106.40
1	1A	850	U	C4-C5-C6	5.35	122.91	119.70
1	1A	1766	G	N3-C2-N2	5.35	123.64	119.90
1	1A	2076	A	C2-N3-C4	-5.35	107.93	110.60
1	1A	2598	C	C6-N1-C2	-5.35	118.16	120.30
1	1A	2635	G	N1-C6-O6	-5.35	116.69	119.90
32	1a	557	G	N3-C4-N9	5.35	129.21	126.00
32	1a	673	G	N7-C8-N9	5.35	115.77	113.10
32	1a	1213	A	C5-C6-N6	5.35	127.98	123.70
1	2A	2174	C	C4-C5-C6	5.35	120.07	117.40
1	2A	2319	G	N7-C8-N9	5.35	115.77	113.10
32	2a	792	A	O4'-C1'-N9	5.35	112.48	108.20
2	1B	39	A	N9-C4-C5	5.35	107.94	105.80
1	2A	329	G	OP1-P-OP2	5.35	127.62	119.60
32	2a	1189	C	C6-N1-C2	5.35	122.44	120.30
1	1A	1019	G	N3-C2-N2	-5.34	116.16	119.90
1	1A	1189	A	N1-C6-N6	5.34	121.81	118.60
1	1A	1282	G	C6-C5-N7	5.34	133.61	130.40
1	1A	1292	A	N7-C8-N9	-5.34	111.13	113.80
1	1A	1803	G	OP1-P-O3'	-5.34	93.44	105.20
1	1A	2193	A	N1-C6-N6	5.34	121.81	118.60
1	1A	2638	C	N3-C4-C5	5.34	124.04	121.90
1	2A	271(Y)	U	O4'-C1'-N1	5.34	112.48	108.20
1	2A	2877	G	N9-C4-C5	-5.34	103.26	105.40
32	2a	1127	G	N9-C4-C5	-5.34	103.26	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	241	G	C5-C6-O6	5.34	131.81	128.60
1	1A	1853	G	C8-N9-C4	5.34	108.54	106.40
32	1a	1181	G	C4-N9-C1'	-5.34	119.55	126.50
1	1A	1200	G	N1-C2-N2	-5.34	111.39	116.20
1	2A	784	A	OP1-P-O3'	5.34	116.95	105.20
1	1A	1354	A	C4-C5-C6	5.34	119.67	117.00
1	1A	1445	C	C6-N1-C2	5.34	122.44	120.30
1	1A	1981	G	OP2-P-O3'	5.34	116.95	105.20
1	1A	2358	A	C6-N1-C2	-5.34	115.40	118.60
32	1a	1358	U	O4'-C1'-N1	5.34	112.47	108.20
1	2A	2023	G	C6-C5-N7	-5.34	127.20	130.40
32	2a	603	U	N3-C2-O2	5.34	125.94	122.20
1	1A	2874	G	N3-C2-N2	5.34	123.64	119.90
32	2a	12	U	OP1-P-OP2	5.34	127.61	119.60
1	1A	89	U	C5-C6-N1	-5.34	120.03	122.70
1	1A	137	G	C4-C5-N7	-5.34	108.67	110.80
1	1A	137	G	N7-C8-N9	-5.34	110.43	113.10
1	1A	354	A	N7-C8-N9	5.34	116.47	113.80
1	1A	1174	A	C6-N1-C2	-5.34	115.40	118.60
1	1A	1993	A	N9-C4-C5	-5.34	103.67	105.80
1	1A	2901	A	O4'-C1'-N9	-5.34	103.93	108.20
2	1B	1	U	C6-N1-C1'	-5.34	113.73	121.20
13	1R	114	VAL	CB-CA-C	-5.34	101.26	111.40
32	1a	343	U	C6-N1-C2	5.34	124.20	121.00
1	2A	271(T)	C	O5'-P-OP2	-5.34	100.90	105.70
1	2A	1070	A	C2-N3-C4	5.34	113.27	110.60
1	2A	2306	C	N3-C2-O2	-5.34	118.17	121.90
32	2a	1092	A	N1-C6-N6	5.34	121.80	118.60
1	1A	217	A	N3-C4-N9	-5.33	123.13	127.40
1	1A	792	G	N1-C6-O6	5.33	123.10	119.90
1	1A	2818	U	C6-N1-C2	5.33	124.20	121.00
19	1X	70	LEU	CA-CB-CG	5.33	127.57	115.30
32	1a	621	A	N1-C6-N6	-5.33	115.40	118.60
1	2A	954	G	N1-C6-O6	-5.33	116.70	119.90
1	2A	2334	G	C5-C6-N1	5.33	114.17	111.50
1	1A	608	G	C5-C6-N1	-5.33	108.83	111.50
1	1A	1927	C	OP1-P-O3'	5.33	116.93	105.20
1	1A	2438	A	C6-N1-C2	-5.33	115.40	118.60
1	1A	2512	U	N3-C4-C5	5.33	117.80	114.60
32	1a	533	A	C8-N9-C1'	-5.33	118.10	127.70
1	2A	669	G	OP1-P-OP2	-5.33	111.60	119.60
1	2A	1208	C	N3-C4-C5	-5.33	119.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1765	C	C6-N1-C2	5.33	122.43	120.30
1	2A	1829	A	C6-N1-C2	-5.33	115.40	118.60
1	2A	2574	G	C4-C5-N7	5.33	112.93	110.80
32	2a	487	A	N1-C6-N6	5.33	121.80	118.60
1	1A	134	G	N3-C4-N9	-5.33	122.80	126.00
1	1A	350	G	O5'-P-OP2	5.33	117.10	110.70
1	1A	1197	G	C8-N9-C4	5.33	108.53	106.40
1	1A	2299	A	P-O3'-C3'	5.33	126.10	119.70
1	1A	2395	G	N1-C6-O6	-5.33	116.70	119.90
32	1a	14	U	N3-C4-O4	5.33	123.13	119.40
32	1a	134	A	O5'-P-OP1	5.33	117.10	110.70
1	2A	554	U	O5'-P-OP1	5.33	117.10	110.70
1	2A	1125	G	C6-C5-N7	-5.33	127.20	130.40
1	2A	1251	C	N3-C4-N4	5.33	121.73	118.00
32	2a	531	U	N1-C2-O2	5.33	126.53	122.80
32	2a	766	A	N7-C8-N9	-5.33	111.14	113.80
1	1A	504	A	C8-N9-C4	-5.33	103.67	105.80
1	1A	794	U	O5'-P-OP1	-5.33	100.90	105.70
1	1A	2506	G	N1-C6-O6	-5.33	116.70	119.90
32	1a	580	U	C5-C4-O4	5.33	129.10	125.90
1	2A	1256	G	N1-C2-N2	5.33	121.00	116.20
2	2B	109	C	OP1-P-OP2	5.33	127.59	119.60
1	1A	1242	G	N3-C2-N2	5.33	123.63	119.90
1	1A	1664	A	C6-C5-N7	5.33	136.03	132.30
1	2A	337	C	O5'-P-OP2	-5.33	100.91	105.70
1	2A	1449	A	N1-C2-N3	-5.33	126.64	129.30
32	2a	267	C	O5'-P-OP1	-5.33	100.91	105.70
1	1A	476	G	C6-N1-C2	-5.33	121.90	125.10
1	1A	2252	C	C2-N3-C4	-5.33	117.24	119.90
32	1a	694	A	O5'-P-OP2	5.33	117.09	110.70
1	2A	476	G	C2-N3-C4	-5.33	109.24	111.90
1	1A	1361	C	N1-C2-N3	5.33	122.93	119.20
1	1A	1361	C	N3-C2-O2	-5.33	118.17	121.90
1	1A	1607	G	OP1-P-O3'	5.33	116.92	105.20
1	1A	2241	C	N3-C4-N4	5.33	121.73	118.00
1	1A	2701	U	P-O3'-C3'	5.33	126.09	119.70
1	1A	2858	G	C5-N7-C8	5.33	106.96	104.30
32	1a	147	G	N9-C4-C5	5.33	107.53	105.40
32	1a	147	G	O4'-C1'-N9	5.33	112.46	108.20
1	2A	1685	C	N1-C2-O2	-5.33	115.70	118.90
1	2A	1777	U	C5-C6-N1	-5.33	120.04	122.70
1	2A	1954	G	N3-C4-N9	-5.33	122.80	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	27	G	C5-C6-O6	-5.33	125.41	128.60
1	1A	215	G	O5'-P-OP2	-5.32	100.91	105.70
1	1A	392	U	N3-C2-O2	5.32	125.93	122.20
1	1A	1853	G	N7-C8-N9	-5.32	110.44	113.10
1	1A	1862	G	N3-C4-N9	-5.32	122.81	126.00
1	1A	2428	C	N3-C4-C5	5.32	124.03	121.90
1	1A	2566	U	C2-N3-C4	-5.32	123.81	127.00
32	1a	575	G	C5-N7-C8	5.32	106.96	104.30
1	2A	1702	G	C4-N9-C1'	-5.32	119.58	126.50
1	2A	1826	G	C5-N7-C8	5.32	106.96	104.30
32	2a	975	A	O4'-C1'-N9	-5.32	103.94	108.20
1	1A	614	C	N1-C2-N3	5.32	122.93	119.20
1	1A	1269	G	N1-C2-N3	-5.32	120.71	123.90
8	2I	75	LEU	CA-CB-CG	5.32	127.54	115.30
32	2a	954	G	O5'-P-OP1	5.32	117.09	110.70
1	1A	283	G	N7-C8-N9	5.32	115.76	113.10
1	1A	1064	C	O5'-P-OP1	-5.32	100.91	105.70
1	1A	1147	U	N1-C2-O2	5.32	126.53	122.80
1	1A	1409	C	N1-C2-O2	5.32	122.09	118.90
1	1A	2361	G	C8-N9-C4	5.32	108.53	106.40
4	1E	77	ILE	CG1-CB-CG2	-5.32	99.69	111.40
1	2A	1602	U	O5'-P-OP1	-5.32	100.91	105.70
1	2A	2454	G	N1-C6-O6	-5.32	116.71	119.90
32	2a	1030(D)	A	N9-C4-C5	5.32	107.93	105.80
32	2a	1505	G	C8-N9-C4	-5.32	104.27	106.40
1	1A	1099	C	C5-C6-N1	5.32	123.66	121.00
1	1A	1537	G	C8-N9-C4	5.32	108.53	106.40
1	2A	1936	A	N9-C4-C5	-5.32	103.67	105.80
3	2D	242	ARG	NE-CZ-NH1	-5.32	117.64	120.30
32	2a	507	C	OP2-P-O3'	5.32	116.90	105.20
32	2a	1099	G	N3-C2-N2	-5.32	116.18	119.90
1	1A	1426	G	C5-C6-O6	-5.32	125.41	128.60
1	1A	1543	U	N1-C2-N3	5.32	118.09	114.90
1	1A	1567	G	N7-C8-N9	5.32	115.76	113.10
1	1A	2519	C	N3-C2-O2	-5.32	118.18	121.90
2	1B	112	U	N3-C4-C5	-5.32	111.41	114.60
5	1F	77	ASP	CB-CG-OD2	-5.32	113.51	118.30
32	1a	549	C	C6-N1-C2	5.32	122.43	120.30
32	1a	960	U	OP1-P-O3'	5.32	116.90	105.20
32	1a	968	A	C8-N9-C4	5.32	107.93	105.80
2	2B	93	G	OP2-P-O3'	5.32	116.90	105.20
32	2a	36	C	N3-C4-C5	-5.32	119.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1527	C	O5'-P-OP1	5.32	117.08	110.70
1	1A	1321	A	OP2-P-O3'	5.32	116.89	105.20
1	1A	1705	C	C2-N1-C1'	5.32	124.65	118.80
1	1A	2827	G	O5'-P-OP2	-5.32	100.92	105.70
1	1A	2832	G	C8-N9-C4	5.32	108.53	106.40
32	1a	189(G)	G	N3-C4-C5	5.32	131.26	128.60
32	1a	1473	A	C5-C6-N6	5.32	127.95	123.70
1	2A	217	G	C6-N1-C2	-5.32	121.91	125.10
1	2A	2022	U	N1-C2-O2	-5.32	119.08	122.80
1	1A	1620	G	N1-C6-O6	5.31	123.09	119.90
1	1A	2580	C	C5-C6-N1	-5.31	118.34	121.00
1	1A	2837	C	O5'-P-OP1	5.31	117.08	110.70
32	1a	1201	A	P-O3'-C3'	5.31	126.08	119.70
1	2A	553	G	N9-C4-C5	5.31	107.53	105.40
1	2A	1226	A	N7-C8-N9	-5.31	111.14	113.80
1	2A	1264	G	OP1-P-OP2	5.31	127.57	119.60
1	2A	1744	C	C6-N1-C2	-5.31	118.17	120.30
1	2A	2447	G	N1-C2-N3	5.31	127.09	123.90
1	1A	1857	G	C5-C6-O6	5.31	131.79	128.60
1	2A	271(W)	G	C5-C6-N1	-5.31	108.84	111.50
1	2A	906	G	C8-N9-C1'	5.31	133.91	127.00
1	2A	1200	C	C2-N1-C1'	-5.31	112.96	118.80
32	2a	354	G	N7-C8-N9	5.31	115.76	113.10
32	2a	670	G	N1-C6-O6	-5.31	116.71	119.90
1	1A	1364	C	N3-C2-O2	5.31	125.62	121.90
1	1A	2745	G	C8-N9-C4	-5.31	104.28	106.40
1	2A	485	C	N1-C2-O2	5.31	122.09	118.90
1	2A	1759	A	C2-N3-C4	-5.31	107.94	110.60
32	2a	1436	U	N1-C2-O2	-5.31	119.08	122.80
1	1A	1011	G	N1-C2-N2	-5.31	111.42	116.20
1	1A	1420	G	N1-C6-O6	5.31	123.09	119.90
1	1A	2249	G	N1-C2-N2	-5.31	111.42	116.20
1	1A	2576	A	N9-C4-C5	-5.31	103.68	105.80
1	1A	2791	A	C2-N3-C4	-5.31	107.94	110.60
32	1a	377	G	O5'-P-OP2	-5.31	100.92	105.70
32	1a	1416	G	O5'-P-OP1	-5.31	100.92	105.70
1	2A	2146	C	C2-N1-C1'	5.31	124.64	118.80
1	2A	2435	A	C8-N9-C4	-5.31	103.68	105.80
32	2a	772	U	OP2-P-O3'	5.31	116.88	105.20
1	1A	308	U	C5-C4-O4	-5.31	122.72	125.90
1	1A	844	C	C6-N1-C2	5.31	122.42	120.30
1	1A	1573	G	C4-C5-N7	-5.31	108.68	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2728	C	OP1-P-OP2	5.31	127.56	119.60
32	1a	1129	C	N1-C2-O2	5.31	122.08	118.90
32	1a	1202	G	C4-C5-N7	-5.31	108.68	110.80
32	1a	1461	G	N1-C6-O6	5.31	123.08	119.90
1	2A	855	G	C8-N9-C4	-5.31	104.28	106.40
1	2A	2221	G	C8-N9-C4	-5.31	104.28	106.40
1	2A	2896	C	C6-N1-C2	-5.31	118.18	120.30
32	2a	1493	A	C8-N9-C4	5.31	107.92	105.80
1	1A	590	A	N1-C2-N3	-5.31	126.65	129.30
1	1A	1746	G	N1-C2-N2	-5.31	111.42	116.20
1	1A	1790	A	C4-C5-C6	5.31	119.65	117.00
32	1a	235	C	OP1-P-OP2	5.31	127.56	119.60
1	2A	1285	G	N1-C6-O6	5.31	123.08	119.90
1	2A	2035	G	C4-N9-C1'	-5.31	119.60	126.50
1	1A	201	G	C4-C5-N7	5.30	112.92	110.80
1	1A	354	A	C6-C5-N7	-5.30	128.59	132.30
1	1A	672	G	C5-C6-O6	5.30	131.78	128.60
1	1A	854	U	N3-C4-O4	5.30	123.11	119.40
1	1A	1006	C	OP1-P-OP2	5.30	127.56	119.60
1	1A	1301	U	N3-C4-C5	-5.30	111.42	114.60
1	1A	1821	C	C6-N1-C2	5.30	122.42	120.30
1	1A	2184	G	N1-C6-O6	-5.30	116.72	119.90
1	1A	2691	A	C6-N1-C2	-5.30	115.42	118.60
1	1A	2703	C	C2-N3-C4	-5.30	117.25	119.90
1	1A	2774	G	C5-C6-O6	-5.30	125.42	128.60
1	1A	989	G	C8-N9-C1'	-5.30	120.11	127.00
1	1A	2737	C	C6-N1-C1'	5.30	127.16	120.80
1	2A	2661	G	O5'-P-OP2	5.30	117.06	110.70
1	1A	47	G	N9-C4-C5	5.30	107.52	105.40
1	1A	622	G	C5-N7-C8	5.30	106.95	104.30
1	1A	1330	A	C2-N3-C4	-5.30	107.95	110.60
1	1A	2022	G	O5'-P-OP2	-5.30	100.93	105.70
1	1A	2333	G	O5'-P-OP1	5.30	117.06	110.70
1	1A	2574	U	C5-C6-N1	-5.30	120.05	122.70
32	1a	509	A	C8-N9-C4	-5.30	103.68	105.80
1	2A	204	A	OP1-P-O3'	5.30	116.86	105.20
1	2A	243	U	O5'-P-OP1	-5.30	100.93	105.70
1	2A	1084	A	N1-C6-N6	5.30	121.78	118.60
2	2B	33	G	N1-C6-O6	5.30	123.08	119.90
32	2a	769	G	C5-C6-N1	-5.30	108.85	111.50
1	1A	436	C	N3-C4-C5	5.30	124.02	121.90
1	1A	1079	U	C5-C6-N1	-5.30	120.05	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1294	G	C2-N3-C4	-5.30	109.25	111.90
32	1a	664	G	C5-C6-O6	5.30	131.78	128.60
32	1a	1504	G	OP2-P-O3'	5.30	116.86	105.20
1	2A	801	G	O5'-P-OP2	-5.30	100.93	105.70
32	2a	121	C	C6-N1-C2	5.30	122.42	120.30
1	1A	195	U	C5-C6-N1	-5.30	120.05	122.70
1	1A	1629	C	C6-N1-C2	5.30	122.42	120.30
32	1a	729	A	OP1-P-O3'	5.30	116.86	105.20
32	1a	1008	C	N3-C2-O2	-5.30	118.19	121.90
1	2A	2070	G	C5'-C4'-O4'	5.30	115.46	109.10
1	2A	2730	C	C6-N1-C2	-5.30	118.18	120.30
32	2a	802	A	C8-N9-C4	-5.30	103.68	105.80
32	2a	830	G	O5'-P-OP2	5.30	117.06	110.70
1	1A	1151	U	C5-C4-O4	-5.30	122.72	125.90
1	1A	2468	C	O5'-P-OP2	5.30	117.06	110.70
1	1A	2802	C	O4'-C1'-N1	5.30	112.44	108.20
1	2A	1563	G	O5'-P-OP1	-5.30	100.93	105.70
1	2A	1567	A	C5-C6-N6	5.30	127.94	123.70
1	2A	1992	G	C5-C6-N1	5.30	114.15	111.50
1	2A	2102	U	N1-C2-O2	5.30	126.51	122.80
1	1A	16	G	OP1-P-OP2	-5.29	111.66	119.60
1	1A	561	A	C8-N9-C4	-5.29	103.68	105.80
1	1A	2250	G	C2-N3-C4	5.29	114.55	111.90
1	2A	2823	A	C8-N9-C4	5.29	107.92	105.80
1	2A	2858	C	C6-N1-C2	5.29	122.42	120.30
32	2a	1048	G	N9-C1'-C2'	-5.29	106.17	112.00
1	1A	231	G	OP1-P-OP2	-5.29	111.66	119.60
1	1A	251	A	N3-C4-N9	-5.29	123.17	127.40
1	1A	1027	A	N7-C8-N9	-5.29	111.15	113.80
1	1A	1212	C	C4-C5-C6	5.29	120.05	117.40
1	1A	1842	G	C8-N9-C4	-5.29	104.28	106.40
1	1A	2019	G	C5-C6-O6	5.29	131.78	128.60
1	1A	2311	G	OP1-P-O3'	5.29	116.85	105.20
1	1A	2671	G	C5-C6-N1	-5.29	108.85	111.50
1	1A	2843	G	N3-C4-C5	-5.29	125.95	128.60
1	1A	2886	G	N7-C8-N9	5.29	115.75	113.10
32	1a	975	A	O4'-C1'-N9	-5.29	103.97	108.20
32	2a	1078	U	N3-C2-O2	-5.29	118.50	122.20
32	2a	1301	U	C6-N1-C2	5.29	124.18	121.00
32	2a	1489	G	C4-N9-C1'	-5.29	119.62	126.50
1	1A	99	G	N3-C4-C5	5.29	131.25	128.60
1	1A	2176	G	N9-C1'-C2'	-5.29	106.18	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2416	C	OP2-P-O3'	5.29	116.84	105.20
1	1A	2596	U	N3-C4-C5	5.29	117.78	114.60
32	1a	1461	G	N3-C4-C5	5.29	131.25	128.60
32	2a	1500	A	OP1-P-OP2	5.29	127.54	119.60
1	1A	1868	C	N1-C2-O2	-5.29	115.73	118.90
1	1A	2390	A	C6-C5-N7	-5.29	128.60	132.30
1	2A	789	A	C4-C5-N7	5.29	113.34	110.70
1	2A	2206	G	C4-N9-C1'	-5.29	119.62	126.50
1	1A	786	G	N1-C2-N2	5.29	120.96	116.20
1	1A	855	G	C5-N7-C8	5.29	106.94	104.30
1	1A	1128	U	C5-C6-N1	5.29	125.34	122.70
1	1A	1870	G	N9-C4-C5	-5.29	103.28	105.40
32	1a	894	G	C5-C6-O6	-5.29	125.43	128.60
1	2A	1341	U	OP1-P-O3'	5.29	116.83	105.20
32	2a	533	A	C6-C5-N7	-5.29	128.60	132.30
32	2a	1445	C	C5-C6-N1	-5.29	118.36	121.00
1	1A	696	C	N3-C4-C5	-5.29	119.79	121.90
1	1A	1246	C	C2-N3-C4	-5.29	117.26	119.90
1	1A	1509	C	N1-C2-O2	5.29	122.07	118.90
1	1A	2243	C	C6-N1-C2	-5.29	118.19	120.30
1	1A	2452	C	C5-C6-N1	-5.29	118.36	121.00
32	1a	435	C	O5'-P-OP2	5.29	117.04	110.70
45	1n	3	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	2A	686	G	C8-N9-C4	-5.29	104.29	106.40
1	2A	743	G	C5-C6-O6	5.29	131.77	128.60
1	2A	1116	C	N1-C2-O2	5.29	122.07	118.90
1	2A	2146	C	C5-C6-N1	5.29	123.64	121.00
1	1A	1138	C	O4'-C1'-N1	5.28	112.43	108.20
1	1A	1278	G	O5'-P-OP2	5.28	117.04	110.70
32	1a	1231	G	N1-C6-O6	5.28	123.07	119.90
32	1a	1523	G	O5'-P-OP2	-5.28	100.94	105.70
1	2A	1348	G	C5-C6-O6	-5.28	125.43	128.60
1	1A	796	C	C5-C6-N1	-5.28	118.36	121.00
1	1A	1332	A	N1-C6-N6	-5.28	115.43	118.60
1	1A	1474	C	N3-C2-O2	5.28	125.60	121.90
1	1A	2004	C	C5-C6-N1	-5.28	118.36	121.00
1	1A	2726	A	C5-C6-N6	5.28	127.93	123.70
1	2A	97	C	C2-N1-C1'	-5.28	112.99	118.80
1	2A	1343	G	C5-C6-O6	5.28	131.77	128.60
1	2A	1900	A	N3-C4-C5	-5.28	123.10	126.80
1	2A	1990	C	OP2-P-O3'	5.28	116.82	105.20
32	2a	240	C	C2-N3-C4	-5.28	117.26	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	718	C	C6-N1-C1'	5.28	127.14	120.80
1	1A	765	A	C4-C5-C6	5.28	119.64	117.00
1	1A	1007	G	OP2-P-O3'	5.28	116.82	105.20
1	1A	1694	G	O4'-C1'-N9	-5.28	103.97	108.20
1	1A	1701	A	OP2-P-O3'	5.28	116.82	105.20
1	1A	2657	G	N1-C6-O6	5.28	123.07	119.90
32	1a	293	G	C6-C5-N7	-5.28	127.23	130.40
32	1a	1375	A	C4-C5-C6	5.28	119.64	117.00
1	2A	230	U	O5'-P-OP2	-5.28	100.95	105.70
1	2A	555	U	N3-C2-O2	5.28	125.90	122.20
1	2A	2332	U	C5-C4-O4	5.28	129.07	125.90
1	1A	67	G	N9-C4-C5	5.28	107.51	105.40
1	1A	801	C	N1-C2-O2	-5.28	115.73	118.90
1	1A	2110	G	N1-C6-O6	5.28	123.07	119.90
1	1A	2460	A	N9-C4-C5	-5.28	103.69	105.80
2	1B	87	G	N7-C8-N9	-5.28	110.46	113.10
1	1A	493	G	N7-C8-N9	-5.28	110.46	113.10
1	1A	1033	G	N1-C2-N2	5.28	120.95	116.20
1	1A	1050	C	N1-C2-N3	5.28	122.89	119.20
1	1A	1296	G	C5-C6-O6	5.28	131.77	128.60
1	1A	2652	G	C4-C5-N7	-5.28	108.69	110.80
21	1Z	77	ASP	CB-CG-OD1	5.28	123.05	118.30
32	1a	890	G	N3-C2-N2	5.28	123.59	119.90
1	2A	731	C	C6-N1-C2	5.28	122.41	120.30
1	2A	2427	C	C6-N1-C2	5.28	122.41	120.30
32	2a	659	U	N3-C4-O4	-5.28	115.71	119.40
1	1A	16	G	C5-N7-C8	5.28	106.94	104.30
1	1A	696	C	C5-C6-N1	5.28	123.64	121.00
1	1A	1097	G	C6-N1-C2	5.28	128.26	125.10
1	1A	2278	A	O5'-P-OP1	-5.28	100.95	105.70
1	1A	2902	G	C4-C5-N7	5.28	112.91	110.80
1	2A	213	A	OP2-P-O3'	5.28	116.81	105.20
1	2A	271(M)	G	C8-N9-C4	-5.28	104.29	106.40
32	2a	644	G	N7-C8-N9	-5.28	110.46	113.10
1	1A	14	A	N1-C6-N6	5.27	121.76	118.60
1	1A	594	A	N7-C8-N9	-5.27	111.16	113.80
1	1A	1198	C	N3-C4-N4	-5.27	114.31	118.00
1	1A	2179	G	C2-N3-C4	5.27	114.54	111.90
1	1A	2751	A	C8-N9-C4	5.27	107.91	105.80
1	2A	1145	C	N1-C2-O2	-5.27	115.74	118.90
1	1A	1359	U	C2-N1-C1'	5.27	124.03	117.70
1	1A	2879	G	N1-C2-N2	5.27	120.94	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	18	42	ARG	NE-CZ-NH2	-5.27	117.66	120.30
32	1a	1370	G	C2-N3-C4	-5.27	109.26	111.90
32	2a	510	A	C8-N9-C4	-5.27	103.69	105.80
1	1A	762	G	C4-C5-N7	5.27	112.91	110.80
1	1A	1753	U	C6-N1-C2	5.27	124.16	121.00
32	1a	405	U	O5'-P-OP1	-5.27	100.96	105.70
1	2A	1428	C	N3-C4-C5	-5.27	119.79	121.90
1	2A	2262	U	OP1-P-OP2	-5.27	111.69	119.60
1	1A	758	G	C5-C6-N1	-5.27	108.86	111.50
1	1A	2253	A	OP1-P-O3'	5.27	116.79	105.20
32	1a	339	C	C2-N1-C1'	-5.27	113.00	118.80
1	1A	34	C	C6-N1-C1'	5.27	127.12	120.80
1	1A	129	G	N3-C2-N2	5.27	123.59	119.90
1	1A	800	C	N3-C2-O2	-5.27	118.21	121.90
1	1A	1359	U	O4'-C1'-N1	5.27	112.42	108.20
1	1A	2093	A	O5'-P-OP1	-5.27	100.96	105.70
2	1B	56	G	O5'-P-OP1	5.27	117.02	110.70
14	1S	17	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	2A	271(G)	C	C6-N1-C2	-5.27	118.19	120.30
1	2A	1771	C	C5-C4-N4	-5.27	116.51	120.20
1	2A	2056	G	C8-N9-C1'	-5.27	120.15	127.00
32	2a	993	G	C8-N9-C1'	-5.27	120.15	127.00
32	2a	1062	U	O5'-P-OP2	-5.27	100.96	105.70
32	2a	1370	G	C4-C5-N7	5.27	112.91	110.80
1	1A	389	G	C4-C5-N7	5.27	112.91	110.80
1	1A	1980	C	N3-C2-O2	5.27	125.59	121.90
1	2A	614	U	C5-C4-O4	5.27	129.06	125.90
2	2B	119	G	N1-C6-O6	5.27	123.06	119.90
32	2a	1528	U	N3-C4-C5	5.27	117.76	114.60
1	1A	497	A	C6-N1-C2	-5.26	115.44	118.60
1	1A	1131	A	O4'-C1'-N9	5.26	112.41	108.20
1	1A	1179	U	N3-C2-O2	5.26	125.89	122.20
1	1A	1343	C	OP1-P-O3'	5.26	116.78	105.20
1	1A	1794	G	N3-C4-N9	-5.26	122.84	126.00
1	1A	1975	A	C8-N9-C4	5.26	107.91	105.80
1	1A	2194	U	O4'-C1'-N1	5.26	112.41	108.20
1	1A	2464	C	N3-C2-O2	5.26	125.58	121.90
1	1A	2720	G	N9-C4-C5	-5.26	103.30	105.40
1	2A	788	A	C5-C6-N6	-5.26	119.49	123.70
1	2A	1421	G	C5-C6-N1	-5.26	108.87	111.50
1	2A	1613	G	O5'-P-OP2	-5.26	100.96	105.70
1	2A	2070	G	O5'-P-OP2	-5.26	100.96	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2375	G	C2-N3-C4	-5.26	109.27	111.90
1	2A	2611	U	OP1-P-OP2	5.26	127.50	119.60
2	2B	56	G	C4-N9-C1'	5.26	133.34	126.50
32	2a	798	G	C8-N9-C4	-5.26	104.29	106.40
1	1A	1382	A	N1-C6-N6	-5.26	115.44	118.60
1	1A	2189	U	C6-N1-C2	-5.26	117.84	121.00
1	1A	2637	G	C5-N7-C8	5.26	106.93	104.30
32	1a	368	U	C5-C4-O4	-5.26	122.74	125.90
1	2A	2397	G	N1-C6-O6	-5.26	116.74	119.90
1	1A	239	G	C5-N7-C8	-5.26	101.67	104.30
1	1A	1080	G	C6-N1-C2	-5.26	121.94	125.10
1	1A	1228	G	C5-C6-O6	5.26	131.76	128.60
1	1A	1392	G	C4-C5-N7	-5.26	108.69	110.80
32	1a	618	C	C2-N3-C4	5.26	122.53	119.90
32	1a	915	A	C2-N3-C4	5.26	113.23	110.60
1	2A	2172	U	C2-N3-C4	-5.26	123.84	127.00
1	2A	2582	G	N7-C8-N9	5.26	115.73	113.10
32	2a	191	G	C8-N9-C4	-5.26	104.30	106.40
32	2a	879	C	O5'-P-OP2	-5.26	100.97	105.70
32	2a	1158	C	C2-N1-C1'	5.26	124.59	118.80
1	1A	75	C	O5'-P-OP1	-5.26	100.97	105.70
1	1A	348	A	N1-C6-N6	5.26	121.76	118.60
1	1A	1652	G	N7-C8-N9	-5.26	110.47	113.10
1	1A	1746	G	N1-C6-O6	-5.26	116.74	119.90
1	1A	1820	A	N3-C4-C5	5.26	130.48	126.80
1	1A	1856	A	C5-C6-N1	5.26	120.33	117.70
1	1A	2221	A	OP1-P-OP2	-5.26	111.71	119.60
1	2A	1092	C	C5-C6-N1	5.26	123.63	121.00
1	2A	1441	G	C8-N9-C4	5.26	108.50	106.40
1	2A	1930	G	N1-C6-O6	5.26	123.06	119.90
32	2a	310	G	O5'-P-OP1	-5.26	100.97	105.70
32	2a	1013	G	N1-C6-O6	5.26	123.06	119.90
1	1A	904	C	N1-C2-O2	-5.26	115.75	118.90
1	1A	1167	C	OP2-P-O3'	5.26	116.77	105.20
1	1A	1342	G	N7-C8-N9	-5.26	110.47	113.10
1	2A	753	C	C2-N3-C4	-5.26	117.27	119.90
32	2a	402	G	OP2-P-O3'	5.26	116.77	105.20
32	2a	1001	A	O4'-C1'-N9	5.26	112.41	108.20
1	1A	596	G	N9-C4-C5	5.26	107.50	105.40
1	1A	751	G	N3-C2-N2	-5.26	116.22	119.90
1	1A	1190	G	N3-C2-N2	5.26	123.58	119.90
1	1A	1451	U	O5'-P-OP2	-5.26	100.97	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2193	A	N3-C4-N9	5.26	131.61	127.40
1	1A	2725	A	C4-C5-N7	5.26	113.33	110.70
1	1A	2844	G	C5-N7-C8	5.26	106.93	104.30
1	2A	130	C	C6-N1-C2	5.26	122.40	120.30
1	2A	244	A	OP2-P-O3'	5.26	116.77	105.20
1	2A	1052	C	C5-C6-N1	5.26	123.63	121.00
32	2a	1394	A	N9-C4-C5	-5.26	103.70	105.80
32	2a	1528	U	C5-C6-N1	-5.26	120.07	122.70
1	1A	322	G	O5'-P-OP1	5.25	117.01	110.70
1	1A	794	U	OP1-P-O3'	5.25	116.76	105.20
1	1A	952	G	C6-C5-N7	5.25	133.55	130.40
1	1A	1184	G	N3-C4-N9	-5.25	122.85	126.00
1	1A	1726	U	N3-C4-O4	5.25	123.08	119.40
1	1A	2068	G	N3-C2-N2	5.25	123.58	119.90
32	1a	1049	U	C5-C4-O4	-5.25	122.75	125.90
1	2A	920	G	C8-N9-C4	-5.25	104.30	106.40
1	2A	1964	G	O4'-C1'-N9	-5.25	104.00	108.20
1	1A	498	A	O5'-P-OP2	-5.25	100.97	105.70
1	1A	1107	U	N1-C2-O2	5.25	126.48	122.80
1	1A	1670	G	OP1-P-OP2	-5.25	111.72	119.60
1	1A	1698	G	O5'-P-OP2	-5.25	100.97	105.70
1	1A	1739	U	C6-N1-C2	5.25	124.15	121.00
1	1A	2824	C	C5-C6-N1	-5.25	118.37	121.00
2	1B	55	U	N1-C2-O2	-5.25	119.12	122.80
2	1B	84	C	N3-C2-O2	5.25	125.58	121.90
32	1a	668	G	O5'-P-OP2	5.25	117.00	110.70
48	1q	53	LEU	CA-CB-CG	5.25	127.38	115.30
1	2A	228	A	C4-C5-C6	-5.25	114.37	117.00
1	2A	2114	A	N7-C8-N9	5.25	116.43	113.80
1	2A	2139	C	N3-C2-O2	-5.25	118.22	121.90
32	2a	176	C	N3-C4-C5	-5.25	119.80	121.90
32	2a	302	G	N7-C8-N9	-5.25	110.47	113.10
32	2a	572	A	C2-N3-C4	-5.25	107.97	110.60
32	2a	1495	U	C6-N1-C2	-5.25	117.85	121.00
1	1A	474	U	C5-C6-N1	-5.25	120.07	122.70
1	1A	484	G	O4'-C1'-N9	5.25	112.40	108.20
1	1A	910	A	OP2-P-O3'	5.25	116.75	105.20
1	1A	1826	C	C2-N3-C4	-5.25	117.27	119.90
1	1A	2663	C	C5-C4-N4	-5.25	116.52	120.20
1	1A	2664	C	OP1-P-OP2	-5.25	111.72	119.60
32	1a	506	G	O5'-P-OP2	5.25	117.00	110.70
32	1a	718	G	N3-C4-C5	5.25	131.23	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	726	C	N3-C4-C5	-5.25	119.80	121.90
32	1a	748	C	O5'-P-OP1	-5.25	100.97	105.70
1	2A	1902	C	N3-C4-C5	5.25	124.00	121.90
32	2a	343	U	N3-C4-C5	5.25	117.75	114.60
1	1A	201	G	C5-N7-C8	-5.25	101.67	104.30
1	1A	271	U	N3-C4-O4	-5.25	115.72	119.40
1	1A	1692	G	C5-N7-C8	5.25	106.92	104.30
27	15	16	ARG	CG-CD-NE	5.25	122.83	111.80
32	1a	502	G	N1-C6-O6	5.25	123.05	119.90
32	1a	738	C	N3-C4-C5	-5.25	119.80	121.90
1	2A	1327	C	C2-N1-C1'	5.25	124.58	118.80
1	2A	1511	C	C6-N1-C2	-5.25	118.20	120.30
1	2A	2162	G	N3-C4-N9	5.25	129.15	126.00
1	1A	134	G	OP2-P-O3'	5.25	116.75	105.20
1	1A	720	C	N3-C2-O2	5.25	125.57	121.90
1	1A	1242	G	C5-C6-O6	5.25	131.75	128.60
1	1A	1494	G	N3-C2-N2	-5.25	116.23	119.90
1	1A	1810	U	OP2-P-O3'	5.25	116.75	105.20
4	1E	101	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	2A	766	C	C6-N1-C2	5.25	122.40	120.30
1	2A	1062	G	O4'-C1'-N9	5.25	112.40	108.20
1	2A	1275	A	C2-N3-C4	-5.25	107.98	110.60
1	2A	1601	G	O5'-P-OP2	-5.25	100.98	105.70
32	2a	395	C	O5'-P-OP1	-5.25	100.98	105.70
1	1A	694	G	C5-C6-N1	-5.25	108.88	111.50
1	1A	1031	C	OP1-P-OP2	5.25	127.47	119.60
1	1A	2453	C	N3-C2-O2	-5.25	118.23	121.90
1	1A	2628	C	N1-C2-N3	5.25	122.87	119.20
2	1B	93	G	C6-C5-N7	5.25	133.55	130.40
32	1a	1213	A	N1-C6-N6	-5.25	115.45	118.60
1	2A	1823	G	C8-N9-C4	5.25	108.50	106.40
32	2a	428	G	C4-C5-N7	-5.25	108.70	110.80
32	2a	1019	C	C6-N1-C2	-5.25	118.20	120.30
1	1A	747	G	N3-C2-N2	5.25	123.57	119.90
1	1A	972	A	O5'-P-OP2	-5.25	100.98	105.70
1	1A	2483	C	C5-C4-N4	5.25	123.87	120.20
1	1A	2510	C	C5-C4-N4	5.25	123.87	120.20
32	1a	112	G	N1-C2-N2	5.25	120.92	116.20
1	2A	736	C	C6-N1-C2	5.25	122.40	120.30
1	2A	772	C	N3-C4-C5	-5.25	119.80	121.90
1	2A	803	U	O5'-P-OP1	5.25	116.99	110.70
1	2A	1302	A	O5'-P-OP1	-5.25	100.98	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2718	G	C8-N9-C4	-5.25	104.30	106.40
1	1A	58	U	O5'-P-OP2	-5.24	100.98	105.70
1	1A	520	G	OP2-P-O3'	5.24	116.73	105.20
1	1A	522	A	C4-C5-N7	5.24	113.32	110.70
1	1A	645	G	OP1-P-O3'	5.24	116.74	105.20
1	1A	773	G	N9-C4-C5	-5.24	103.30	105.40
1	1A	1555	C	C2-N1-C1'	5.24	124.57	118.80
1	1A	1993	A	O5'-P-OP1	5.24	116.99	110.70
32	1a	1106	G	N7-C8-N9	5.24	115.72	113.10
1	2A	1618	A	C8-N9-C4	-5.24	103.70	105.80
1	2A	2483	C	C5-C6-N1	5.24	123.62	121.00
32	2a	813	U	OP2-P-O3'	5.24	116.74	105.20
1	1A	394	C	OP1-P-OP2	-5.24	111.74	119.60
32	1a	726	C	OP1-P-O3'	5.24	116.73	105.20
1	2A	736	C	OP2-P-O3'	5.24	116.73	105.20
1	2A	2029	G	N1-C6-O6	5.24	123.05	119.90
32	2a	1303	C	N1-C2-O2	5.24	122.05	118.90
32	2a	1469	G	N1-C6-O6	5.24	123.05	119.90
1	1A	52	A	N1-C2-N3	5.24	131.92	129.30
1	1A	740	C	C2-N3-C4	-5.24	117.28	119.90
1	1A	1009	C	C4-C5-C6	5.24	120.02	117.40
1	1A	2278	A	C8-N9-C4	-5.24	103.70	105.80
1	1A	2692	C	C2-N3-C4	5.24	122.52	119.90
1	2A	2429	G	O5'-P-OP1	5.24	116.99	110.70
32	2a	217	C	N3-C2-O2	5.24	125.57	121.90
1	1A	109	A	C5-N7-C8	-5.24	101.28	103.90
1	1A	641	G	N1-C6-O6	-5.24	116.76	119.90
1	1A	978	A	C8-N9-C4	-5.24	103.70	105.80
1	1A	1087	C	C5-C6-N1	5.24	123.62	121.00
1	1A	1648	U	C5-C6-N1	-5.24	120.08	122.70
1	1A	1665	G	O4'-C1'-N9	-5.24	104.01	108.20
1	2A	698	C	C5-C6-N1	-5.24	118.38	121.00
1	2A	877	U	N1-C2-N3	5.24	118.04	114.90
1	1A	178	G	C5-C6-O6	-5.24	125.46	128.60
1	1A	1268	C	C4-C5-C6	5.24	120.02	117.40
1	1A	2421	G	N3-C4-N9	5.24	129.14	126.00
1	1A	2510	C	C5-C6-N1	-5.24	118.38	121.00
32	1a	748	C	C6-N1-C2	-5.24	118.20	120.30
1	1A	88	G	N7-C8-N9	5.24	115.72	113.10
1	1A	1287	A	N1-C6-N6	5.24	121.74	118.60
1	1A	2084	A	N1-C6-N6	5.24	121.74	118.60
1	1A	2118	U	OP2-P-O3'	5.24	116.72	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2496	G	C5-C6-O6	-5.24	125.46	128.60
1	1A	2595	G	O5'-P-OP2	5.24	116.98	110.70
32	1a	903	G	OP2-P-O3'	5.24	116.72	105.20
1	2A	673	C	C5-C4-N4	-5.24	116.53	120.20
1	2A	855	G	N7-C8-N9	5.24	115.72	113.10
1	2A	1276	A	C2-N3-C4	-5.24	107.98	110.60
1	2A	2060	A	C8-N9-C4	-5.24	103.71	105.80
1	1A	2284	U	O5'-P-OP2	-5.23	100.99	105.70
1	2A	1388	G	O5'-P-OP2	-5.23	100.99	105.70
1	2A	1865	G	C4-C5-N7	-5.23	108.71	110.80
32	2a	79	G	C4-N9-C1'	-5.23	119.70	126.50
32	2a	644	G	C8-N9-C4	5.23	108.49	106.40
32	2a	1498	UR3	OP2-P-O3'	5.23	116.72	105.20
1	1A	1018	A	C5-C6-N1	-5.23	115.08	117.70
1	1A	1285	G	C5-C6-O6	5.23	131.74	128.60
1	1A	1914	C	N1-C2-O2	-5.23	115.76	118.90
1	1A	2627	U	C5-C6-N1	-5.23	120.08	122.70
32	1a	1054	C	N3-C4-N4	-5.23	114.34	118.00
1	2A	738	G	OP1-P-O3'	5.23	116.71	105.20
32	2a	1499	A	N1-C2-N3	-5.23	126.68	129.30
1	1A	435	G	C5-N7-C8	5.23	106.92	104.30
1	1A	1060	U	O5'-P-OP1	5.23	116.98	110.70
1	1A	1613	A	N1-C2-N3	-5.23	126.68	129.30
1	1A	1977	U	N3-C2-O2	5.23	125.86	122.20
1	1A	1982	A	C6-N1-C2	5.23	121.74	118.60
2	1B	59	A	C5-C6-N1	5.23	120.31	117.70
32	1a	630	G	N1-C2-N3	-5.23	120.76	123.90
1	2A	731	C	C5-C6-N1	-5.23	118.38	121.00
1	2A	746	A	O5'-P-OP1	-5.23	100.99	105.70
1	2A	1690	A	C4-C5-N7	5.23	113.32	110.70
1	2A	1721	G	N9-C4-C5	-5.23	103.31	105.40
1	2A	1745	C	N3-C2-O2	5.23	125.56	121.90
1	2A	2261	C	N3-C2-O2	5.23	125.56	121.90
1	2A	2538	C	C6-N1-C2	5.23	122.39	120.30
32	2a	354	G	C8-N9-C1'	-5.23	120.20	127.00
32	2a	453	A	O5'-P-OP1	-5.23	100.99	105.70
32	2a	1138	G	C4-N9-C1'	5.23	133.30	126.50
1	1A	641	G	N1-C2-N2	-5.23	111.49	116.20
1	1A	1749	G	OP2-P-O3'	5.23	116.70	105.20
1	1A	601	A	N9-C4-C5	5.23	107.89	105.80
1	1A	984	G	C6-N1-C2	-5.23	121.96	125.10
1	1A	1302	G	N3-C2-N2	5.23	123.56	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1663	C	N1-C2-O2	-5.23	115.76	118.90
1	1A	1920	U	C5-C6-N1	-5.23	120.09	122.70
1	1A	2791	A	O5'-P-OP2	-5.23	101.00	105.70
1	1A	2870	A	OP1-P-OP2	-5.23	111.76	119.60
32	1a	668	G	OP1-P-OP2	-5.23	111.76	119.60
1	2A	944	G	C4-N9-C1'	5.23	133.29	126.50
1	2A	1241	A	C8-N9-C4	-5.23	103.71	105.80
1	2A	1258	C	N3-C4-C5	5.23	123.99	121.90
32	2a	610	G	N3-C2-N2	-5.23	116.24	119.90
1	1A	1094	A	N1-C6-N6	-5.23	115.46	118.60
1	1A	2418	U	O4'-C1'-N1	-5.23	104.02	108.20
32	1a	288	A	OP1-P-O3'	5.23	116.70	105.20
32	1a	675	A	OP1-P-O3'	5.23	116.70	105.20
32	1a	1159	U	C5-C4-O4	5.23	129.03	125.90
1	2A	956	G	N3-C2-N2	-5.23	116.24	119.90
1	1A	155	C	N1-C2-O2	5.22	122.03	118.90
1	1A	657	A	C2-N3-C4	-5.22	107.99	110.60
1	1A	1644	C	O5'-P-OP1	-5.22	101.00	105.70
1	1A	2335	G	C8-N9-C4	-5.22	104.31	106.40
1	1A	2483	C	N3-C4-N4	-5.22	114.34	118.00
1	1A	2522	C	C5-C4-N4	5.22	123.86	120.20
32	1a	1145	C	C5-C6-N1	5.22	123.61	121.00
1	2A	794	G	C5-C6-N1	-5.22	108.89	111.50
1	2A	1226	A	C8-N9-C4	5.22	107.89	105.80
1	2A	1818	U	O5'-P-OP2	5.22	116.97	110.70
1	2A	2249	U	N1-C2-O2	5.22	126.46	122.80
1	1A	345	G	C8-N9-C4	5.22	108.49	106.40
1	1A	531	G	O5'-P-OP2	-5.22	101.00	105.70
1	1A	810	G	C8-N9-C4	5.22	108.49	106.40
1	1A	995	G	C2-N3-C4	-5.22	109.29	111.90
1	1A	1098	C	OP2-P-O3'	5.22	116.69	105.20
1	1A	1206	G	N9-C4-C5	-5.22	103.31	105.40
1	1A	2158	C	C2-N1-C1'	5.22	124.54	118.80
1	1A	2534	U	C2-N3-C4	-5.22	123.87	127.00
1	1A	2629	C	N3-C4-C5	-5.22	119.81	121.90
1	1A	705	C	OP1-P-OP2	5.22	127.43	119.60
1	1A	1306	G	C5-C6-O6	5.22	131.73	128.60
1	1A	1995	G	N9-C4-C5	5.22	107.49	105.40
1	1A	2782	C	N1-C2-O2	-5.22	115.77	118.90
1	2A	201	C	C6-N1-C2	5.22	122.39	120.30
32	2a	1185	G	C2-N3-C4	5.22	114.51	111.90
1	1A	593	G	OP2-P-O3'	5.22	116.68	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	893	C	C2-N3-C4	-5.22	117.29	119.90
1	1A	1187	U	N1-C2-O2	5.22	126.45	122.80
1	1A	1710	C	C2-N3-C4	-5.22	117.29	119.90
1	1A	1823	G	C5-N7-C8	5.22	106.91	104.30
1	1A	2348	A	C4-C5-C6	-5.22	114.39	117.00
32	1a	979	C	N3-C4-C5	-5.22	119.81	121.90
1	2A	888	C	C5-C6-N1	5.22	123.61	121.00
1	2A	2241	A	C5-C6-N6	5.22	127.88	123.70
1	2A	2729	G	N1-C6-O6	-5.22	116.77	119.90
32	2a	49	U	N1-C2-O2	5.22	126.45	122.80
32	2a	105	G	N7-C8-N9	5.22	115.71	113.10
1	1A	494	G	C5-N7-C8	5.22	106.91	104.30
1	1A	855	G	N1-C6-O6	-5.22	116.77	119.90
1	1A	1035	G	N3-C4-N9	5.22	129.13	126.00
1	1A	1639	G	N3-C2-N2	-5.22	116.25	119.90
1	1A	2576	A	C5-C6-N6	-5.22	119.53	123.70
32	1a	777	A	O5'-P-OP2	-5.22	101.00	105.70
1	2A	540	C	C6-N1-C2	-5.22	118.21	120.30
1	2A	1275	A	C8-N9-C4	5.22	107.89	105.80
1	2A	1361	G	C5-C6-O6	5.22	131.73	128.60
1	2A	2515	C	C5-C6-N1	-5.22	118.39	121.00
32	2a	269	C	C5-C6-N1	-5.22	118.39	121.00
1	1A	1104	G	N3-C4-N9	5.22	129.13	126.00
1	1A	2093	A	C2-N3-C4	-5.22	107.99	110.60
1	1A	2250	G	N3-C2-N2	5.22	123.55	119.90
1	1A	2262	G	O4'-C1'-N9	5.22	112.37	108.20
1	2A	994	C	C5-C6-N1	-5.22	118.39	121.00
1	2A	1445(A)	C	C6-N1-C2	-5.22	118.21	120.30
1	2A	2332	U	N3-C2-O2	-5.22	118.55	122.20
32	2a	288	A	OP2-P-O3'	-5.22	93.72	105.20
32	2a	1500	A	C6-N1-C2	5.22	121.73	118.60
32	2a	1529	G	N1-C2-N2	-5.22	111.51	116.20
1	1A	2546	A	N3-C4-N9	5.21	131.57	127.40
1	1A	2768	C	N1-C2-N3	5.21	122.85	119.20
1	1A	2534	U	C5-C4-O4	-5.21	122.77	125.90
32	1a	910	C	C2-N3-C4	-5.21	117.29	119.90
32	1a	948	C	C6-N1-C2	5.21	122.39	120.30
1	2A	1201	C	OP1-P-OP2	5.21	127.42	119.60
18	2W	94	ASP	CB-CA-C	5.21	120.82	110.40
32	2a	625	G	N7-C8-N9	5.21	115.71	113.10
32	2a	869	G	O5'-P-OP2	5.21	116.95	110.70
32	2a	998	G	C6-C5-N7	5.21	133.53	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1789	G	OP2-P-O3'	5.21	116.66	105.20
1	1A	1790	A	N9-C4-C5	-5.21	103.72	105.80
32	1a	224	C	OP1-P-OP2	5.21	127.42	119.60
1	2A	989	G	O5'-P-OP1	-5.21	101.01	105.70
1	2A	1091	G	C2-N3-C4	5.21	114.50	111.90
1	1A	276	C	OP2-P-O3'	5.21	116.66	105.20
1	1A	532	A	OP1-P-O3'	5.21	116.66	105.20
1	1A	1039	G	C5-C6-O6	5.21	131.72	128.60
1	1A	1597	C	N1-C2-O2	-5.21	115.78	118.90
1	1A	1649	A	OP1-P-O3'	5.21	116.66	105.20
32	1a	189(G)	G	N1-C6-O6	5.21	123.03	119.90
32	1a	598	U	OP1-P-O3'	5.21	116.66	105.20
1	2A	866	A	C8-N9-C1'	-5.21	118.32	127.70
1	2A	2182	G	N9-C4-C5	5.21	107.48	105.40
32	2a	587	G	N7-C8-N9	5.21	115.70	113.10
32	2a	709	G	C8-N9-C4	-5.21	104.32	106.40
32	2a	758	G	C2-N3-C4	-5.21	109.30	111.90
1	1A	30	G	N1-C2-N3	5.21	127.02	123.90
1	1A	848	G	N1-C6-O6	-5.21	116.78	119.90
1	1A	1856	A	C2-N3-C4	5.21	113.20	110.60
1	1A	1858	C	N3-C4-N4	-5.21	114.36	118.00
1	1A	2048	C	N1-C2-N3	5.21	122.84	119.20
2	1B	91	C	C4-C5-C6	-5.21	114.80	117.40
1	2A	1821	A	N1-C6-N6	-5.21	115.48	118.60
1	2A	2708	G	C8-N9-C4	5.21	108.48	106.40
2	2B	35	U	N1-C2-O2	5.21	126.44	122.80
32	2a	1465	C	N3-C4-C5	5.21	123.98	121.90
1	1A	2001	C	C5-C4-N4	-5.21	116.56	120.20
1	1A	2556	G	OP1-P-OP2	-5.21	111.79	119.60
32	1a	385	C	N1-C2-O2	-5.21	115.78	118.90
1	1A	987	G	OP2-P-O3'	-5.20	93.75	105.20
1	1A	1369	U	OP1-P-O3'	5.20	116.65	105.20
1	1A	1679	A	C5-N7-C8	5.20	106.50	103.90
1	1A	2030	C	C5-C6-N1	-5.20	118.40	121.00
1	1A	2062	C	N3-C4-N4	5.20	121.64	118.00
2	1B	4	C	N1-C2-O2	-5.20	115.78	118.90
32	1a	1530	G	C8-N9-C4	5.20	108.48	106.40
1	2A	567	A	C5-C6-N6	-5.20	119.54	123.70
32	2a	921	U	O5'-P-OP1	5.20	116.94	110.70
1	1A	1314	A	O5'-P-OP2	-5.20	101.02	105.70
1	1A	1892	G	O5'-P-OP2	-5.20	101.02	105.70
1	1A	2015	U	C5-C4-O4	5.20	129.02	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2479	C	O5'-P-OP2	-5.20	101.02	105.70
32	1a	776	G	O5'-P-OP1	-5.20	101.02	105.70
32	2a	290	C	C6-N1-C2	5.20	122.38	120.30
32	2a	1415	G	O5'-P-OP2	-5.20	101.02	105.70
1	1A	62	U	N1-C2-N3	5.20	118.02	114.90
1	1A	383	A	OP1-P-OP2	5.20	127.40	119.60
1	1A	1006	C	N1-C2-N3	5.20	122.84	119.20
1	1A	1245	C	C2-N1-C1'	-5.20	113.08	118.80
1	1A	1443	U	N3-C4-O4	-5.20	115.76	119.40
1	1A	1838	G	N3-C2-N2	-5.20	116.26	119.90
1	1A	1902	C	OP2-P-O3'	5.20	116.64	105.20
1	1A	1903	C	O5'-P-OP1	-5.20	101.02	105.70
1	1A	2900	G	N1-C6-O6	5.20	123.02	119.90
10	1O	23	ARG	CA-CB-CG	5.20	124.84	113.40
32	1a	152	A	N9-C4-C5	-5.20	103.72	105.80
32	1a	192	U	C6-N1-C2	-5.20	117.88	121.00
1	2A	2576	G	C8-N9-C4	5.20	108.48	106.40
32	2a	1029	C	C2-N3-C4	5.20	122.50	119.90
1	1A	11	G	C8-N9-C1'	5.20	133.76	127.00
1	1A	243	G	C4-C5-N7	-5.20	108.72	110.80
1	1A	1503	G	N1-C6-O6	5.20	123.02	119.90
1	1A	1517	G	C5-C6-O6	-5.20	125.48	128.60
1	1A	1621	C	C5-C6-N1	-5.20	118.40	121.00
1	1A	1986	G	C6-C5-N7	-5.20	127.28	130.40
1	1A	2297	C	N1-C2-O2	5.20	122.02	118.90
1	1A	2628	C	C2-N3-C4	-5.20	117.30	119.90
32	1a	134	A	N9-C4-C5	-5.20	103.72	105.80
32	1a	181	G	O4'-C1'-N9	5.20	112.36	108.20
1	2A	1137	G	C5-C6-N1	-5.20	108.90	111.50
1	2A	2891	G	C5-C6-O6	-5.20	125.48	128.60
13	2R	114	VAL	CB-CA-C	-5.20	101.52	111.40
32	2a	569	C	C5-C6-N1	-5.20	118.40	121.00
32	2a	787	A	N9-C4-C5	-5.20	103.72	105.80
32	2a	1504	G	N3-C4-N9	-5.20	122.88	126.00
1	1A	1781	G	O5'-P-OP1	-5.20	101.02	105.70
1	1A	2373	A	C2-N3-C4	-5.20	108.00	110.60
1	1A	2671	G	N3-C4-N9	-5.20	122.88	126.00
1	2A	1783	A	C6-C5-N7	5.20	135.94	132.30
1	2A	2049	G	C5-C6-O6	5.20	131.72	128.60
1	2A	2419	U	OP1-P-O3'	5.20	116.63	105.20
2	2B	84	C	N3-C2-O2	5.20	125.54	121.90
32	2a	945	G	C4-C5-N7	5.20	112.88	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	478	G	C5-C6-N1	5.20	114.10	111.50
1	1A	752	A	C6-C5-N7	-5.20	128.66	132.30
1	1A	2068	G	N1-C2-N2	-5.20	111.53	116.20
1	1A	2711	C	C5-C6-N1	-5.20	118.40	121.00
32	1a	911	U	N1-C2-N3	5.20	118.02	114.90
32	1a	1192	C	O5'-P-OP2	5.20	116.94	110.70
1	2A	845	G	N3-C4-N9	5.20	129.12	126.00
1	2A	1053	C	P-O3'-C3'	5.20	125.93	119.70
1	2A	2741	A	N1-C6-N6	5.20	121.72	118.60
2	2B	72	G	N3-C4-N9	5.20	129.12	126.00
2	2B	89	G	O5'-P-OP2	-5.20	101.02	105.70
32	2a	24	U	N3-C4-C5	-5.20	111.48	114.60
32	2a	1470	G	O5'-P-OP1	-5.20	101.02	105.70
1	1A	2637	G	C4-C5-N7	-5.19	108.72	110.80
32	1a	1346	A	OP1-P-O3'	5.19	116.63	105.20
1	2A	380	U	N3-C4-O4	5.19	123.04	119.40
1	2A	710	G	N1-C6-O6	5.19	123.02	119.90
1	2A	2794	C	C2-N3-C4	5.19	122.50	119.90
1	1A	779	C	C6-N1-C1'	5.19	127.03	120.80
1	1A	1078	A	OP1-P-OP2	5.19	127.39	119.60
1	1A	1242	G	C4-N9-C1'	-5.19	119.75	126.50
1	1A	1721	G	C8-N9-C1'	-5.19	120.25	127.00
1	1A	1965	U	O5'-P-OP2	-5.19	101.03	105.70
1	1A	2722	C	OP2-P-O3'	5.19	116.62	105.20
32	1a	34	C	C6-N1-C2	5.19	122.38	120.30
32	1a	1510	U	N3-C2-O2	5.19	125.83	122.20
1	2A	125	G	C5-N7-C8	-5.19	101.70	104.30
1	2A	1799	G	C6-N1-C2	-5.19	121.98	125.10
1	1A	322	G	N3-C4-N9	5.19	129.12	126.00
1	1A	474	U	N1-C2-N3	5.19	118.01	114.90
1	1A	600	G	C5-N7-C8	5.19	106.90	104.30
1	1A	1039	G	O5'-P-OP1	-5.19	101.03	105.70
1	1A	1243	U	N3-C2-O2	-5.19	118.57	122.20
1	1A	2822	G	N1-C2-N2	-5.19	111.53	116.20
1	1A	2863	C	C6-N1-C2	5.19	122.38	120.30
1	2A	2179	C	C5-C6-N1	5.19	123.59	121.00
32	2a	561	U	O5'-P-OP1	-5.19	101.03	105.70
1	1A	1785	C	N3-C4-N4	-5.19	114.37	118.00
7	1H	60	ARG	NE-CZ-NH1	-5.19	117.70	120.30
32	1a	158	G	C8-N9-C1'	5.19	133.75	127.00
32	1a	704	A	OP1-P-O3'	5.19	116.62	105.20
32	2a	1103	C	C5-C6-N1	5.19	123.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	813	C	C2-N3-C4	-5.19	117.31	119.90
1	1A	2188	G	C4-N9-C1'	-5.19	119.75	126.50
1	1A	2633	A	N1-C2-N3	-5.19	126.71	129.30
15	1T	124	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	2A	228	A	C8-N9-C1'	5.19	137.04	127.70
1	2A	940	G	C5-C6-O6	5.19	131.71	128.60
1	2A	1667	G	N7-C8-N9	-5.19	110.51	113.10
32	2a	1528	U	O5'-P-OP1	5.19	116.92	110.70
1	1A	169	G	O5'-P-OP1	-5.19	101.03	105.70
1	1A	1312	G	C2-N3-C4	5.19	114.49	111.90
1	1A	2298	A	C8-N9-C4	-5.19	103.73	105.80
1	1A	2708	U	C5-C4-O4	-5.19	122.79	125.90
1	1A	2812	A	C2-N3-C4	5.19	113.19	110.60
1	1A	2832	G	N9-C4-C5	-5.19	103.33	105.40
32	1a	815	A	N7-C8-N9	-5.19	111.21	113.80
32	1a	1278	U	C6-N1-C2	-5.19	117.89	121.00
1	2A	1187	G	OP2-P-O3'	5.19	116.61	105.20
32	2a	332	G	O4'-C1'-N9	-5.19	104.05	108.20
32	2a	424	G	OP1-P-O3'	5.19	116.61	105.20
32	2a	1163	C	N1-C2-O2	5.19	122.01	118.90
1	1A	421	A	C5-N7-C8	5.18	106.49	103.90
1	1A	777	C	N3-C4-C5	5.18	123.97	121.90
1	1A	895	G	C8-N9-C4	5.18	108.47	106.40
1	1A	2272	C	C2-N3-C4	-5.18	117.31	119.90
32	1a	873	A	N1-C6-N6	5.18	121.71	118.60
32	1a	1442	G	P-O3'-C3'	5.18	125.92	119.70
1	2A	10	G	N3-C4-C5	5.18	131.19	128.60
1	2A	1345	C	C5-C6-N1	-5.18	118.41	121.00
1	2A	1359	A	N1-C2-N3	-5.18	126.71	129.30
32	2a	397	A	C8-N9-C4	-5.18	103.73	105.80
32	2a	1314	C	C6-N1-C2	-5.18	118.23	120.30
1	1A	256	C	C2-N3-C4	-5.18	117.31	119.90
1	1A	1615	G	N3-C4-N9	5.18	129.11	126.00
1	1A	1709	C	C2-N3-C4	-5.18	117.31	119.90
1	1A	2179	G	N3-C4-C5	-5.18	126.01	128.60
1	1A	2320	G	C8-N9-C4	-5.18	104.33	106.40
32	1a	121	C	C5-C4-N4	-5.18	116.57	120.20
32	1a	486	U	O4'-C1'-N1	5.18	112.34	108.20
32	1a	1255	G	C8-N9-C4	5.18	108.47	106.40
32	1a	1289	A	N1-C6-N6	5.18	121.71	118.60
48	1q	6	LEU	CA-CB-CG	5.18	127.22	115.30
1	2A	13	A	C5-C6-N6	5.18	127.84	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1238	G	N7-C8-N9	-5.18	110.51	113.10
1	2A	1793	C	C2-N3-C4	-5.18	117.31	119.90
1	2A	1926	U	N3-C4-O4	-5.18	115.77	119.40
1	2A	2508	G	N9-C4-C5	-5.18	103.33	105.40
32	2a	266	G	C2'-C3'-O3'	5.18	121.99	113.70
32	2a	1331	G	O4'-C1'-N9	5.18	112.35	108.20
1	1A	64	C	O5'-P-OP2	-5.18	101.04	105.70
1	1A	1855	G	C5-C6-O6	-5.18	125.49	128.60
1	1A	2188	G	C6-C5-N7	5.18	133.51	130.40
2	1B	62	C	C6-N1-C2	5.18	122.37	120.30
32	1a	1184	G	OP1-P-OP2	-5.18	111.83	119.60
32	1a	1282	C	N1-C2-O2	5.18	122.01	118.90
1	2A	1636	C	OP1-P-O3'	5.18	116.60	105.20
1	2A	2242	G	C5-C6-N1	-5.18	108.91	111.50
1	1A	73	A	C5-C6-N1	5.18	120.29	117.70
1	1A	144	C	N3-C4-C5	-5.18	119.83	121.90
1	1A	706	C	OP2-P-O3'	5.18	116.59	105.20
1	1A	1220	U	OP1-P-OP2	-5.18	111.83	119.60
1	1A	1700	G	C2'-C3'-O3'	5.18	121.99	113.70
32	1a	123	C	C5-C6-N1	-5.18	118.41	121.00
1	2A	363(B)	G	C4-N9-C1'	5.18	133.23	126.50
1	2A	1092	C	OP1-P-OP2	5.18	127.37	119.60
1	2A	1243	G	N1-C2-N3	5.18	127.01	123.90
1	2A	2324	C	N3-C2-O2	5.18	125.53	121.90
32	2a	1134	G	C8-N9-C4	-5.18	104.33	106.40
32	2a	1150	U	N3-C4-C5	-5.18	111.49	114.60
1	1A	566	C	OP1-P-OP2	5.18	127.37	119.60
1	1A	2405	A	C5-C6-N6	-5.18	119.56	123.70
1	1A	2475	C	C5-C6-N1	-5.18	118.41	121.00
2	1B	52	A	C5-C6-N6	-5.18	119.56	123.70
32	1a	1024	G	C8-N9-C4	-5.18	104.33	106.40
46	1o	23	GLY	N-CA-C	5.18	126.05	113.10
1	2A	41	C	C5-C6-N1	-5.18	118.41	121.00
1	2A	2166	G	C4-C5-N7	-5.18	108.73	110.80
1	2A	2886	G	C8-N9-C4	-5.18	104.33	106.40
32	2a	892	A	C6-N1-C2	-5.18	115.49	118.60
1	1A	799	A	O5'-P-OP1	-5.18	101.04	105.70
1	1A	1035	G	C5-N7-C8	5.18	106.89	104.30
1	1A	2455	C	C6-N1-C2	-5.18	118.23	120.30
1	1A	2477	C	C4-C5-C6	-5.18	114.81	117.40
1	1A	2573	A	C5-C6-N6	5.18	127.84	123.70
1	1A	2717	A	C4-C5-N7	5.18	113.29	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	913	A	N1-C6-N6	-5.18	115.49	118.60
1	2A	711	G	C5-C6-N1	-5.18	108.91	111.50
1	2A	2021	C	C6-N1-C2	5.18	122.37	120.30
2	2B	35	U	N3-C2-O2	-5.18	118.58	122.20
1	1A	82	G	N1-C2-N2	-5.17	111.54	116.20
1	1A	305	G	C8-N9-C4	5.17	108.47	106.40
1	1A	308	U	N1-C2-O2	-5.17	119.18	122.80
1	1A	357	G	C4-C5-N7	-5.17	108.73	110.80
1	1A	821	A	N9-C4-C5	5.17	107.87	105.80
1	1A	1546	G	O5'-P-OP2	-5.17	101.04	105.70
1	1A	2308	U	C4-C5-C6	5.17	122.81	119.70
1	1A	2762	A	C2-N3-C4	5.17	113.19	110.60
32	1a	644	G	O5'-P-OP2	-5.17	101.04	105.70
1	2A	129	C	O5'-P-OP2	-5.17	101.04	105.70
1	2A	507	A	C4-C5-C6	-5.17	114.41	117.00
1	2A	527	C	C2-N1-C1'	-5.17	113.11	118.80
1	2A	667	U	N1-C2-O2	-5.17	119.18	122.80
1	2A	2834	G	N3-C2-N2	5.17	123.52	119.90
32	2a	353	A	C4-C5-N7	5.17	113.29	110.70
1	1A	858	U	C5-C4-O4	5.17	129.00	125.90
2	1B	13	A	OP1-P-OP2	5.17	127.36	119.60
32	1a	7	G	N9-C4-C5	-5.17	103.33	105.40
1	2A	652	C	O5'-P-OP2	5.17	116.91	110.70
1	2A	771	G	N3-C4-N9	-5.17	122.90	126.00
1	2A	1701	A	O5'-P-OP1	-5.17	101.05	105.70
1	1A	225	C	O5'-P-OP1	5.17	116.91	110.70
1	1A	1152	G	O4'-C1'-N9	-5.17	104.06	108.20
1	1A	1306	G	C5-C6-N1	-5.17	108.92	111.50
1	1A	2440	G	N1-C6-O6	-5.17	116.80	119.90
18	1W	111	HIS	N-CA-C	5.17	124.96	111.00
1	2A	1772	G	C5-C6-O6	5.17	131.70	128.60
1	2A	2263	C	N3-C2-O2	5.17	125.52	121.90
2	2B	25	A	N1-C6-N6	5.17	121.70	118.60
32	2a	169	C	OP1-P-O3'	5.17	116.58	105.20
1	1A	84	G	N3-C2-N2	-5.17	116.28	119.90
1	1A	92	C	C6-N1-C2	-5.17	118.23	120.30
1	1A	2682	A	O4'-C1'-N9	-5.17	104.06	108.20
32	1a	534	U	C5-C6-N1	-5.17	120.11	122.70
32	1a	1505	G	N3-C4-N9	-5.17	122.90	126.00
1	2A	2371	G	C5-C6-N1	5.17	114.08	111.50
1	1A	858	U	N3-C4-O4	-5.17	115.78	119.40
1	1A	1184	G	C6-C5-N7	5.17	133.50	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1482	G	OP1-P-OP2	-5.17	111.85	119.60
2	1B	105	A	C8-N9-C4	5.17	107.87	105.80
32	1a	365	U	O4'-C1'-N1	5.17	112.33	108.20
32	1a	496	A	C2-N3-C4	5.17	113.18	110.60
1	2A	775	G	N9-C4-C5	-5.17	103.33	105.40
1	2A	1409	C	OP1-P-OP2	5.17	127.35	119.60
32	2a	552	U	OP2-P-O3'	5.17	116.57	105.20
32	2a	854	G	C5-N7-C8	-5.17	101.72	104.30
32	2a	1227	A	C2-N3-C4	-5.17	108.02	110.60
1	1A	809	U	C5-C4-O4	-5.17	122.80	125.90
1	1A	1434	G	C5-C6-O6	5.17	131.70	128.60
1	1A	2394	G	N3-C2-N2	5.17	123.52	119.90
1	1A	2514	G	N3-C4-N9	5.17	129.10	126.00
8	1I	43	ASN	N-CA-CB	5.17	119.90	110.60
32	1a	776	G	N1-C6-O6	5.17	123.00	119.90
32	1a	1117	G	N3-C4-C5	-5.17	126.02	128.60
1	2A	271(K)	U	C6-N1-C2	-5.17	117.90	121.00
1	2A	595	C	C5-C4-N4	-5.17	116.58	120.20
1	2A	1079	C	N1-C2-N3	5.17	122.82	119.20
1	2A	1967	C	C6-N1-C2	5.17	122.37	120.30
1	2A	2177	C	C2-N3-C4	5.17	122.48	119.90
32	2a	572	A	N7-C8-N9	-5.17	111.22	113.80
32	2a	797	C	O5'-P-OP2	5.17	116.90	110.70
32	2a	876	G	C6-C5-N7	5.17	133.50	130.40
1	1A	1478	C	N1-C2-O2	-5.17	115.80	118.90
1	2A	1408	C	N1-C2-O2	-5.17	115.80	118.90
1	2A	1992	G	C4-N9-C1'	5.17	133.21	126.50
1	1A	201	G	C2-N3-C4	-5.16	109.32	111.90
1	1A	1291	G	O5'-P-OP2	5.16	116.90	110.70
1	1A	1673	G	N3-C2-N2	5.16	123.52	119.90
1	1A	2229	A	O4'-C1'-N9	5.16	112.33	108.20
1	1A	2437	A	C6-N1-C2	-5.16	115.50	118.60
1	1A	2792	U	C4-C5-C6	-5.16	116.60	119.70
32	1a	103	C	O5'-P-OP2	5.16	116.90	110.70
1	2A	593	G	N1-C6-O6	5.16	123.00	119.90
1	2A	2520	C	C2-N3-C4	-5.16	117.32	119.90
1	2A	2592	G	N1-C2-N3	5.16	127.00	123.90
1	1A	554	A	N1-C6-N6	5.16	121.70	118.60
1	1A	1222	A	C8-N9-C4	-5.16	103.73	105.80
1	2A	932	G	C4-C5-N7	-5.16	108.73	110.80
2	2B	24	G	C6-C5-N7	-5.16	127.30	130.40
32	2a	1517	G	O5'-P-OP1	5.16	116.89	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	146	G	N1-C2-N2	-5.16	111.56	116.20
1	1A	398	A	N9-C4-C5	-5.16	103.73	105.80
1	1A	1782	C	N1-C2-O2	-5.16	115.80	118.90
1	1A	2054	G	O5'-P-OP1	-5.16	101.06	105.70
1	1A	2372	A	OP1-P-OP2	5.16	127.34	119.60
1	1A	2597	U	C2-N1-C1'	-5.16	111.51	117.70
1	1A	2693	C	C5-C6-N1	-5.16	118.42	121.00
1	1A	2843	G	C8-N9-C4	-5.16	104.34	106.40
32	1a	558	G	C5-C6-O6	-5.16	125.50	128.60
1	2A	127	A	C5-C6-N1	5.16	120.28	117.70
1	2A	866	A	C4-N9-C1'	5.16	135.59	126.30
1	2A	1394	U	OP1-P-OP2	-5.16	111.86	119.60
1	2A	1757	U	N3-C2-O2	5.16	125.81	122.20
1	2A	1772	G	N9-C1'-C2'	-5.16	106.32	112.00
1	2A	1853	A	C5-N7-C8	5.16	106.48	103.90
1	1A	652	A	C2-N3-C4	5.16	113.18	110.60
1	1A	1029	A	C8-N9-C4	5.16	107.86	105.80
1	1A	1170	C	C6-N1-C2	5.16	122.36	120.30
1	1A	1537	G	C4-C5-N7	-5.16	108.74	110.80
1	1A	1544	C	C4-C5-C6	-5.16	114.82	117.40
1	1A	2449	U	C2-N3-C4	-5.16	123.91	127.00
1	1A	2510	C	N1-C2-N3	5.16	122.81	119.20
32	1a	1513	A	C6-N1-C2	-5.16	115.50	118.60
1	2A	1109	C	N1-C2-O2	5.16	122.00	118.90
1	2A	1836	C	O5'-P-OP1	5.16	116.89	110.70
32	2a	575	G	O4'-C1'-N9	-5.16	104.07	108.20
32	2a	884	U	O5'-P-OP2	-5.16	101.06	105.70
1	2A	178	G	C2-N3-C4	5.16	114.48	111.90
1	2A	2328	A	N7-C8-N9	-5.16	111.22	113.80
1	2A	2501	C	C5-C6-N1	-5.16	118.42	121.00
1	1A	335	A	N1-C2-N3	-5.16	126.72	129.30
1	1A	493	G	C5-N7-C8	5.16	106.88	104.30
1	1A	2031	G	N9-C4-C5	5.16	107.46	105.40
1	1A	2082	A	C6-C5-N7	5.16	135.91	132.30
1	1A	2134	G	C6-C5-N7	-5.16	127.31	130.40
1	1A	2630	G	N1-C6-O6	-5.16	116.81	119.90
32	1a	248	C	OP1-P-OP2	5.16	127.33	119.60
1	2A	752	A	C5-N7-C8	-5.16	101.32	103.90
1	2A	1328	G	C6-N1-C2	-5.16	122.01	125.10
1	2A	1926	U	C2-N1-C1'	-5.16	111.51	117.70
1	2A	2805	G	C2-N3-C4	5.16	114.48	111.90
1	2A	2847	U	C5-C6-N1	-5.16	120.12	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	189(J)	G	N9-C4-C5	-5.16	103.34	105.40
1	1A	831	A	C8-N9-C4	5.15	107.86	105.80
1	1A	1382	A	N1-C2-N3	5.15	131.88	129.30
16	1U	3	ARG	NE-CZ-NH2	-5.15	117.72	120.30
32	1a	280	C	C5-C4-N4	-5.15	116.59	120.20
32	1a	523	A	N1-C6-N6	5.15	121.69	118.60
1	1A	572	A	C8-N9-C4	-5.15	103.74	105.80
1	1A	1022	C	OP2-P-O3'	5.15	116.54	105.20
1	1A	1829	U	N3-C4-O4	-5.15	115.79	119.40
32	1a	607	A	C4-C5-C6	5.15	119.58	117.00
32	1a	802	A	C4-C5-N7	5.15	113.28	110.70
32	1a	878	G	N1-C2-N2	-5.15	111.56	116.20
1	2A	1031	G	N1-C6-O6	5.15	122.99	119.90
1	2A	1108	U	C6-N1-C2	-5.15	117.91	121.00
1	2A	2858	C	N3-C4-C5	5.15	123.96	121.90
32	2a	45	U	C6-N1-C2	5.15	124.09	121.00
1	1A	91	G	O5'-P-OP1	-5.15	101.06	105.70
1	1A	881	C	N1-C2-O2	-5.15	115.81	118.90
1	1A	1012	C	N3-C4-C5	5.15	123.96	121.90
1	1A	1472	G	C5-C6-N1	5.15	114.08	111.50
1	1A	2009	G	C2-N3-C4	-5.15	109.33	111.90
1	1A	2058	C	N3-C4-C5	5.15	123.96	121.90
1	1A	2137	G	C2-N3-C4	5.15	114.47	111.90
1	1A	2244	U	N3-C4-O4	-5.15	115.79	119.40
2	1B	25	A	N1-C6-N6	5.15	121.69	118.60
32	1a	1184	G	N1-C6-O6	5.15	122.99	119.90
1	2A	354	G	N9-C4-C5	-5.15	103.34	105.40
1	2A	1755	A	OP1-P-O3'	5.15	116.53	105.20
1	2A	1799	G	C5-C6-O6	-5.15	125.51	128.60
32	2a	562	C	C5-C4-N4	-5.15	116.59	120.20
1	1A	623	G	C8-N9-C4	-5.15	104.34	106.40
1	1A	1800	G	O5'-P-OP1	5.15	116.88	110.70
1	1A	2348	A	C5-C6-N1	5.15	120.27	117.70
1	2A	580	C	N1-C2-O2	-5.15	115.81	118.90
1	2A	675	A	C4-C5-N7	5.15	113.28	110.70
1	2A	1074	G	C4-N9-C1'	-5.15	119.81	126.50
1	2A	1482	G	O5'-P-OP2	-5.15	101.07	105.70
1	1A	646	A	C5-C6-N6	-5.15	119.58	123.70
1	1A	902	G	N9-C4-C5	-5.15	103.34	105.40
1	1A	1998	U	C6-N1-C2	-5.15	117.91	121.00
32	1a	999	C	N1-C2-O2	5.15	121.99	118.90
1	2A	663	G	C8-N9-C4	5.15	108.46	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	554	A	O5'-P-OP1	5.15	116.88	110.70
1	1A	1769	G	C5-C6-O6	5.15	131.69	128.60
1	1A	2534	U	C6-N1-C2	5.15	124.09	121.00
1	1A	2600	G	N3-C2-N2	5.15	123.50	119.90
32	1a	1468	A	C5-C6-N6	-5.15	119.58	123.70
1	2A	206	U	O5'-P-OP2	-5.15	101.07	105.70
1	2A	1091	G	C4-N9-C1'	5.15	133.19	126.50
32	2a	883	C	N1-C2-O2	-5.15	115.81	118.90
1	1A	45	C	O5'-P-OP1	-5.14	101.07	105.70
1	1A	126	C	C2-N3-C4	-5.14	117.33	119.90
1	1A	414	U	C5-C4-O4	-5.14	122.81	125.90
1	1A	832	G	N1-C6-O6	-5.14	116.81	119.90
1	1A	2222	C	O5'-P-OP1	5.14	116.87	110.70
1	1A	2607	G	C4-C5-N7	-5.14	108.74	110.80
32	1a	16	A	OP1-P-O3'	5.14	116.52	105.20
32	1a	533	A	C6-N1-C2	-5.14	115.51	118.60
32	1a	639	G	C8-N9-C4	-5.14	104.34	106.40
32	1a	1193	G	C4-C5-N7	-5.14	108.74	110.80
1	2A	111	A	C2-N3-C4	-5.14	108.03	110.60
1	2A	622	G	C5-N7-C8	5.14	106.87	104.30
32	2a	354	G	C5-N7-C8	-5.14	101.73	104.30
32	2a	776	G	O5'-P-OP2	-5.14	101.07	105.70
1	1A	283	G	C5-C6-N1	-5.14	108.93	111.50
1	1A	540	A	N1-C6-N6	-5.14	115.51	118.60
1	1A	1025	G	C5-C6-O6	5.14	131.69	128.60
1	1A	1211	U	C5-C4-O4	5.14	128.99	125.90
1	1A	1397	C	OP1-P-O3'	5.14	116.51	105.20
1	1A	1474	C	C6-N1-C1'	5.14	126.97	120.80
1	1A	2017	U	N3-C2-O2	5.14	125.80	122.20
1	1A	2435	U	C2-N3-C4	-5.14	123.91	127.00
32	1a	857	C	O5'-P-OP2	-5.14	101.07	105.70
32	1a	1046	A	N1-C6-N6	5.14	121.69	118.60
32	1a	1232	U	C5-C6-N1	5.14	125.27	122.70
32	1a	1525	G	C4-N9-C1'	-5.14	119.81	126.50
32	2a	787	A	C8-N9-C4	5.14	107.86	105.80
32	2a	819	A	O4'-C1'-N9	-5.14	104.09	108.20
32	2a	839	U	N1-C2-N3	-5.14	111.81	114.90
32	2a	1125	U	C6-N1-C2	-5.14	117.92	121.00
1	1A	620	U	OP1-P-OP2	5.14	127.31	119.60
1	2A	633	A	N1-C6-N6	5.14	121.69	118.60
1	2A	1361	G	N1-C6-O6	-5.14	116.81	119.90
1	2A	2119	A	N1-C6-N6	5.14	121.68	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	26	G	O5'-P-OP2	-5.14	101.07	105.70
1	1A	202	A	C4-C5-C6	-5.14	114.43	117.00
1	1A	247	G	C8-N9-C4	-5.14	104.34	106.40
32	1a	224	C	N3-C4-C5	-5.14	119.84	121.90
32	1a	1188	A	OP1-P-OP2	5.14	127.31	119.60
1	2A	391	G	N1-C2-N3	5.14	126.98	123.90
1	2A	537	C	C6-N1-C2	5.14	122.36	120.30
1	2A	1846	G	N3-C4-C5	5.14	131.17	128.60
1	2A	2332	U	N1-C2-N3	5.14	117.98	114.90
32	2a	1504	G	C4-N9-C1'	-5.14	119.82	126.50
1	1A	1255	A	N7-C8-N9	5.14	116.37	113.80
1	1A	2417	G	OP1-P-OP2	5.14	127.31	119.60
32	1a	1493	A	C2-N3-C4	5.14	113.17	110.60
1	2A	195	A	P-O3'-C3'	5.14	125.87	119.70
1	2A	2137	C	C2-N3-C4	5.14	122.47	119.90
32	2a	761	G	N3-C2-N2	-5.14	116.30	119.90
1	1A	262	C	C6-N1-C2	5.14	122.36	120.30
1	1A	503	A	O5'-P-OP2	-5.14	101.08	105.70
1	1A	662	A	C8-N9-C4	5.14	107.86	105.80
1	1A	1069	U	N1-C2-O2	-5.14	119.20	122.80
1	1A	1831	C	N3-C4-C5	-5.14	119.85	121.90
1	1A	2220	A	N7-C8-N9	-5.14	111.23	113.80
1	1A	2637	G	N3-C2-N2	-5.14	116.30	119.90
1	1A	2642	G	O5'-P-OP1	-5.14	101.08	105.70
32	1a	1515	C	N3-C4-C5	-5.14	119.84	121.90
1	2A	2578	G	O5'-P-OP1	-5.14	101.08	105.70
2	2B	88	C	O4'-C1'-N1	5.14	112.31	108.20
2	2B	115	G	N3-C4-C5	5.14	131.17	128.60
1	1A	39	C	O5'-P-OP2	-5.13	101.08	105.70
1	1A	1121	C	C2-N1-C1'	5.13	124.45	118.80
1	1A	1664	A	N9-C4-C5	5.13	107.85	105.80
1	1A	1683	C	O5'-P-OP2	5.13	116.86	110.70
1	1A	1849	U	C2-N3-C4	-5.13	123.92	127.00
1	1A	2160	C	C5-C6-N1	5.13	123.57	121.00
1	1A	2394	G	C4-C5-N7	5.13	112.85	110.80
1	1A	2640	C	N3-C4-C5	5.13	123.95	121.90
12	1Q	6	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	2A	2586	C	OP1-P-OP2	-5.13	111.90	119.60
1	2A	2593	U	OP2-P-O3'	5.13	116.50	105.20
32	2a	242	C	C4-C5-C6	5.13	119.97	117.40
32	2a	441	A	OP2-P-O3'	5.13	116.50	105.20
32	2a	622	A	OP2-P-O3'	5.13	116.50	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	856	C	N3-C4-C5	-5.13	119.85	121.90
1	1A	591	U	C2-N3-C4	-5.13	123.92	127.00
1	1A	2470	G	C4-C5-N7	-5.13	108.75	110.80
1	1A	2896	G	N3-C2-N2	-5.13	116.31	119.90
1	1A	187	C	N3-C2-O2	-5.13	118.31	121.90
1	1A	546	G	OP2-P-O3'	5.13	116.49	105.20
1	1A	567	C	C6-N1-C2	5.13	122.35	120.30
1	1A	780	G	N7-C8-N9	-5.13	110.53	113.10
1	1A	1992	A	O4'-C1'-N9	-5.13	104.09	108.20
1	1A	2437	A	O5'-P-OP2	-5.13	101.08	105.70
1	1A	2757	G	N1-C6-O6	5.13	122.98	119.90
2	1B	113	G	N3-C2-N2	5.13	123.49	119.90
1	2A	466	A	O5'-P-OP1	5.13	116.86	110.70
1	2A	807	U	N1-C2-O2	-5.13	119.21	122.80
1	2A	911	A	OP1-P-OP2	5.13	127.30	119.60
1	2A	2271	G	OP2-P-O3'	5.13	116.49	105.20
1	2A	2406	U	O4'-C1'-N1	-5.13	104.09	108.20
1	2A	2623	G	N1-C6-O6	5.13	122.98	119.90
1	2A	2897	U	C6-N1-C2	-5.13	117.92	121.00
32	2a	563	A	N1-C2-N3	5.13	131.87	129.30
32	2a	1131	G	C2-N3-C4	5.13	114.47	111.90
32	2a	1442	G	N3-C4-N9	5.13	129.08	126.00
1	1A	536	U	N1-C2-N3	5.13	117.98	114.90
1	1A	1832	G	O4'-C1'-N9	5.13	112.30	108.20
1	1A	2440	G	N7-C8-N9	5.13	115.67	113.10
1	2A	212	G	C8-N9-C4	-5.13	104.35	106.40
1	2A	817	C	OP1-P-O3'	5.13	116.49	105.20
1	2A	843	G	O5'-P-OP2	-5.13	101.08	105.70
1	1A	1054	C	C4-C5-C6	5.13	119.97	117.40
1	1A	1167	C	N1-C2-N3	5.13	122.79	119.20
1	1A	1228	G	N1-C6-O6	-5.13	116.82	119.90
1	1A	1561	C	C6-N1-C2	5.13	122.35	120.30
1	1A	1655	A	OP2-P-O3'	5.13	116.48	105.20
1	1A	2262	G	N7-C8-N9	5.13	115.66	113.10
1	1A	2777	A	N3-C4-C5	5.13	130.39	126.80
1	2A	1580	A	OP2-P-O3'	5.13	116.48	105.20
32	2a	255	G	O5'-P-OP1	-5.13	101.08	105.70
32	2a	406	G	C4-C5-N7	5.13	112.85	110.80
32	2a	1158	C	N3-C2-O2	-5.13	118.31	121.90
32	2a	1365	G	C8-N9-C4	-5.13	104.35	106.40
1	1A	37	C	N3-C4-N4	-5.13	114.41	118.00
1	1A	500	G	C5-C6-O6	5.13	131.68	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	785	G	OP1-P-OP2	5.13	127.29	119.60
1	1A	1093	G	C8-N9-C1'	-5.13	120.34	127.00
1	1A	1394	G	C6-N1-C2	-5.13	122.02	125.10
1	1A	1895	U	N1-C2-O2	-5.13	119.21	122.80
1	1A	1932	G	N3-C4-C5	5.13	131.16	128.60
1	1A	1959	A	N1-C2-N3	5.13	131.86	129.30
1	1A	2433	G	C8-N9-C4	5.13	108.45	106.40
32	1a	252	U	OP2-P-O3'	5.13	116.48	105.20
32	1a	658	G	O5'-P-OP1	-5.13	101.09	105.70
32	1a	1394	A	N1-C6-N6	5.13	121.68	118.60
33	1b	111	ARG	NE-CZ-NH1	-5.13	117.74	120.30
1	2A	116	C	C6-N1-C2	-5.13	118.25	120.30
1	2A	1354	A	O5'-P-OP1	5.13	116.85	110.70
1	2A	1883	G	N3-C4-N9	5.13	129.08	126.00
1	2A	2557	G	OP1-P-OP2	-5.13	111.91	119.60
1	1A	425	G	N1-C2-N2	-5.12	111.59	116.20
1	1A	479	C	N3-C4-C5	5.12	123.95	121.90
1	1A	892	G	O5'-P-OP2	-5.12	101.09	105.70
1	2A	2060	A	N9-C4-C5	5.12	107.85	105.80
1	2A	2286	A	N1-C6-N6	-5.12	115.53	118.60
1	1A	1629	C	C2-N3-C4	-5.12	117.34	119.90
1	1A	1896	G	C6-C5-N7	-5.12	127.33	130.40
1	1A	1965	U	N3-C4-O4	-5.12	115.81	119.40
1	1A	2470	G	N3-C2-N2	-5.12	116.31	119.90
1	1A	2554	A	C2-N3-C4	-5.12	108.04	110.60
1	1A	2558	U	N3-C2-O2	5.12	125.79	122.20
32	1a	115	G	C8-N9-C4	-5.12	104.35	106.40
32	1a	150	C	N3-C4-C5	-5.12	119.85	121.90
32	1a	545	C	OP1-P-OP2	5.12	127.28	119.60
1	2A	2319	G	N9-C1'-C2'	5.12	120.66	114.00
2	2B	113	G	C5-C6-O6	-5.12	125.53	128.60
1	1A	1175	A	N3-C4-C5	-5.12	123.22	126.80
1	1A	1219	A	N9-C1'-C2'	5.12	120.66	114.00
1	1A	2282	G	C5-C6-O6	-5.12	125.53	128.60
1	1A	2436	C	N3-C4-C5	-5.12	119.85	121.90
1	1A	2732	G	N3-C2-N2	5.12	123.48	119.90
32	1a	442	C	C2-N1-C1'	5.12	124.43	118.80
1	2A	195	A	OP2-P-O3'	5.12	116.47	105.20
1	2A	1657	C	OP1-P-O3'	-5.12	93.93	105.20
1	2A	1963	U	N3-C2-O2	-5.12	118.61	122.20
32	2a	774	G	N1-C6-O6	5.12	122.97	119.90
1	1A	122	G	N1-C6-O6	5.12	122.97	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	890	G	O5'-P-OP2	-5.12	101.09	105.70
1	2A	711	G	N1-C6-O6	5.12	122.97	119.90
1	2A	1992	G	N9-C4-C5	5.12	107.45	105.40
32	2a	1038	C	C6-N1-C2	-5.12	118.25	120.30
32	2a	1391	U	N1-C2-N3	5.12	117.97	114.90
1	1A	958	C	OP1-P-OP2	5.12	127.28	119.60
1	1A	1382	A	C6-N1-C2	-5.12	115.53	118.60
1	1A	2030	C	C6-N1-C2	-5.12	118.25	120.30
1	1A	2540	U	C5-C4-O4	-5.12	122.83	125.90
17	1V	13	ARG	NE-CZ-NH1	-5.12	117.74	120.30
32	1a	701	C	O5'-P-OP2	-5.12	101.09	105.70
1	2A	308	G	C5-C6-O6	-5.12	125.53	128.60
1	2A	896	A	C8-N9-C4	5.12	107.85	105.80
1	2A	1087	G	C6-C5-N7	5.12	133.47	130.40
1	2A	1615	C	C6-N1-C2	-5.12	118.25	120.30
1	2A	2599	G	C4-C5-N7	-5.12	108.75	110.80
32	2a	52	G	OP1-P-O3'	5.12	116.46	105.20
32	2a	129(A)	G	O5'-P-OP1	-5.12	101.09	105.70
32	2a	961	U	C5-C4-O4	-5.12	122.83	125.90
32	2a	1079	G	N9-C4-C5	5.12	107.45	105.40
1	1A	2447	A	C2-N3-C4	5.12	113.16	110.60
1	2A	1233	C	C5-C6-N1	5.12	123.56	121.00
2	2B	119	G	C5-C6-O6	-5.12	125.53	128.60
32	2a	923	A	O5'-P-OP1	-5.12	101.09	105.70
32	2a	1023	G	C8-N9-C4	-5.12	104.35	106.40
1	1A	132	C	N3-C2-O2	-5.12	118.32	121.90
1	1A	405	C	N3-C4-C5	5.12	123.95	121.90
1	1A	614	C	C5-C6-N1	-5.12	118.44	121.00
1	1A	711	C	N3-C4-C5	5.12	123.95	121.90
1	1A	958	C	N1-C2-O2	5.12	121.97	118.90
1	1A	1757	C	N1-C2-O2	-5.12	115.83	118.90
1	1A	2771	A	C8-N9-C4	5.12	107.85	105.80
2	1B	60	C	C5-C6-N1	5.12	123.56	121.00
1	2A	329	G	C8-N9-C4	-5.12	104.35	106.40
1	2A	675	A	N9-C4-C5	-5.12	103.75	105.80
1	2A	1312	U	C6-N1-C2	-5.12	117.93	121.00
1	2A	2880	C	OP1-P-OP2	5.12	127.27	119.60
1	1A	36	G	N7-C8-N9	-5.11	110.54	113.10
1	1A	1455	C	C2-N3-C4	-5.11	117.34	119.90
1	1A	1455	C	C4-C5-C6	5.11	119.96	117.40
1	1A	1652	G	OP1-P-O3'	5.11	116.45	105.20
1	1A	1994	A	OP2-P-O3'	5.11	116.45	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2004	C	OP1-P-OP2	5.11	127.27	119.60
1	1A	2420	U	N3-C4-O4	-5.11	115.82	119.40
1	1A	2519	C	C5-C4-N4	5.11	123.78	120.20
1	1A	2529	C	OP2-P-O3'	5.11	116.45	105.20
32	1a	685	G	C6-C5-N7	-5.11	127.33	130.40
1	2A	2056	G	N9-C4-C5	-5.11	103.36	105.40
32	2a	204	U	O4'-C1'-N1	5.11	112.29	108.20
1	1A	590	A	O5'-P-OP1	5.11	116.83	110.70
1	1A	975	U	N3-C2-O2	5.11	125.78	122.20
1	1A	2331	G	N1-C2-N3	5.11	126.97	123.90
1	1A	2440	G	OP2-P-O3'	5.11	116.45	105.20
32	1a	1447	A	O4'-C1'-N9	5.11	112.29	108.20
1	2A	154	G	N7-C8-N9	-5.11	110.54	113.10
32	2a	977	A	O4'-C1'-N9	5.11	112.29	108.20
32	2a	1128	C	P-O3'-C3'	5.11	125.83	119.70
1	1A	1335	C	C6-N1-C2	5.11	122.34	120.30
1	1A	1735	U	C2-N3-C4	-5.11	123.93	127.00
1	1A	2019	G	N1-C2-N2	-5.11	111.60	116.20
1	1A	2412	G	C5-C6-O6	5.11	131.67	128.60
32	1a	192	U	C5-C4-O4	5.11	128.97	125.90
32	1a	1397	C	C6-N1-C2	-5.11	118.26	120.30
1	2A	529	A	N3-C4-C5	5.11	130.38	126.80
1	2A	1973	G	N3-C2-N2	5.11	123.48	119.90
1	2A	2198	A	C5-C6-N6	-5.11	119.61	123.70
32	2a	656	C	C6-N1-C2	-5.11	118.26	120.30
1	1A	1287	A	N9-C4-C5	-5.11	103.76	105.80
32	1a	1279	A	N7-C8-N9	5.11	116.36	113.80
1	2A	1767	C	C5-C4-N4	5.11	123.78	120.20
1	1A	323	A	N1-C6-N6	-5.11	115.53	118.60
1	1A	447	C	N3-C4-C5	5.11	123.94	121.90
1	1A	639	G	N3-C2-N2	-5.11	116.33	119.90
1	1A	1107	U	O4'-C1'-N1	5.11	112.29	108.20
1	1A	1882	U	C5-C6-N1	-5.11	120.15	122.70
1	1A	2054	G	C4-C5-N7	-5.11	108.76	110.80
1	1A	2247	G	C5-C6-O6	5.11	131.66	128.60
1	1A	2339	A	C4-C5-N7	-5.11	108.15	110.70
32	1a	1186	G	N9-C4-C5	5.11	107.44	105.40
1	2A	1466	G	C8-N9-C4	5.11	108.44	106.40
1	2A	2069	G	C6-C5-N7	5.11	133.47	130.40
1	2A	2382	G	C8-N9-C4	5.11	108.44	106.40
1	1A	1666	G	C6-C5-N7	5.11	133.46	130.40
1	1A	1726	U	C2-N3-C4	-5.11	123.94	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1899	A	OP2-P-O3'	5.11	116.43	105.20
1	1A	2734	A	N1-C6-N6	5.11	121.66	118.60
1	1A	2879	G	C4-C5-C6	5.11	121.86	118.80
2	1B	115	G	N7-C8-N9	-5.11	110.55	113.10
32	1a	474	G	C4-C5-N7	-5.11	108.76	110.80
32	1a	858	G	C6-C5-N7	-5.11	127.34	130.40
32	1a	1030(B)	C	C5-C6-N1	5.11	123.55	121.00
1	2A	467	G	N9-C4-C5	-5.11	103.36	105.40
1	2A	737	C	C5-C6-N1	-5.11	118.45	121.00
1	2A	1179	C	N1-C2-N3	-5.11	115.63	119.20
1	2A	2474	C	N1-C2-O2	5.11	121.96	118.90
1	2A	2829	C	C6-N1-C2	5.11	122.34	120.30
32	2a	572	A	N3-C4-C5	5.11	130.37	126.80
32	2a	1125	U	O4'-C1'-N1	5.11	112.28	108.20
1	1A	385	G	N3-C4-C5	5.10	131.15	128.60
32	1a	482	A	OP1-P-O3'	5.10	116.43	105.20
1	2A	1279	G	O5'-P-OP1	5.10	116.82	110.70
1	2A	2419	U	N3-C4-C5	5.10	117.66	114.60
1	1A	508	A	N1-C6-N6	5.10	121.66	118.60
1	1A	980	C	C6-N1-C2	5.10	122.34	120.30
1	1A	1543	U	O4'-C1'-N1	5.10	112.28	108.20
1	1A	1609	A	O5'-P-OP1	-5.10	101.11	105.70
1	1A	1650	C	C5-C4-N4	-5.10	116.63	120.20
32	1a	343	U	N3-C2-O2	-5.10	118.63	122.20
32	1a	533	A	C4-N9-C1'	5.10	135.48	126.30
32	1a	1082	G	N9-C4-C5	-5.10	103.36	105.40
32	1a	1087	G	N3-C4-C5	-5.10	126.05	128.60
32	1a	1233	G	C5-C6-O6	5.10	131.66	128.60
1	2A	36	G	C5-C6-N1	-5.10	108.95	111.50
1	2A	531	C	O5'-P-OP1	-5.10	101.11	105.70
1	2A	1652	A	N3-C4-C5	5.10	130.37	126.80
32	2a	715	A	N3-C4-C5	5.10	130.37	126.80
1	1A	184	A	C4-C5-C6	-5.10	114.45	117.00
1	1A	2621	U	C4-C5-C6	5.10	122.76	119.70
32	2a	1063	C	C6-N1-C2	-5.10	118.26	120.30
1	1A	826	U	N3-C2-O2	5.10	125.77	122.20
32	1a	350	G	C8-N9-C4	-5.10	104.36	106.40
1	2A	599	G	N1-C2-N3	5.10	126.96	123.90
1	2A	1844	C	C5-C4-N4	-5.10	116.63	120.20
1	2A	2446	G	C8-N9-C4	5.10	108.44	106.40
32	2a	764	C	N3-C4-N4	-5.10	114.43	118.00
1	1A	1355	G	C5-N7-C8	5.10	106.85	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2332	A	O5'-P-OP2	-5.10	101.11	105.70
1	2A	1609	A	OP2-P-O3'	5.10	116.42	105.20
1	2A	1890	A	N7-C8-N9	-5.10	111.25	113.80
1	2A	2585	U	OP1-P-O3'	5.10	116.41	105.20
1	1A	113	C	N3-C4-N4	-5.10	114.43	118.00
1	1A	868	A	N9-C4-C5	5.09	107.84	105.80
1	1A	2181	G	C4-N9-C1'	5.09	133.12	126.50
2	1B	32	C	OP2-P-O3'	5.09	116.41	105.20
1	2A	517	C	OP2-P-O3'	5.09	116.41	105.20
1	2A	2448	A	OP1-P-OP2	-5.09	111.96	119.60
2	2B	59	A	C5-C6-N6	-5.09	119.62	123.70
32	2a	522	C	N3-C2-O2	-5.09	118.33	121.90
1	1A	1952	G	C4-C5-N7	-5.09	108.76	110.80
1	1A	2735	G	N1-C6-O6	5.09	122.96	119.90
32	1a	65	U	O4'-C1'-N1	-5.09	104.12	108.20
1	2A	2489	G	OP2-P-O3'	5.09	116.41	105.20
1	1A	1409	C	OP1-P-O3'	-5.09	94.00	105.20
1	1A	1890	A	OP1-P-OP2	-5.09	111.96	119.60
1	1A	2063	U	OP1-P-OP2	5.09	127.24	119.60
1	1A	2076	A	N1-C6-N6	5.09	121.66	118.60
1	1A	2375	C	C5-C6-N1	-5.09	118.45	121.00
1	2A	405	U	N1-C2-O2	5.09	126.36	122.80
1	2A	645	C	C2-N3-C4	5.09	122.45	119.90
1	2A	2555	U	N3-C2-O2	5.09	125.76	122.20
32	2a	117	G	O5'-P-OP1	5.09	116.81	110.70
32	2a	929	G	N3-C4-N9	-5.09	122.95	126.00
1	1A	238	C	OP1-P-O3'	5.09	116.40	105.20
1	1A	825	G	C6-C5-N7	-5.09	127.35	130.40
1	1A	1513	G	O4'-C1'-N9	5.09	112.27	108.20
1	1A	1688	A	O5'-P-OP1	-5.09	101.12	105.70
1	1A	2522	C	N3-C4-N4	-5.09	114.44	118.00
32	1a	455	C	N3-C4-C5	5.09	123.94	121.90
32	1a	474	G	N1-C6-O6	-5.09	116.85	119.90
1	2A	788	A	N7-C8-N9	5.09	116.34	113.80
1	2A	1170	G	C5-N7-C8	-5.09	101.76	104.30
1	2A	1702	G	N9-C4-C5	5.09	107.44	105.40
1	2A	2690	C	C2-N1-C1'	-5.09	113.20	118.80
1	2A	2771	C	C6-N1-C2	-5.09	118.26	120.30
32	2a	768	A	C6-C5-N7	-5.09	128.74	132.30
32	2a	785	G	C8-N9-C1'	5.09	133.62	127.00
32	2a	1128	C	C5-C6-N1	5.09	123.54	121.00
32	1a	380	G	N1-C6-O6	-5.09	116.85	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	913	A	C8-N9-C4	-5.09	103.77	105.80
1	2A	1818	U	O5'-P-OP1	-5.09	101.12	105.70
1	2A	2337	G	N3-C2-N2	-5.09	116.34	119.90
1	1A	694	G	N1-C6-O6	5.09	122.95	119.90
1	1A	806	G	N9-C4-C5	5.09	107.43	105.40
1	1A	1270	C	C5-C4-N4	-5.09	116.64	120.20
1	1A	1646	C	O5'-P-OP2	-5.09	101.12	105.70
1	1A	1662	A	N1-C2-N3	-5.09	126.76	129.30
2	1B	15	A	C8-N9-C4	5.09	107.83	105.80
2	1B	108	U	N3-C2-O2	-5.09	118.64	122.20
32	1a	502	G	C5-C6-O6	-5.09	125.55	128.60
1	2A	1367	A	N1-C2-N3	5.09	131.84	129.30
1	2A	1494	A	C2-N3-C4	-5.09	108.06	110.60
1	2A	2227	A	OP1-P-OP2	-5.09	111.97	119.60
32	2a	839	U	C5-C6-N1	5.09	125.24	122.70
32	2a	898	G	C4-C5-N7	5.09	112.83	110.80
32	2a	1489	G	C8-N9-C1'	5.09	133.61	127.00
1	1A	36	G	C5-C6-O6	5.08	131.65	128.60
1	1A	1099	C	N1-C1'-C2'	-5.08	106.41	112.00
1	1A	1137	G	O4'-C1'-N9	5.08	112.27	108.20
1	1A	1381	U	C5-C6-N1	-5.08	120.16	122.70
1	1A	2466	G	N1-C6-O6	-5.08	116.85	119.90
1	1A	2880	C	C6-N1-C2	-5.08	118.27	120.30
32	1a	1499	A	O5'-P-OP1	5.08	116.80	110.70
1	1A	217	A	C4-C5-C6	-5.08	114.46	117.00
1	1A	1244	U	C5-C4-O4	5.08	128.95	125.90
1	1A	1249	A	C6-C5-N7	-5.08	128.74	132.30
1	1A	1406	A	C5-C6-N6	-5.08	119.63	123.70
1	1A	1877	G	OP2-P-O3'	5.08	116.38	105.20
1	1A	2194	U	N3-C2-O2	-5.08	118.64	122.20
1	1A	2559	U	C5-C6-N1	-5.08	120.16	122.70
32	1a	901	A	N7-C8-N9	5.08	116.34	113.80
1	2A	265	A	N1-C2-N3	5.08	131.84	129.30
1	2A	581	C	N3-C2-O2	-5.08	118.34	121.90
1	2A	833	U	OP2-P-O3'	5.08	116.39	105.20
32	2a	196	A	O5'-P-OP1	-5.08	101.12	105.70
32	2a	1033	G	N1-C6-O6	5.08	122.95	119.90
32	2a	1472	U	O5'-P-OP2	-5.08	101.12	105.70
1	1A	72	A	C6-N1-C2	-5.08	115.55	118.60
1	1A	1215	G	OP2-P-O3'	5.08	116.38	105.20
1	1A	1371	G	C4-C5-N7	-5.08	108.77	110.80
1	1A	1838	G	OP1-P-OP2	-5.08	111.98	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2203	G	C6-C5-N7	5.08	133.45	130.40
1	1A	2266	C	C4-C5-C6	5.08	119.94	117.40
2	1B	38	C	OP2-P-O3'	5.08	116.38	105.20
9	1N	35	ARG	CA-CB-CG	5.08	124.58	113.40
32	1a	561	U	C6-N1-C2	5.08	124.05	121.00
32	1a	859	A	OP1-P-O3'	5.08	116.38	105.20
1	2A	10	G	N1-C6-O6	5.08	122.95	119.90
1	2A	2172	U	C5-C6-N1	-5.08	120.16	122.70
29	27	35	ARG	NE-CZ-NH1	-5.08	117.76	120.30
32	2a	858	G	C8-N9-C1'	-5.08	120.39	127.00
1	1A	1283	A	C8-N9-C4	-5.08	103.77	105.80
1	1A	1393	G	N1-C6-O6	-5.08	116.85	119.90
1	1A	1883	C	OP2-P-O3'	5.08	116.38	105.20
32	1a	244	U	C5-C4-O4	-5.08	122.85	125.90
1	2A	652	C	O5'-P-OP1	-5.08	101.13	105.70
1	1A	289	G	C8-N9-C4	5.08	108.43	106.40
1	1A	484	G	OP1-P-OP2	5.08	127.22	119.60
1	1A	999	G	N1-C6-O6	-5.08	116.85	119.90
1	1A	1414	G	C5-C6-N1	5.08	114.04	111.50
1	1A	1457	C	N3-C4-N4	-5.08	114.45	118.00
1	1A	2340	A	C8-N9-C4	-5.08	103.77	105.80
1	1A	2774	G	N7-C8-N9	-5.08	110.56	113.10
16	1U	19	LYS	CD-CE-NZ	-5.08	100.02	111.70
32	1a	549	C	OP1-P-OP2	-5.08	111.98	119.60
1	2A	228	A	N3-C4-N9	-5.08	123.34	127.40
1	2A	1671	U	C5-C6-N1	-5.08	120.16	122.70
1	2A	2207	G	N3-C4-N9	5.08	129.05	126.00
1	2A	2716	U	C6-N1-C2	-5.08	117.95	121.00
1	2A	2832	U	C6-N1-C2	5.08	124.05	121.00
1	1A	514	G	C5-N7-C8	5.08	106.84	104.30
1	1A	1243	U	C2-N3-C4	-5.08	123.95	127.00
1	1A	1699	A	O5'-P-OP1	-5.08	101.13	105.70
1	1A	2478	C	N3-C2-O2	5.08	125.45	121.90
32	1a	1417	G	C6-C5-N7	-5.08	127.35	130.40
1	2A	966	G	C4-C5-N7	5.08	112.83	110.80
32	2a	738	C	C5-C6-N1	5.08	123.54	121.00
1	1A	907	U	O5'-P-OP1	5.08	116.79	110.70
1	1A	1128	U	C6-N1-C2	-5.08	117.95	121.00
1	1A	1366	C	N3-C2-O2	-5.08	118.35	121.90
1	1A	1732	C	C2-N3-C4	-5.08	117.36	119.90
1	1A	2080	A	C4-C5-C6	5.08	119.54	117.00
1	1A	2378	A	C6-C5-N7	-5.08	128.75	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	139	G	N7-C8-N9	5.08	115.64	113.10
32	1a	894	G	N7-C8-N9	-5.08	110.56	113.10
1	2A	871	U	N3-C4-O4	5.08	122.95	119.40
32	2a	1452	C	N3-C2-O2	-5.08	118.35	121.90
1	1A	71	U	C2-N1-C1'	-5.07	111.61	117.70
1	1A	184	A	C6-N1-C2	5.07	121.64	118.60
1	1A	1144	A	C2-N3-C4	5.07	113.14	110.60
1	1A	2387	G	N9-C1'-C2'	-5.07	106.42	112.00
1	1A	2855	G	N3-C4-C5	-5.07	126.06	128.60
2	1B	108	U	OP1-P-OP2	5.07	127.21	119.60
32	1a	149	A	C5-C6-N1	-5.07	115.16	117.70
32	1a	567	G	O5'-P-OP1	-5.07	101.13	105.70
1	2A	2268	A	C8-N9-C4	5.07	107.83	105.80
1	2A	2587	A	N1-C6-N6	5.07	121.64	118.60
32	2a	917	G	O5'-P-OP2	5.07	116.79	110.70
1	1A	1409	C	O5'-P-OP2	-5.07	101.14	105.70
1	1A	2355	C	N1-C2-O2	-5.07	115.86	118.90
1	1A	2573	A	N9-C4-C5	5.07	107.83	105.80
1	2A	2010	G	C5-C6-N1	-5.07	108.96	111.50
1	2A	2483	C	O5'-P-OP1	-5.07	101.14	105.70
1	1A	194	G	N3-C4-N9	5.07	129.04	126.00
1	1A	363	U	C6-N1-C2	5.07	124.04	121.00
1	1A	543	G	N9-C4-C5	5.07	107.43	105.40
1	1A	1357	G	C4-C5-N7	5.07	112.83	110.80
1	1A	2065	C	C2-N3-C4	-5.07	117.36	119.90
2	1B	99	G	C5-N7-C8	5.07	106.84	104.30
3	1D	99	ASP	CB-CA-C	-5.07	100.26	110.40
32	1a	291	C	N1-C2-O2	-5.07	115.86	118.90
32	1a	811	C	N3-C2-O2	5.07	125.45	121.90
1	2A	1681	G	N3-C4-C5	5.07	131.13	128.60
1	2A	1745	C	N1-C2-O2	-5.07	115.86	118.90
1	2A	1806	C	OP2-P-O3'	5.07	116.35	105.20
1	2A	1968	G	C4-C5-N7	5.07	112.83	110.80
1	2A	2075	U	N3-C2-O2	-5.07	118.65	122.20
32	2a	550	G	N1-C6-O6	5.07	122.94	119.90
1	1A	725	C	OP1-P-OP2	-5.07	112.00	119.60
1	1A	818	G	N9-C4-C5	-5.07	103.37	105.40
37	1f	19	LEU	CA-CB-CG	5.07	126.96	115.30
1	2A	989	G	C6-C5-N7	-5.07	127.36	130.40
1	1A	540	A	C5-C6-N1	5.07	120.23	117.70
1	1A	2188	G	C8-N9-C1'	5.07	133.59	127.00
1	1A	2227	G	C1'-O4'-C4'	-5.07	105.85	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2390	A	C8-N9-C1'	-5.07	118.58	127.70
1	1A	2597	U	P-O3'-C3'	5.07	125.78	119.70
32	1a	120	A	O4'-C1'-N9	-5.07	104.15	108.20
32	1a	1436	U	N1-C2-O2	-5.07	119.25	122.80
1	2A	2487	G	C8-N9-C4	5.07	108.43	106.40
2	2B	56	G	C8-N9-C4	-5.07	104.37	106.40
1	1A	43	A	C5-C6-N1	-5.07	115.17	117.70
1	1A	670	C	N3-C4-N4	-5.07	114.45	118.00
1	1A	790	G	N7-C8-N9	-5.07	110.57	113.10
1	1A	904	C	OP2-P-O3'	5.07	116.34	105.20
1	1A	1883	C	O5'-P-OP2	-5.07	101.14	105.70
1	1A	2285	A	O5'-P-OP2	-5.07	101.14	105.70
1	1A	2576	A	C6-C5-N7	-5.07	128.75	132.30
1	1A	2605	U	N3-C2-O2	-5.07	118.65	122.20
1	1A	2882	G	N3-C4-N9	5.07	129.04	126.00
32	1a	751	U	N1-C2-O2	-5.07	119.25	122.80
32	1a	825	G	C5-C6-O6	5.07	131.64	128.60
32	1a	1495	U	N3-C4-C5	-5.07	111.56	114.60
1	2A	1693	U	N3-C4-C5	5.07	117.64	114.60
1	2A	2449	U	N1-C2-O2	5.07	126.35	122.80
32	2a	397	A	N1-C2-N3	5.07	131.83	129.30
32	2a	1031	G	C8-N9-C4	-5.07	104.37	106.40
32	2a	1391	U	C5-C6-N1	-5.07	120.17	122.70
1	1A	893	C	C6-N1-C2	5.06	122.33	120.30
1	1A	1852	A	N1-C6-N6	-5.06	115.56	118.60
1	2A	386	G	C6-N1-C2	-5.06	122.06	125.10
1	2A	2095	C	N3-C4-N4	-5.06	114.45	118.00
32	2a	84	U	N1-C2-O2	5.06	126.34	122.80
32	2a	1124	G	C8-N9-C4	-5.06	104.37	106.40
1	1A	149	A	C8-N9-C4	5.06	107.83	105.80
1	1A	634	C	C5-C6-N1	-5.06	118.47	121.00
1	1A	1645	C	N3-C4-N4	-5.06	114.46	118.00
1	1A	2307	C	N1-C2-O2	-5.06	115.86	118.90
2	1B	74	U	N1-C2-N3	5.06	117.94	114.90
32	1a	880	C	C6-N1-C2	5.06	122.33	120.30
32	1a	912	C	C5-C4-N4	-5.06	116.66	120.20
1	2A	271(M)	G	P-O3'-C3'	5.06	125.77	119.70
1	2A	482	A	C8-N9-C4	5.06	107.83	105.80
1	2A	489	G	C6-C5-N7	-5.06	127.36	130.40
1	2A	766	C	C5-C6-N1	-5.06	118.47	121.00
1	2A	1838	C	O5'-P-OP1	-5.06	101.14	105.70
1	2A	2511	U	C6-N1-C2	-5.06	117.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2553	G	O5'-P-OP2	5.06	116.78	110.70
1	2A	2725	A	OP2-P-O3'	5.06	116.34	105.20
1	2A	2827	C	N1-C2-O2	-5.06	115.86	118.90
32	2a	530	G	C2-N3-C4	5.06	114.43	111.90
1	1A	2425	G	OP2-P-O3'	5.06	116.33	105.20
32	1a	977	A	O5'-P-OP2	-5.06	101.14	105.70
1	2A	1450(A)	C	C6-N1-C2	-5.06	118.28	120.30
1	2A	2321	G	N7-C8-N9	5.06	115.63	113.10
2	2B	52	A	N1-C6-N6	5.06	121.64	118.60
1	1A	114	C	OP1-P-OP2	5.06	127.19	119.60
1	1A	729	G	C8-N9-C1'	-5.06	120.42	127.00
1	1A	786	G	C8-N9-C4	5.06	108.42	106.40
1	1A	1604	C	C5-C6-N1	-5.06	118.47	121.00
1	1A	2184	G	C2-N3-C4	5.06	114.43	111.90
1	1A	2621	U	C6-N1-C2	5.06	124.04	121.00
2	1B	97	G	C2-N3-C4	5.06	114.43	111.90
2	1B	101	G	C8-N9-C4	5.06	108.42	106.40
32	1a	565	U	OP1-P-OP2	-5.06	112.01	119.60
1	2A	492	A	N1-C2-N3	5.06	131.83	129.30
1	1A	256	C	N1-C2-O2	-5.06	115.86	118.90
1	1A	540	A	OP1-P-O3'	5.06	116.33	105.20
1	1A	541	C	OP1-P-OP2	-5.06	112.01	119.60
1	1A	1874	C	N3-C2-O2	5.06	125.44	121.90
1	1A	1986	G	N3-C4-N9	5.06	129.03	126.00
32	1a	1201	A	N1-C2-N3	5.06	131.83	129.30
1	2A	9	U	P-O3'-C3'	5.06	125.77	119.70
1	2A	321	G	O4'-C1'-N9	5.06	112.25	108.20
1	2A	1567	A	N9-C4-C5	5.06	107.82	105.80
1	2A	1753	G	O5'-P-OP2	-5.06	101.15	105.70
1	2A	2385	C	OP1-P-OP2	5.06	127.19	119.60
1	2A	2885	C	OP2-P-O3'	5.06	116.33	105.20
32	2a	622	A	C5-C6-N1	5.06	120.23	117.70
32	2a	1476	G	C4-C5-N7	5.06	112.82	110.80
1	1A	2406	C	N1-C2-N3	5.06	122.74	119.20
1	2A	450	G	N1-C6-O6	-5.06	116.87	119.90
1	2A	1478	G	OP1-P-O3'	5.06	116.32	105.20
1	2A	1771	C	C2-N3-C4	-5.06	117.37	119.90
1	1A	98	U	N3-C2-O2	-5.05	118.66	122.20
1	1A	578	U	C5-C4-O4	-5.05	122.87	125.90
1	1A	1003	U	N1-C2-N3	5.05	117.93	114.90
1	1A	1838	G	C5-N7-C8	-5.05	101.77	104.30
1	1A	2562	G	C4-C5-C6	5.05	121.83	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	74	U	C5-C6-N1	-5.05	120.17	122.70
32	1a	740	U	O5'-P-OP2	-5.05	101.15	105.70
1	2A	467	G	N9-C1'-C2'	-5.05	106.44	112.00
1	2A	660	G	C5-C6-N1	-5.05	108.97	111.50
1	2A	684	G	C8-N9-C4	-5.05	104.38	106.40
1	2A	1137	G	N1-C6-O6	5.05	122.93	119.90
1	2A	1685	C	N3-C2-O2	5.05	125.44	121.90
32	2a	306	G	N1-C2-N2	5.05	120.75	116.20
32	2a	741	G	O5'-P-OP2	-5.05	101.15	105.70
1	1A	2267	G	N9-C4-C5	-5.05	103.38	105.40
32	1a	423	G	N3-C4-N9	5.05	129.03	126.00
32	1a	1033	G	N1-C2-N3	-5.05	120.87	123.90
1	1A	423	G	C6-N1-C2	-5.05	122.07	125.10
1	1A	436	C	C5-C6-N1	-5.05	118.47	121.00
1	1A	1051	C	OP1-P-OP2	5.05	127.18	119.60
1	1A	1787	G	C5-C6-O6	5.05	131.63	128.60
2	1B	31	C	C5-C4-N4	5.05	123.74	120.20
32	1a	774	G	C5-C6-N1	-5.05	108.97	111.50
32	1a	885	G	C8-N9-C4	5.05	108.42	106.40
1	2A	520	G	O5'-P-OP2	-5.05	101.15	105.70
1	2A	1186	G	C4-C5-C6	5.05	121.83	118.80
1	2A	2599	G	N7-C8-N9	-5.05	110.57	113.10
32	2a	811	C	OP2-P-O3'	5.05	116.31	105.20
32	2a	947	G	N3-C2-N2	5.05	123.44	119.90
1	1A	392	U	N1-C2-O2	-5.05	119.27	122.80
1	1A	934	A	C2-N3-C4	5.05	113.12	110.60
1	1A	1063	G	OP2-P-O3'	5.05	116.31	105.20
1	1A	1184	G	N1-C6-O6	-5.05	116.87	119.90
1	1A	2390	A	N3-C4-N9	5.05	131.44	127.40
1	1A	2565	G	C5-C6-N1	5.05	114.03	111.50
1	1A	2717	A	N3-C4-C5	5.05	130.34	126.80
1	1A	2859	U	N3-C2-O2	5.05	125.73	122.20
14	1S	30	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	2A	6	A	N3-C4-C5	-5.05	123.27	126.80
1	2A	1229	G	N9-C4-C5	-5.05	103.38	105.40
1	2A	1672	C	OP1-P-O3'	5.05	116.31	105.20
1	2A	1975	G	O5'-P-OP1	5.05	116.76	110.70
1	1A	1025	G	C8-N9-C4	5.05	108.42	106.40
1	1A	1674	G	N3-C4-C5	-5.05	126.08	128.60
1	1A	2375	C	N3-C4-N4	-5.05	114.47	118.00
1	1A	2782	C	C4-C5-C6	5.05	119.92	117.40
32	1a	297	G	N3-C4-C5	5.05	131.12	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	871	U	N3-C4-C5	-5.05	111.57	114.60
1	2A	492	A	C6-N1-C2	-5.05	115.57	118.60
1	2A	1671	U	N3-C4-C5	5.05	117.63	114.60
1	2A	2058	A	C4-C5-C6	5.05	119.52	117.00
1	2A	2337	G	N1-C6-O6	5.05	122.93	119.90
1	2A	2820	A	OP1-P-O3'	5.05	116.31	105.20
48	2q	6	LEU	CA-CB-CG	5.05	126.91	115.30
1	1A	167	G	C4-C5-N7	-5.05	108.78	110.80
1	1A	1145	G	N9-C1'-C2'	-5.05	106.45	112.00
1	1A	1249	A	C4-C5-N7	5.05	113.22	110.70
1	1A	1706	U	C6-N1-C2	-5.05	117.97	121.00
1	1A	2463	A	N7-C8-N9	5.05	116.32	113.80
1	1A	2748	G	C8-N9-C4	-5.05	104.38	106.40
2	1B	48	A	C8-N9-C4	5.05	107.82	105.80
1	2A	95	G	C5-C6-O6	-5.05	125.57	128.60
1	2A	277	C	N3-C2-O2	-5.05	118.37	121.90
1	2A	1663	C	O5'-P-OP1	5.05	116.76	110.70
32	2a	485	G	N3-C4-N9	5.05	129.03	126.00
1	1A	1152	G	N9-C4-C5	-5.04	103.38	105.40
1	2A	297	C	O5'-P-OP2	-5.04	101.16	105.70
1	2A	1586	A	N1-C6-N6	5.04	121.63	118.60
32	2a	29	G	OP1-P-OP2	5.04	127.17	119.60
32	2a	100	C	C6-N1-C2	-5.04	118.28	120.30
32	2a	819	A	C4-C5-N7	5.04	113.22	110.70
1	1A	13	A	N9-C4-C5	5.04	107.82	105.80
1	1A	350	G	C4-C5-N7	-5.04	108.78	110.80
1	1A	449	A	OP1-P-OP2	-5.04	112.03	119.60
1	1A	837	C	OP1-P-OP2	5.04	127.16	119.60
1	1A	1382	A	OP1-P-OP2	5.04	127.17	119.60
1	1A	1898	A	OP1-P-O3'	5.04	116.30	105.20
1	1A	1919	G	C4-C5-N7	5.04	112.82	110.80
1	1A	2268	G	OP2-P-O3'	5.04	116.29	105.20
1	1A	2784	C	C5-C6-N1	-5.04	118.48	121.00
29	17	28	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	2A	771	G	N9-C4-C5	5.04	107.42	105.40
1	2A	2505	G	C8-N9-C4	-5.04	104.38	106.40
1	1A	725	C	O5'-P-OP1	5.04	116.75	110.70
1	1A	741	U	N1-C2-N3	5.04	117.92	114.90
1	1A	1007	G	C4-C5-N7	-5.04	108.78	110.80
1	1A	1030	A	O5'-P-OP2	-5.04	101.16	105.70
1	1A	1617	A	C2-N3-C4	-5.04	108.08	110.60
1	1A	2278	A	N7-C8-N9	5.04	116.32	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	475	U	C5-C6-N1	5.04	125.22	122.70
1	2A	486	C	C6-N1-C2	5.04	122.32	120.30
1	2A	713	G	C4-C5-N7	5.04	112.82	110.80
1	2A	1372	U	C5-C6-N1	5.04	125.22	122.70
1	2A	1780	A	N1-C2-N3	5.04	131.82	129.30
1	2A	1865	G	N3-C2-N2	-5.04	116.37	119.90
1	2A	2588	G	N1-C6-O6	5.04	122.92	119.90
1	2A	2867	G	N3-C4-C5	5.04	131.12	128.60
32	2a	332	G	OP1-P-OP2	5.04	127.16	119.60
1	1A	8	A	O5'-P-OP2	5.04	116.75	110.70
1	1A	409	G	N1-C6-O6	-5.04	116.88	119.90
1	1A	786	G	N1-C6-O6	5.04	122.92	119.90
32	1a	1232	U	C6-N1-C2	-5.04	117.98	121.00
1	2A	1343	G	N1-C6-O6	-5.04	116.88	119.90
1	2A	1989	G	O5'-P-OP2	-5.04	101.16	105.70
1	1A	166	G	O4'-C1'-N9	5.04	112.23	108.20
1	1A	390	G	N3-C4-N9	5.04	129.02	126.00
1	1A	896	A	C8-N9-C4	5.04	107.81	105.80
1	1A	948	C	C5-C6-N1	-5.04	118.48	121.00
1	1A	983	G	N1-C6-O6	-5.04	116.88	119.90
1	1A	1006	C	N3-C2-O2	-5.04	118.37	121.90
1	1A	1113	A	C2-N3-C4	5.04	113.12	110.60
1	1A	2428	C	C4-C5-C6	-5.04	114.88	117.40
1	1A	2635	G	C5-C6-O6	5.04	131.62	128.60
32	1a	73	G	C8-N9-C4	5.04	108.42	106.40
32	1a	174	C	C2-N1-C1'	5.04	124.34	118.80
32	1a	1054	C	N1-C2-O2	5.04	121.92	118.90
1	2A	1052	C	C6-N1-C2	-5.04	118.28	120.30
1	2A	1092	C	C2-N1-C1'	5.04	124.34	118.80
1	2A	1740	G	N1-C6-O6	-5.04	116.88	119.90
32	2a	381	C	N1-C2-O2	5.04	121.92	118.90
32	2a	1436	U	C4-C5-C6	5.04	122.72	119.70
1	1A	581	G	N1-C2-N2	-5.04	111.67	116.20
1	1A	1985	U	O5'-P-OP2	-5.04	101.17	105.70
32	1a	363	A	O5'-P-OP2	-5.04	101.17	105.70
32	1a	635	G	C4-C5-N7	5.04	112.81	110.80
1	2A	794	G	C8-N9-C4	5.04	108.42	106.40
32	2a	1030(D)	A	N3-C4-C5	-5.04	123.27	126.80
1	1A	2129	C	C6-N1-C2	-5.04	118.29	120.30
32	1a	183	G	N3-C4-C5	-5.04	126.08	128.60
32	1a	928	G	O5'-P-OP1	-5.04	101.17	105.70
32	1a	1067	A	C8-N9-C4	-5.04	103.78	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	62	C	C5-C6-N1	-5.04	118.48	121.00
1	2A	2177	C	N1-C2-O2	5.04	121.92	118.90
1	2A	2894	G	C4-N9-C1'	-5.04	119.95	126.50
32	2a	728	A	C8-N9-C4	-5.04	103.79	105.80
32	2a	754	C	O5'-P-OP1	-5.04	101.17	105.70
1	1A	153	C	OP1-P-O3'	-5.03	94.13	105.20
1	1A	1093	G	P-O3'-C3'	5.03	125.74	119.70
32	1a	427	U	C6-N1-C2	-5.03	117.98	121.00
32	1a	596	C	N3-C2-O2	-5.03	118.38	121.90
1	2A	44	G	OP1-P-OP2	5.03	127.15	119.60
1	2A	575	A	O4'-C1'-N9	5.03	112.23	108.20
1	2A	1109	C	N3-C2-O2	-5.03	118.38	121.90
1	1A	292	G	C8-N9-C4	5.03	108.41	106.40
1	2A	383	U	O4'-C1'-N1	5.03	112.22	108.20
32	2a	1065	U	P-O3'-C3'	5.03	125.74	119.70
32	2a	1346	A	OP1-P-O3'	5.03	116.27	105.20
1	1A	198	C	C6-N1-C1'	-5.03	114.76	120.80
1	1A	247	G	N1-C2-N2	-5.03	111.67	116.20
1	1A	447	C	C2-N3-C4	-5.03	117.39	119.90
1	1A	722	A	C8-N9-C1'	-5.03	118.65	127.70
1	1A	1456	G	OP1-P-O3'	-5.03	94.13	105.20
1	1A	2611	G	N1-C2-N2	-5.03	111.67	116.20
32	1a	552	U	C2-N3-C4	-5.03	123.98	127.00
1	2A	1097	U	N3-C4-O4	5.03	122.92	119.40
1	2A	1516	C	N3-C4-C5	5.03	123.91	121.90
1	2A	1936	A	C5-N7-C8	-5.03	101.39	103.90
32	2a	570	G	C8-N9-C4	-5.03	104.39	106.40
32	2a	900	A	O5'-P-OP1	-5.03	101.17	105.70
1	1A	1788	U	N3-C2-O2	5.03	125.72	122.20
1	1A	2379	G	OP2-P-O3'	5.03	116.26	105.20
1	1A	2614	A	OP2-P-O3'	5.03	116.26	105.20
1	1A	2641	A	N9-C1'-C2'	5.03	120.54	114.00
1	2A	421	U	OP1-P-O3'	5.03	116.26	105.20
1	2A	704	G	C8-N9-C4	-5.03	104.39	106.40
32	2a	1392	G	N1-C6-O6	-5.03	116.88	119.90
32	2a	1524	C	N3-C2-O2	5.03	125.42	121.90
1	1A	75	C	C6-N1-C2	-5.03	118.29	120.30
1	1A	454	U	O3'-P-O5'	-5.03	94.45	104.00
1	1A	977	G	N3-C2-N2	5.03	123.42	119.90
1	1A	1407	G	N1-C6-O6	-5.03	116.88	119.90
1	1A	2242	G	N1-C6-O6	5.03	122.92	119.90
1	1A	2789	A	C8-N9-C4	5.03	107.81	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	276	G	N7-C8-N9	5.03	115.61	113.10
32	1a	713	G	OP2-P-O3'	5.03	116.26	105.20
32	1a	1231	G	N3-C2-N2	-5.03	116.38	119.90
32	1a	1456	G	N9-C4-C5	-5.03	103.39	105.40
1	2A	2391	G	O4'-C1'-N9	5.03	112.22	108.20
1	2A	2700	C	O5'-P-OP1	5.03	116.73	110.70
1	2A	2765	A	C6-N1-C2	-5.03	115.58	118.60
2	2B	104	U	C5-C6-N1	-5.03	120.19	122.70
32	2a	568	G	O5'-P-OP2	5.03	116.73	110.70
32	2a	991	U	P-O3'-C3'	5.03	125.73	119.70
1	1A	206	G	C4-C5-N7	-5.03	108.79	110.80
1	1A	702	A	N9-C4-C5	5.03	107.81	105.80
1	1A	874	U	C2-N3-C4	-5.03	123.98	127.00
1	1A	1040	C	C4-C5-C6	5.03	119.91	117.40
1	1A	2094	G	C6-N1-C2	5.03	128.12	125.10
1	1A	2598	C	C2-N3-C4	-5.03	117.39	119.90
32	1a	523	A	C2-N3-C4	-5.03	108.09	110.60
1	2A	417	C	C5-C6-N1	5.03	123.51	121.00
1	2A	772	C	N3-C4-N4	5.03	121.52	118.00
1	2A	1300	U	OP1-P-O3'	5.03	116.25	105.20
32	2a	461	A	N1-C6-N6	-5.03	115.58	118.60
47	2p	25	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	1A	146	G	C5-C6-O6	5.02	131.62	128.60
1	1A	295	C	N1-C2-O2	5.02	121.91	118.90
1	1A	1016	C	OP1-P-OP2	-5.02	112.06	119.60
1	1A	1294	G	N7-C8-N9	-5.02	110.59	113.10
1	1A	2595	G	OP1-P-OP2	-5.02	112.06	119.60
32	1a	266	G	C8-N9-C1'	-5.02	120.47	127.00
32	1a	1012	U	O5'-P-OP2	-5.02	101.18	105.70
1	2A	1305	C	OP1-P-OP2	-5.02	112.06	119.60
1	2A	2690	C	OP1-P-O3'	5.02	116.25	105.20
1	1A	1041	C	C6-N1-C2	-5.02	118.29	120.30
1	1A	1067	A	C4-C5-C6	5.02	119.51	117.00
1	1A	1310	G	OP1-P-OP2	5.02	127.13	119.60
1	1A	2472	U	O5'-P-OP1	-5.02	101.18	105.70
1	1A	2633	A	C5-N7-C8	5.02	106.41	103.90
1	1A	2745	G	N3-C4-C5	-5.02	126.09	128.60
1	2A	1334	G	N9-C4-C5	5.02	107.41	105.40
1	2A	1618	A	C5-C6-N6	5.02	127.72	123.70
1	2A	2148	G	N3-C4-C5	-5.02	126.09	128.60
32	2a	310	G	N1-C6-O6	5.02	122.91	119.90
32	2a	585	G	C5-C6-N1	5.02	114.01	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1221	G	P-O3'-C3'	5.02	125.72	119.70
32	1a	674	G	OP1-P-O3'	5.02	116.25	105.20
1	2A	882	G	N3-C4-N9	-5.02	122.99	126.00
1	2A	2084	C	C5-C6-N1	-5.02	118.49	121.00
1	1A	410	U	N1-C2-N3	-5.02	111.89	114.90
1	1A	433	G	O5'-P-OP1	-5.02	101.18	105.70
1	1A	509	A	N1-C2-N3	5.02	131.81	129.30
1	1A	557	A	C5-C6-N6	5.02	127.72	123.70
1	1A	1318	A	N1-C2-N3	5.02	131.81	129.30
1	1A	1705	C	C5-C4-N4	-5.02	116.69	120.20
1	1A	2052	A	C6-C5-N7	-5.02	128.79	132.30
1	1A	2299	A	N1-C6-N6	-5.02	115.59	118.60
32	1a	928	G	C5-N7-C8	-5.02	101.79	104.30
32	2a	509	A	N7-C8-N9	5.02	116.31	113.80
1	1A	107	G	N1-C6-O6	-5.02	116.89	119.90
1	1A	292	G	N9-C4-C5	-5.02	103.39	105.40
1	1A	1371	G	O4'-C1'-N9	5.02	112.21	108.20
1	1A	2117	C	OP2-P-O3'	5.02	116.24	105.20
32	1a	1352	C	N3-C4-C5	-5.02	119.89	121.90
1	2A	512	G	OP1-P-OP2	5.02	127.13	119.60
1	2A	2716	U	N1-C2-N3	5.02	117.91	114.90
32	2a	1205	U	C5-C6-N1	5.02	125.21	122.70
1	1A	812	G	O5'-P-OP2	-5.02	101.19	105.70
1	1A	1400	A	N1-C2-N3	5.02	131.81	129.30
1	2A	1084	A	N9-C4-C5	-5.02	103.79	105.80
1	2A	1378	A	N3-C4-N9	-5.02	123.39	127.40
32	2a	147	G	C5-C6-O6	5.02	131.61	128.60
1	1A	1167	C	N3-C2-O2	-5.01	118.39	121.90
1	1A	1235	G	N3-C2-N2	5.01	123.41	119.90
1	1A	1838	G	N9-C1'-C2'	-5.01	106.48	112.00
32	1a	221	C	C5-C6-N1	5.01	123.51	121.00
1	2A	1186	G	C6-C5-N7	-5.01	127.39	130.40
1	2A	1776	G	C6-C5-N7	-5.01	127.39	130.40
2	2B	41	U	P-O3'-C3'	5.01	125.72	119.70
32	2a	472	A	N7-C8-N9	5.01	116.31	113.80
32	2a	947	G	N9-C4-C5	-5.01	103.39	105.40
1	1A	1440	U	O5'-P-OP1	-5.01	101.19	105.70
1	1A	1626	A	C4-C5-N7	5.01	113.21	110.70
32	1a	235	C	C6-N1-C2	5.01	122.31	120.30
32	1a	1027	C	C2-N3-C4	5.01	122.41	119.90
32	2a	1370	G	N3-C4-N9	5.01	129.01	126.00
1	1A	203	G	N3-C2-N2	5.01	123.41	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1067	A	C6-N1-C2	-5.01	115.59	118.60
1	1A	1268	C	N3-C2-O2	5.01	125.41	121.90
1	1A	2087	C	OP1-P-OP2	5.01	127.12	119.60
1	1A	2276	C	OP2-P-O3'	5.01	116.22	105.20
1	1A	2353	G	N7-C8-N9	5.01	115.61	113.10
2	1B	28	C	N1-C2-O2	5.01	121.91	118.90
1	2A	458	G	N1-C2-N2	-5.01	111.69	116.20
1	1A	100	G	C8-N9-C4	5.01	108.40	106.40
1	1A	458	U	OP2-P-O3'	5.01	116.22	105.20
1	1A	652	A	OP1-P-O3'	5.01	116.22	105.20
1	1A	1326	G	OP1-P-OP2	-5.01	112.09	119.60
1	1A	2873	C	OP1-P-OP2	5.01	127.11	119.60
1	2A	6	A	C4-C5-N7	-5.01	108.20	110.70
1	2A	103	A	N9-C4-C5	-5.01	103.80	105.80
1	2A	271(L)	U	O4'-C1'-N1	-5.01	104.19	108.20
1	2A	496	G	C2-N3-C4	-5.01	109.39	111.90
1	2A	1066	U	N3-C2-O2	-5.01	118.69	122.20
1	2A	1346	G	N1-C6-O6	-5.01	116.89	119.90
1	2A	1443	G	C4-C5-N7	-5.01	108.80	110.80
1	1A	718	C	C6-N1-C2	-5.01	118.30	120.30
1	1A	1425	A	N9-C4-C5	-5.01	103.80	105.80
1	1A	1957	G	N3-C4-C5	5.01	131.10	128.60
1	1A	2706	G	N9-C4-C5	-5.01	103.40	105.40
32	1a	1010	G	C4-N9-C1'	-5.01	119.99	126.50
1	2A	694	U	O5'-P-OP2	-5.01	101.19	105.70
1	2A	733	G	C2-N3-C4	-5.01	109.40	111.90
1	1A	1820	A	C2-N3-C4	-5.01	108.10	110.60
1	1A	2103	C	O5'-P-OP2	-5.01	101.19	105.70
1	1A	2111	U	C5-C6-N1	-5.01	120.20	122.70
2	1B	9	G	N3-C4-N9	-5.01	123.00	126.00
1	2A	746	A	O4'-C1'-N9	5.01	112.20	108.20
1	2A	1114	G	N1-C6-O6	-5.01	116.90	119.90
1	2A	2351	G	N3-C4-N9	5.01	129.00	126.00
32	2a	310	G	C5-C6-O6	-5.01	125.60	128.60
32	2a	361	G	OP1-P-O3'	5.01	116.22	105.20
32	2a	473	G	C5-C6-O6	5.01	131.60	128.60
32	2a	1478	C	C6-N1-C2	-5.01	118.30	120.30
2	1B	31	C	N3-C2-O2	-5.00	118.40	121.90
1	2A	877	U	C6-N1-C2	-5.00	118.00	121.00
1	2A	1547	C	N3-C4-C5	-5.00	119.90	121.90
1	2A	1747(A)	G	N1-C6-O6	5.00	122.90	119.90
2	2B	90	A	N1-C6-N6	5.00	121.60	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	27	G	OP2-P-O3'	5.00	116.21	105.20
1	1A	1274	G	N3-C4-N9	-5.00	123.00	126.00
1	1A	1331	G	N3-C2-N2	5.00	123.40	119.90
1	1A	2462	A	C2-N3-C4	5.00	113.10	110.60
1	1A	2772	G	N9-C4-C5	5.00	107.40	105.40
32	1a	147	G	C8-N9-C1'	5.00	133.50	127.00
1	2A	684	G	N7-C8-N9	5.00	115.60	113.10
1	2A	1207	C	N3-C4-C5	-5.00	119.90	121.90
1	2A	1291	C	C6-N1-C2	5.00	122.30	120.30
1	2A	1689	A	C5-N7-C8	-5.00	101.40	103.90
2	2B	1	U	N1-C2-O2	5.00	126.30	122.80
1	1A	1166	G	C5-C6-O6	5.00	131.60	128.60
1	1A	1586	G	N3-C4-C5	5.00	131.10	128.60
1	1A	2031	G	N1-C2-N2	5.00	120.70	116.20
1	1A	2402	U	C4-C5-C6	5.00	122.70	119.70
1	1A	2860	A	C6-N1-C2	-5.00	115.60	118.60
32	1a	472	A	C5-C6-N1	-5.00	115.20	117.70
32	1a	1392	G	C5-C6-N1	-5.00	109.00	111.50
32	1a	1496	C	C5-C6-N1	-5.00	118.50	121.00
32	1a	1517	G	C5-C6-O6	-5.00	125.60	128.60
1	2A	635	C	N3-C4-C5	-5.00	119.90	121.90
1	2A	1056	G	N3-C4-N9	-5.00	123.00	126.00
1	2A	1213	A	O4'-C1'-N9	-5.00	104.20	108.20
1	2A	1253	A	O4'-C1'-N9	-5.00	104.20	108.20
1	2A	1835	G	N3-C4-C5	-5.00	126.10	128.60
1	2A	2755	C	N3-C4-C5	-5.00	119.90	121.90
32	2a	728	A	N9-C4-C5	5.00	107.80	105.80
32	2a	1471	G	O5'-P-OP2	-5.00	101.20	105.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	1X	93	GLU	Peptide
33	1b	124	SER	Peptide
19	2X	93	GLU	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/275 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/275 (99%)	256 (94%)	17 (6%)	0	100	100
4	1E	202/204 (99%)	192 (95%)	9 (4%)	1 (0%)	29	61
4	2E	202/204 (99%)	191 (95%)	10 (5%)	1 (0%)	29	61
5	1F	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	29	61
5	2F	201/203 (99%)	192 (96%)	7 (4%)	2 (1%)	15	45
6	1G	179/181 (99%)	163 (91%)	12 (7%)	4 (2%)	6	24
6	2G	179/181 (99%)	163 (91%)	13 (7%)	3 (2%)	9	31
7	1H	172/174 (99%)	163 (95%)	9 (5%)	0	100	100
7	2H	171/174 (98%)	164 (96%)	7 (4%)	0	100	100
8	1I	145/147 (99%)	127 (88%)	15 (10%)	3 (2%)	7	26
8	2I	144/147 (98%)	125 (87%)	16 (11%)	3 (2%)	7	26
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19	51
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	51
11	1P	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	22	54
12	1Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22	54
12	2Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22	54
13	1R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
14	1S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	17	48
14	2S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	17	48
15	1T	129/131 (98%)	125 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
16	1U	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/116 (98%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	45
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	45
18	1W	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
20	2Y	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
21	1Z	201/203 (99%)	187 (93%)	14 (7%)	0	100	100
21	2Z	199/203 (98%)	189 (95%)	10 (5%)	0	100	100
22	10	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
22	20	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
23	11	95/97 (98%)	94 (99%)	0	1 (1%)	14	42
23	21	95/97 (98%)	93 (98%)	1 (1%)	1 (1%)	14	42
24	12	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
24	22	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
25	13	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
25	23	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
26	14	67/69 (97%)	52 (78%)	11 (16%)	4 (6%)	1	4
26	24	67/69 (97%)	52 (78%)	10 (15%)	5 (8%)	1	2
27	15	57/59 (97%)	57 (100%)	0	0	100	100
27	25	57/59 (97%)	57 (100%)	0	0	100	100
28	16	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
28	26	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
29	17	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
29	27	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
30	18	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
30	28	62/64 (97%)	60 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/231 (99%)	190 (83%)	27 (12%)	12 (5%)	2	6
33	2b	229/231 (99%)	192 (84%)	27 (12%)	10 (4%)	2	10
34	1c	204/206 (99%)	171 (84%)	31 (15%)	2 (1%)	15	45
34	2c	204/206 (99%)	176 (86%)	25 (12%)	3 (2%)	10	34
35	1d	206/208 (99%)	183 (89%)	19 (9%)	4 (2%)	8	28
35	2d	206/208 (99%)	186 (90%)	17 (8%)	3 (2%)	10	34
36	1e	146/148 (99%)	126 (86%)	19 (13%)	1 (1%)	22	54
36	2e	146/148 (99%)	129 (88%)	16 (11%)	1 (1%)	22	54
37	1f	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
37	2f	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/155 (99%)	143 (94%)	9 (6%)	1 (1%)	22	54
38	2g	153/155 (99%)	142 (93%)	8 (5%)	3 (2%)	7	27
39	1h	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
39	2h	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/127 (98%)	107 (86%)	15 (12%)	3 (2%)	6	22
40	2i	124/127 (98%)	105 (85%)	15 (12%)	4 (3%)	4	16
41	1j	95/97 (98%)	79 (83%)	13 (14%)	3 (3%)	4	16
41	2j	94/97 (97%)	79 (84%)	12 (13%)	3 (3%)	4	16
42	1k	112/114 (98%)	100 (89%)	11 (10%)	1 (1%)	17	48
42	2k	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
43	1l	119/122 (98%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/122 (98%)	113 (95%)	6 (5%)	0	100	100
44	1m	114/116 (98%)	104 (91%)	5 (4%)	5 (4%)	2	10
44	2m	112/116 (97%)	103 (92%)	7 (6%)	2 (2%)	8	29
45	1n	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
45	2n	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	13	40
46	2o	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	13	40
47	1p	80/82 (98%)	67 (84%)	12 (15%)	1 (1%)	12	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/82 (98%)	65 (81%)	15 (19%)	0	100	100
48	1q	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/68 (97%)	61 (92%)	4 (6%)	1 (2%)	10	34
49	2r	66/68 (97%)	62 (94%)	3 (4%)	1 (2%)	10	34
50	1s	81/83 (98%)	73 (90%)	6 (7%)	2 (2%)	5	21
50	2s	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
51	1t	94/98 (96%)	87 (93%)	6 (6%)	1 (1%)	14	42
51	2t	96/98 (98%)	85 (88%)	8 (8%)	3 (3%)	4	16
52	1u	21/23 (91%)	19 (90%)	0	2 (10%)	0	1
52	2u	21/23 (91%)	17 (81%)	3 (14%)	1 (5%)	2	8
53	1x	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
53	2x	94/97 (97%)	90 (96%)	4 (4%)	0	100	100
54	1y	8/10 (80%)	8 (100%)	0	0	100	100
54	2y	8/10 (80%)	8 (100%)	0	0	100	100
All	All	11645/11862 (98%)	10762 (92%)	770 (7%)	113 (1%)	15	45

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	52	LEU
6	1G	49	ASP
6	1G	51	ARG
6	1G	78	SER
8	1I	73	GLU
14	1S	59	LYS
23	11	3	LYS
26	14	49	PHE
26	14	60	GLN
33	1b	17	PHE
33	1b	20	GLU
33	1b	37	ASN
33	1b	124	SER
33	1b	125	PRO
34	1c	156	ARG
41	1j	79	ARG
44	1m	3	ARG

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Mol	Chain	Res	Type
44	1m	11	ARG
44	1m	12	ASN
50	1s	12	ASP
5	2F	21	ALA
5	2F	130	ALA
6	2G	81	LYS
8	2I	105	HIS
26	24	45	GLY
26	24	65	ASP
33	2b	10	LEU
33	2b	17	PHE
33	2b	125	PRO
38	2g	7	ALA
40	2i	44	VAL
40	2i	54	ASP
41	2j	32	ALA
41	2j	79	ARG
44	2m	67	GLU
5	1F	130	ALA
26	14	45	GLY
33	1b	127	ILE
33	1b	190	THR
35	1d	171	GLY
38	1g	55	GLY
41	1j	31	GLY
44	1m	67	GLU
46	1o	23	GLY
51	1t	95	ALA
6	2G	78	SER
8	2I	10	GLU
23	21	3	LYS
33	2b	16	HIS
33	2b	190	THR
34	2c	156	ARG
35	2d	171	GLY
38	2g	55	GLY
52	2u	7	ARG
6	1G	124	SER
10	1O	5	GLN
33	1b	28	PHE
49	1r	25	THR
4	2E	51	PHE

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Mol	Chain	Res	Type
6	2G	124	SER
12	2Q	59	ARG
17	2V	79	VAL
26	24	47	GLN
33	2b	20	GLU
33	2b	228	GLY
34	2c	61	ALA
40	2i	11	LYS
46	2o	88	ARG
12	1Q	59	ARG
26	14	55	ARG
33	1b	16	HIS
33	1b	22	LYS
33	1b	202	PRO
35	1d	3	ARG
52	1u	7	ARG
10	2O	5	GLN
26	24	49	PHE
35	2d	108	LEU
38	2g	6	ARG
44	2m	5	ALA
8	1I	85	GLU
8	1I	105	HIS
33	1b	83	MET
40	1i	33	PHE
40	1i	107	ARG
42	1k	117	ASN
50	1s	13	ASP
8	2I	85	GLU
14	2S	89	ARG
26	24	48	ARG
33	2b	8	LYS
41	2j	77	PRO
49	2r	36	ASN
51	2t	100	ILE
51	2t	102	GLY
36	1e	147	ASP
40	1i	44	VAL
44	1m	21	TYR
47	1p	69	THR
52	1u	3	LYS
11	2P	29	LYS

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Mol	Chain	Res	Type
34	2c	129	ALA
40	2i	33	PHE
51	2t	10	LEU
17	1V	79	VAL
41	1j	77	PRO
33	2b	127	ILE
35	2d	136	PRO
34	1c	108	ASN
33	2b	202	PRO
36	2e	96	PRO
35	1d	5	ILE
35	1d	136	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	214/217 (99%)	190 (89%)	24 (11%)	6 18
3	2D	215/217 (99%)	195 (91%)	20 (9%)	9 27
4	1E	164/165 (99%)	147 (90%)	17 (10%)	7 21
4	2E	164/165 (99%)	144 (88%)	20 (12%)	5 15
5	1F	160/161 (99%)	136 (85%)	24 (15%)	3 9
5	2F	158/161 (98%)	142 (90%)	16 (10%)	7 23
6	1G	144/155 (93%)	127 (88%)	17 (12%)	5 16
6	2G	142/155 (92%)	133 (94%)	9 (6%)	18 46
7	1H	144/145 (99%)	132 (92%)	12 (8%)	11 32
7	2H	143/145 (99%)	121 (85%)	22 (15%)	2 8
8	1I	111/123 (90%)	97 (87%)	14 (13%)	4 13
8	2I	108/123 (88%)	95 (88%)	13 (12%)	5 15
9	1N	119/119 (100%)	105 (88%)	14 (12%)	5 16
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1O	100/100 (100%)	91 (91%)	9 (9%)	9	29
10	2O	100/100 (100%)	94 (94%)	6 (6%)	19	49
11	1P	115/116 (99%)	107 (93%)	8 (7%)	15	41
11	2P	115/116 (99%)	106 (92%)	9 (8%)	12	34
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	14	39
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	8	24
13	1R	101/101 (100%)	88 (87%)	13 (13%)	4	13
13	2R	101/101 (100%)	87 (86%)	14 (14%)	3	10
14	1S	87/87 (100%)	77 (88%)	10 (12%)	5	17
14	2S	85/87 (98%)	75 (88%)	10 (12%)	5	16
15	1T	115/115 (100%)	109 (95%)	6 (5%)	23	55
15	2T	113/115 (98%)	108 (96%)	5 (4%)	28	61
16	1U	93/93 (100%)	82 (88%)	11 (12%)	5	16
16	2U	93/93 (100%)	86 (92%)	7 (8%)	13	37
17	1V	81/82 (99%)	70 (86%)	11 (14%)	3	11
17	2V	80/82 (98%)	69 (86%)	11 (14%)	3	10
18	1W	89/91 (98%)	81 (91%)	8 (9%)	9	29
18	2W	88/91 (97%)	83 (94%)	5 (6%)	20	51
19	1X	77/77 (100%)	71 (92%)	6 (8%)	12	34
19	2X	77/77 (100%)	75 (97%)	2 (3%)	46	77
20	1Y	86/88 (98%)	79 (92%)	7 (8%)	11	33
20	2Y	86/88 (98%)	76 (88%)	10 (12%)	5	16
21	1Z	169/176 (96%)	147 (87%)	22 (13%)	4	12
21	2Z	165/176 (94%)	149 (90%)	16 (10%)	8	25
22	10	61/62 (98%)	56 (92%)	5 (8%)	11	32
22	20	61/62 (98%)	58 (95%)	3 (5%)	25	57
23	11	79/82 (96%)	72 (91%)	7 (9%)	9	29
23	21	81/82 (99%)	72 (89%)	9 (11%)	6	19
24	12	65/66 (98%)	61 (94%)	4 (6%)	18	47
24	22	66/66 (100%)	60 (91%)	6 (9%)	9	28
25	13	51/51 (100%)	49 (96%)	2 (4%)	32	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	23	50/51 (98%)	46 (92%)	4 (8%)	12	33
26	14	58/62 (94%)	49 (84%)	9 (16%)	2	8
26	24	54/62 (87%)	45 (83%)	9 (17%)	2	6
27	15	51/51 (100%)	45 (88%)	6 (12%)	5	16
27	25	50/51 (98%)	47 (94%)	3 (6%)	19	49
28	16	51/51 (100%)	46 (90%)	5 (10%)	8	24
28	26	50/51 (98%)	45 (90%)	5 (10%)	7	23
29	17	41/41 (100%)	36 (88%)	5 (12%)	5	15
29	27	41/41 (100%)	38 (93%)	3 (7%)	14	38
30	18	54/54 (100%)	48 (89%)	6 (11%)	6	19
30	28	54/54 (100%)	47 (87%)	7 (13%)	4	12
31	19	34/34 (100%)	32 (94%)	2 (6%)	19	49
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	49
33	1b	191/199 (96%)	170 (89%)	21 (11%)	6	19
33	2b	187/199 (94%)	156 (83%)	31 (17%)	2	7
34	1c	144/160 (90%)	135 (94%)	9 (6%)	18	46
34	2c	140/160 (88%)	127 (91%)	13 (9%)	9	27
35	1d	171/180 (95%)	151 (88%)	20 (12%)	5	16
35	2d	172/180 (96%)	159 (92%)	13 (8%)	13	36
36	1e	114/114 (100%)	104 (91%)	10 (9%)	10	30
36	2e	114/114 (100%)	107 (94%)	7 (6%)	18	48
37	1f	85/90 (94%)	80 (94%)	5 (6%)	19	49
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	59
38	1g	120/126 (95%)	111 (92%)	9 (8%)	13	37
38	2g	119/126 (94%)	112 (94%)	7 (6%)	19	49
39	1h	116/118 (98%)	104 (90%)	12 (10%)	7	22
39	2h	114/118 (97%)	106 (93%)	8 (7%)	15	41
40	1i	91/98 (93%)	81 (89%)	10 (11%)	6	19
40	2i	88/98 (90%)	79 (90%)	9 (10%)	7	22
41	1j	68/87 (78%)	61 (90%)	7 (10%)	7	22
41	2j	68/87 (78%)	62 (91%)	6 (9%)	10	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	1k	83/86 (96%)	79 (95%)	4 (5%)	25 58
42	2k	83/86 (96%)	75 (90%)	8 (10%)	8 25
43	1l	96/102 (94%)	90 (94%)	6 (6%)	18 46
43	2l	96/102 (94%)	89 (93%)	7 (7%)	14 38
44	1m	90/94 (96%)	83 (92%)	7 (8%)	12 34
44	2m	87/94 (93%)	77 (88%)	10 (12%)	5 17
45	1n	49/49 (100%)	43 (88%)	6 (12%)	5 15
45	2n	49/49 (100%)	45 (92%)	4 (8%)	11 32
46	1o	78/79 (99%)	73 (94%)	5 (6%)	17 45
46	2o	78/79 (99%)	72 (92%)	6 (8%)	13 35
47	1p	69/71 (97%)	57 (83%)	12 (17%)	2 6
47	2p	68/71 (96%)	61 (90%)	7 (10%)	7 22
48	1q	94/94 (100%)	88 (94%)	6 (6%)	17 45
48	2q	94/94 (100%)	88 (94%)	6 (6%)	17 45
49	1r	59/59 (100%)	54 (92%)	5 (8%)	10 31
49	2r	59/59 (100%)	51 (86%)	8 (14%)	3 11
50	1s	68/72 (94%)	62 (91%)	6 (9%)	10 30
50	2s	67/72 (93%)	62 (92%)	5 (8%)	13 37
51	1t	71/76 (93%)	65 (92%)	6 (8%)	10 31
51	2t	70/76 (92%)	66 (94%)	4 (6%)	20 51
52	1u	18/18 (100%)	17 (94%)	1 (6%)	21 52
52	2u	18/18 (100%)	15 (83%)	3 (17%)	2 6
53	1x	82/83 (99%)	77 (94%)	5 (6%)	18 48
53	2x	79/83 (95%)	67 (85%)	12 (15%)	3 8
54	1y	10/10 (100%)	9 (90%)	1 (10%)	7 23
54	2y	10/10 (100%)	9 (90%)	1 (10%)	7 23
All	All	9540/9882 (96%)	8626 (90%)	914 (10%)	8 25

All (914) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	13	ARG

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Mol	Chain	Res	Type
3	1D	37	LEU
3	1D	38	LYS
3	1D	61	LEU
3	1D	69	ARG
3	1D	88	ARG
3	1D	94	LEU
3	1D	99	ASP
3	1D	103	ARG
3	1D	106	ILE
3	1D	111	LEU
3	1D	113	VAL
3	1D	115	GLN
3	1D	126	GLN
3	1D	141	VAL
3	1D	155	LEU
3	1D	211	ARG
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	260	ARG
4	1E	1	MET
4	1E	7	VAL
4	1E	9	VAL
4	1E	49	LEU
4	1E	73	GLU
4	1E	75	VAL
4	1E	78	LEU
4	1E	113	PHE
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	154	LYS
4	1E	163	GLU
4	1E	170	LEU
4	1E	175	VAL
4	1E	178	GLU
4	1E	181	LEU
5	1F	14	PRO
5	1F	18	ARG
5	1F	24	LEU

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Mol	Chain	Res	Type
5	1F	28	ILE
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	60	SER
5	1F	62	ARG
5	1F	74	ARG
5	1F	94	PRO
5	1F	110	LEU
5	1F	125	LEU
5	1F	132	VAL
5	1F	137	LYS
5	1F	140	LEU
5	1F	158	THR
5	1F	162	LEU
5	1F	168	ARG
5	1F	170	LEU
5	1F	191	ARG
5	1F	192	LEU
5	1F	197	ASP
5	1F	200	GLU
6	1G	5	VAL
6	1G	7	LEU
6	1G	28	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	45	GLU
6	1G	52	ILE
6	1G	53	LEU
6	1G	78	SER
6	1G	82	LEU
6	1G	126	ASP
6	1G	133	LEU
6	1G	140	ILE
6	1G	145	THR
6	1G	159	VAL
6	1G	165	THR
6	1G	167	GLU
7	1H	6	ARG
7	1H	13	LYS
7	1H	15	VAL
7	1H	45	VAL

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Mol	Chain	Res	Type
7	1H	71	LEU
7	1H	105	LEU
7	1H	107	VAL
7	1H	119	GLU
7	1H	122	THR
7	1H	134	SER
7	1H	139	GLN
7	1H	153	LYS
8	1I	3	VAL
8	1I	5	LEU
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	38	LEU
8	1I	47	LEU
8	1I	52	ARG
8	1I	75	LEU
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	109	ILE
8	1I	140	LEU
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	46	VAL
9	1N	48	MET
9	1N	62	VAL
9	1N	67	LEU
9	1N	73	THR
9	1N	87	LEU
9	1N	97	ARG
9	1N	99	LEU
9	1N	121	LYS
9	1N	138	LEU
9	1N	140	VAL
10	1O	8	LEU
10	1O	10	VAL
10	1O	20	MET
10	1O	28	SER
10	1O	64	ARG
10	1O	69	ILE

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Mol	Chain	Res	Type
10	1O	97	ARG
10	1O	108	GLU
10	1O	113	LYS
11	1P	1	MET
11	1P	3	LEU
11	1P	59	LEU
11	1P	83	VAL
11	1P	112	LEU
11	1P	125	VAL
11	1P	147	LEU
11	1P	149	GLU
12	1Q	2	LEU
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	21	THR
12	1Q	35	VAL
12	1Q	59	ARG
12	1Q	75	THR
12	1Q	133	ARG
13	1R	6	SER
13	1R	17	ARG
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	59	ASP
13	1R	67	LEU
13	1R	71	GLN
13	1R	73	VAL
13	1R	75	LEU
13	1R	111	LEU
14	1S	14	VAL
14	1S	17	ARG
14	1S	25	ARG
14	1S	36	TYR
14	1S	46	VAL
14	1S	52	SER
14	1S	59	LYS
14	1S	69	VAL
14	1S	85	VAL
14	1S	110	LEU

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Mol	Chain	Res	Type
15	1T	13	ARG
15	1T	28	VAL
15	1T	59	THR
15	1T	74	ARG
15	1T	89	VAL
15	1T	108	ARG
16	1U	8	VAL
16	1U	27	LEU
16	1U	31	SER
16	1U	52	ARG
16	1U	59	ARG
16	1U	74	LEU
16	1U	83	LEU
16	1U	95	LEU
16	1U	104	GLN
16	1U	112	ARG
16	1U	117	GLN
17	1V	28	GLU
17	1V	35	LEU
17	1V	46	VAL
17	1V	51	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
17	1V	82	ARG
17	1V	95	LEU
17	1V	100	ARG
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	67	ASP
18	1W	100	THR
18	1W	107	LEU
19	1X	15	GLU
19	1X	33	LYS
19	1X	40	LYS
19	1X	45	THR
19	1X	57	LEU
19	1X	66	LEU

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Mol	Chain	Res	Type
20	1Y	43	ASN
20	1Y	47	LYS
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	90	LEU
20	1Y	92	ASN
20	1Y	99	CYS
21	1Z	11	GLU
21	1Z	14	LYS
21	1Z	18	LEU
21	1Z	31	ARG
21	1Z	33	LEU
21	1Z	37	VAL
21	1Z	42	VAL
21	1Z	46	LYS
21	1Z	58	VAL
21	1Z	61	LEU
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	93	ASP
21	1Z	94	GLU
21	1Z	102	LEU
21	1Z	103	ARG
21	1Z	126	VAL
21	1Z	150	LEU
21	1Z	161	VAL
21	1Z	170	THR
21	1Z	203	GLU
22	10	10	THR
22	10	14	ARG
22	10	39	ARG
22	10	55	ARG
22	10	59	LEU
23	11	11	ARG
23	11	30	VAL
23	11	33	LYS
23	11	35	THR
23	11	59	THR
23	11	83	GLU
23	11	95	LEU
24	12	3	LEU

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Mol	Chain	Res	Type
24	12	53	LEU
24	12	68	ARG
24	12	70	GLN
25	13	8	LEU
25	13	23	LEU
26	14	23	GLU
26	14	30	GLU
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
26	14	57	GLU
26	14	58	ARG
26	14	59	PHE
26	14	65	ASP
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	57	VAL
27	15	58	LEU
27	15	60	VAL
28	16	6	ARG
28	16	14	THR
28	16	19	ARG
28	16	48	VAL
28	16	52	VAL
29	17	1	MET
29	17	10	ARG
29	17	24	THR
29	17	43	THR
29	17	47	ARG
30	18	14	VAL
30	18	23	VAL
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
30	18	37	SER
31	19	4	ARG
31	19	17	ILE
33	1b	9	GLU
33	1b	15	VAL
33	1b	17	PHE
33	1b	19	HIS

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Mol	Chain	Res	Type
33	1b	24	TRP
33	1b	28	PHE
33	1b	67	THR
33	1b	71	VAL
33	1b	73	THR
33	1b	80	ILE
33	1b	82	ARG
33	1b	111	ARG
33	1b	122	PHE
33	1b	157	ARG
33	1b	178	ARG
33	1b	185	ILE
33	1b	200	ILE
33	1b	208	ILE
33	1b	221	LEU
33	1b	226	ARG
33	1b	230	VAL
34	1c	21	ARG
34	1c	29	TYR
34	1c	36	ASP
34	1c	52	LEU
34	1c	64	VAL
34	1c	67	THR
34	1c	104	GLN
34	1c	115	LEU
34	1c	202	ILE
35	1d	25	ARG
35	1d	28	SER
35	1d	34	GLU
35	1d	47	ARG
35	1d	49	ARG
35	1d	59	ARG
35	1d	80	GLU
35	1d	85	LYS
35	1d	107	ARG
35	1d	110	PHE
35	1d	123	HIS
35	1d	127	THR
35	1d	135	LEU
35	1d	150	GLU
35	1d	158	ILE
35	1d	168	ARG

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Mol	Chain	Res	Type
35	1d	182	LYS
35	1d	184	LYS
35	1d	194	LEU
35	1d	196	LEU
36	1e	16	THR
36	1e	20	GLN
36	1e	31	LEU
36	1e	41	VAL
36	1e	75	THR
36	1e	78	HIS
36	1e	91	LEU
36	1e	120	THR
36	1e	135	THR
36	1e	148	VAL
37	1f	17	SER
37	1f	40	VAL
37	1f	57	GLN
37	1f	63	TYR
37	1f	70	ASP
38	1g	9	VAL
38	1g	13	GLN
38	1g	15	ASP
38	1g	58	PRO
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	138	LYS
38	1g	155	ARG
39	1h	25	ASP
39	1h	26	VAL
39	1h	51	VAL
39	1h	63	LEU
39	1h	99	GLU
39	1h	102	ARG
39	1h	104	ARG
39	1h	112	LEU
39	1h	120	THR
39	1h	121	ASP
39	1h	122	ARG
39	1h	137	VAL
40	1i	25	LYS
40	1i	27	THR

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Mol	Chain	Res	Type
40	1i	41	VAL
40	1i	42	ARG
40	1i	50	LEU
40	1i	56	LEU
40	1i	60	ASP
40	1i	81	ILE
40	1i	92	TYR
40	1i	114	TYR
41	1j	5	ARG
41	1j	13	HIS
41	1j	34	VAL
41	1j	56	HIS
41	1j	94	VAL
41	1j	95	GLU
41	1j	100	THR
42	1k	14	VAL
42	1k	18	ARG
42	1k	31	THR
42	1k	109	VAL
43	1l	18	VAL
43	1l	27	LEU
43	1l	33	ARG
43	1l	60	LEU
43	1l	89	ARG
43	1l	113	ARG
44	1m	17	VAL
44	1m	19	LEU
44	1m	55	ARG
44	1m	56	LEU
44	1m	70	LEU
44	1m	102	ARG
44	1m	111	LYS
45	1n	3	ARG
45	1n	12	ARG
45	1n	18	VAL
45	1n	32	SER
45	1n	33	VAL
45	1n	44	LEU
46	1o	5	LYS
46	1o	28	GLN
46	1o	39	LEU
46	1o	66	LEU

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Mol	Chain	Res	Type
46	1o	88	ARG
47	1p	1	MET
47	1p	2	VAL
47	1p	8	ARG
47	1p	25	ARG
47	1p	45	THR
47	1p	58	TYR
47	1p	60	LEU
47	1p	62	VAL
47	1p	67	THR
47	1p	69	THR
47	1p	76	GLN
47	1p	79	VAL
48	1q	9	VAL
48	1q	52	LYS
48	1q	63	ARG
48	1q	70	ARG
48	1q	87	LYS
48	1q	98	LEU
49	1r	37	VAL
49	1r	42	ARG
49	1r	54	ARG
49	1r	65	ILE
49	1r	76	LEU
50	1s	4	SER
50	1s	16	LEU
50	1s	37	ARG
50	1s	41	VAL
50	1s	77	THR
50	1s	79	THR
51	1t	10	LEU
51	1t	15	ARG
51	1t	58	LYS
51	1t	62	LEU
51	1t	80	ARG
51	1t	84	LEU
52	1u	24	ARG
53	1x	23	ARG
53	1x	24	LEU
53	1x	41	LEU
53	1x	46	GLN
53	1x	66	LYS

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Mol	Chain	Res	Type
54	1y	6	TYR
3	2D	61	LEU
3	2D	88	ARG
3	2D	94	LEU
3	2D	103	ARG
3	2D	106	ILE
3	2D	111	LEU
3	2D	113	VAL
3	2D	116	GLN
3	2D	138	VAL
3	2D	155	LEU
3	2D	211	ARG
3	2D	217	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	260	ARG
3	2D	274	ARG
3	2D	275	LYS
3	2D	276	LYS
4	2E	1	MET
4	2E	21	VAL
4	2E	24	THR
4	2E	33	VAL
4	2E	34	VAL
4	2E	47	VAL
4	2E	49	LEU
4	2E	75	VAL
4	2E	78	LEU
4	2E	87	GLU
4	2E	89	ASP
4	2E	113	PHE
4	2E	116	VAL
4	2E	144	ARG
4	2E	154	LYS
4	2E	163	GLU
4	2E	170	LEU
4	2E	175	VAL
4	2E	181	LEU
4	2E	184	VAL
5	2F	18	ARG

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Mol	Chain	Res	Type
5	2F	24	LEU
5	2F	33	LEU
5	2F	38	ARG
5	2F	53	THR
5	2F	57	VAL
5	2F	74	ARG
5	2F	88	VAL
5	2F	95	ARG
5	2F	108	LYS
5	2F	132	VAL
5	2F	140	LEU
5	2F	158	THR
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
6	2G	3	LEU
6	2G	5	VAL
6	2G	28	VAL
6	2G	49	ASP
6	2G	113	ARG
6	2G	124	SER
6	2G	145	THR
6	2G	159	VAL
6	2G	165	THR
7	2H	6	ARG
7	2H	13	LYS
7	2H	15	VAL
7	2H	23	ARG
7	2H	25	LYS
7	2H	33	LEU
7	2H	47	GLU
7	2H	49	VAL
7	2H	59	ARG
7	2H	63	SER
7	2H	71	LEU
7	2H	81	GLU
7	2H	88	LEU
7	2H	95	ARG
7	2H	105	LEU
7	2H	107	VAL
7	2H	122	THR
7	2H	136	ILE

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Mol	Chain	Res	Type
7	2H	139	GLN
7	2H	148	ILE
7	2H	153	LYS
7	2H	172	LYS
8	2I	5	LEU
8	2I	9	LEU
8	2I	38	LEU
8	2I	44	LEU
8	2I	52	ARG
8	2I	54	GLN
8	2I	75	LEU
8	2I	92	VAL
8	2I	99	GLU
8	2I	101	LEU
8	2I	116	LEU
8	2I	123	LEU
8	2I	140	LEU
9	2N	5	VAL
9	2N	10	GLU
9	2N	33	LEU
9	2N	34	LEU
9	2N	46	VAL
9	2N	48	MET
9	2N	62	VAL
9	2N	67	LEU
9	2N	73	THR
9	2N	87	LEU
9	2N	99	LEU
9	2N	115	ARG
9	2N	138	LEU
10	2O	10	VAL
10	2O	24	VAL
10	2O	28	SER
10	2O	69	ILE
10	2O	90	GLN
10	2O	108	GLU
11	2P	1	MET
11	2P	3	LEU
11	2P	32	THR
11	2P	59	LEU
11	2P	74	GLU
11	2P	83	VAL

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Mol	Chain	Res	Type
11	2P	95	VAL
11	2P	99	LEU
11	2P	112	LEU
12	2Q	2	LEU
12	2Q	16	ARG
12	2Q	21	THR
12	2Q	22	LYS
12	2Q	35	VAL
12	2Q	55	VAL
12	2Q	59	ARG
12	2Q	60	ARG
12	2Q	63	LYS
12	2Q	75	THR
12	2Q	85	LYS
13	2R	6	SER
13	2R	18	LEU
13	2R	24	GLN
13	2R	29	LEU
13	2R	36	THR
13	2R	44	LEU
13	2R	54	LEU
13	2R	65	LEU
13	2R	75	LEU
13	2R	79	LEU
13	2R	96	ARG
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	14	VAL
14	2S	17	ARG
14	2S	25	ARG
14	2S	36	TYR
14	2S	38	GLN
14	2S	52	SER
14	2S	68	GLN
14	2S	75	GLU
14	2S	85	VAL
14	2S	110	LEU
15	2T	28	VAL
15	2T	74	ARG
15	2T	89	VAL
15	2T	95	ARG

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Mol	Chain	Res	Type
15	2T	115	ARG
16	2U	5	LYS
16	2U	31	SER
16	2U	52	ARG
16	2U	74	LEU
16	2U	83	LEU
16	2U	85	LYS
16	2U	117	GLN
17	2V	35	LEU
17	2V	46	VAL
17	2V	51	VAL
17	2V	52	VAL
17	2V	53	GLU
17	2V	57	VAL
17	2V	72	VAL
17	2V	73	SER
17	2V	79	VAL
17	2V	82	ARG
17	2V	95	LEU
18	2W	11	ARG
18	2W	17	VAL
18	2W	27	LYS
18	2W	100	THR
18	2W	107	LEU
19	2X	57	LEU
19	2X	68	ARG
20	2Y	6	HIS
20	2Y	47	LYS
20	2Y	64	GLU
20	2Y	70	SER
20	2Y	73	ARG
20	2Y	81	LYS
20	2Y	88	LYS
20	2Y	90	LEU
20	2Y	92	ASN
20	2Y	99	CYS
21	2Z	18	LEU
21	2Z	28	MET
21	2Z	31	ARG
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	54	HIS

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Mol	Chain	Res	Type
21	2Z	61	LEU
21	2Z	72	ARG
21	2Z	86	VAL
21	2Z	87	ASP
21	2Z	91	LEU
21	2Z	94	GLU
21	2Z	97	GLU
21	2Z	107	THR
21	2Z	150	LEU
21	2Z	182	LYS
22	20	10	THR
22	20	14	ARG
22	20	39	ARG
23	21	4	VAL
23	21	21	ARG
23	21	30	VAL
23	21	35	THR
23	21	59	THR
23	21	62	VAL
23	21	75	GLU
23	21	85	LEU
23	21	95	LEU
24	22	3	LEU
24	22	8	LYS
24	22	15	LYS
24	22	32	LEU
24	22	45	SER
24	22	53	LEU
25	23	23	LEU
25	23	31	LEU
25	23	44	ARG
25	23	54	VAL
26	24	13	ARG
26	24	52	THR
26	24	53	GLU
26	24	56	VAL
26	24	60	GLN
26	24	62	ARG
26	24	63	TYR
26	24	67	TYR
26	24	69	LYS
27	25	16	ARG

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Mol	Chain	Res	Type
27	25	29	THR
27	25	57	VAL
28	26	6	ARG
28	26	14	THR
28	26	19	ARG
28	26	48	VAL
28	26	52	VAL
29	27	1	MET
29	27	43	THR
29	27	46	VAL
30	28	6	THR
30	28	14	VAL
30	28	23	VAL
30	28	31	HIS
30	28	34	TRP
30	28	37	SER
30	28	46	ARG
31	29	4	ARG
31	29	17	ILE
33	2b	10	LEU
33	2b	11	LEU
33	2b	15	VAL
33	2b	16	HIS
33	2b	17	PHE
33	2b	19	HIS
33	2b	23	ARG
33	2b	24	TRP
33	2b	28	PHE
33	2b	37	ASN
33	2b	44	LEU
33	2b	45	GLN
33	2b	58	ILE
33	2b	80	ILE
33	2b	81	VAL
33	2b	93	VAL
33	2b	94	ASN
33	2b	111	ARG
33	2b	126	GLU
33	2b	128	GLU
33	2b	144	ARG
33	2b	145	LEU
33	2b	154	LEU

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Mol	Chain	Res	Type
33	2b	157	ARG
33	2b	158	LEU
33	2b	191	ASP
33	2b	200	ILE
33	2b	209	ARG
33	2b	224	GLN
33	2b	226	ARG
33	2b	230	VAL
34	2c	15	THR
34	2c	52	LEU
34	2c	82	GLU
34	2c	89	GLU
34	2c	102	ASN
34	2c	105	GLU
34	2c	128	PHE
34	2c	131	ARG
34	2c	132	ARG
34	2c	152	ILE
34	2c	162	GLN
34	2c	192	THR
34	2c	202	ILE
35	2d	13	ARG
35	2d	25	ARG
35	2d	28	SER
35	2d	31	CYS
35	2d	49	ARG
35	2d	59	ARG
35	2d	96	LEU
35	2d	107	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	170	VAL
35	2d	178	VAL
36	2e	20	GLN
36	2e	31	LEU
36	2e	41	VAL
36	2e	69	VAL
36	2e	72	GLN
36	2e	91	LEU
36	2e	135	THR
37	2f	22	GLU

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Mol	Chain	Res	Type
37	2f	40	VAL
37	2f	63	TYR
37	2f	94	GLN
38	2g	9	VAL
38	2g	13	GLN
38	2g	15	ASP
38	2g	50	ILE
38	2g	104	LEU
38	2g	113	GLU
38	2g	115	ARG
39	2h	2	LEU
39	2h	26	VAL
39	2h	39	LEU
39	2h	63	LEU
39	2h	91	ARG
39	2h	97	VAL
39	2h	104	ARG
39	2h	112	LEU
40	2i	14	VAL
40	2i	27	THR
40	2i	35	GLU
40	2i	50	LEU
40	2i	53	VAL
40	2i	54	ASP
40	2i	64	THR
40	2i	87	GLN
40	2i	93	ARG
41	2j	19	SER
41	2j	74	ILE
41	2j	84	GLN
41	2j	92	THR
41	2j	95	GLU
41	2j	100	THR
42	2k	14	VAL
42	2k	28	THR
42	2k	33	THR
42	2k	48	ILE
42	2k	103	LEU
42	2k	112	THR
42	2k	114	VAL
42	2k	117	ASN
43	2l	5	PRO

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Mol	Chain	Res	Type
43	2l	18	VAL
43	2l	33	ARG
43	2l	52	LEU
43	2l	55	VAL
43	2l	113	ARG
43	2l	116	SER
44	2m	8	GLU
44	2m	12	ASN
44	2m	14	ARG
44	2m	19	LEU
44	2m	35	GLU
44	2m	56	LEU
44	2m	70	LEU
44	2m	88	ARG
44	2m	115	LYS
44	2m	116	THR
45	2n	3	ARG
45	2n	12	ARG
45	2n	18	VAL
45	2n	44	LEU
46	2o	10	LYS
46	2o	28	GLN
46	2o	38	ARG
46	2o	39	LEU
46	2o	64	ARG
46	2o	66	LEU
47	2p	1	MET
47	2p	2	VAL
47	2p	54	GLU
47	2p	60	LEU
47	2p	62	VAL
47	2p	67	THR
47	2p	69	THR
48	2q	9	VAL
48	2q	14	LYS
48	2q	63	ARG
48	2q	70	ARG
48	2q	74	LEU
48	2q	87	LYS
49	2r	25	THR
49	2r	28	GLU
49	2r	37	VAL

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Mol	Chain	Res	Type
49	2r	54	ARG
49	2r	65	ILE
49	2r	76	LEU
49	2r	85	LEU
49	2r	86	VAL
50	2s	5	LEU
50	2s	33	THR
50	2s	64	GLU
50	2s	77	THR
50	2s	79	THR
51	2t	10	LEU
51	2t	62	LEU
51	2t	80	ARG
51	2t	84	LEU
52	2u	7	ARG
52	2u	15	ARG
52	2u	24	ARG
53	2x	3	MET
53	2x	5	ILE
53	2x	13	THR
53	2x	16	ILE
53	2x	23	ARG
53	2x	24	LEU
53	2x	29	LYS
53	2x	41	LEU
53	2x	42	SER
53	2x	60	VAL
53	2x	62	VAL
53	2x	96	ARG
54	2y	6	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	143	HIS
3	1D	253	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	75	HIS
7	1H	139	GLN
8	1I	104	GLN

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Mol	Chain	Res	Type
8	1I	105	HIS
10	1O	3	GLN
14	1S	95	HIS
15	1T	58	ASN
16	1U	104	GLN
17	1V	80	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	73	GLN
21	1Z	151	HIS
22	10	35	ASN
24	12	9	GLN
25	13	32	GLN
26	14	47	GLN
26	14	60	GLN
34	1c	6	HIS
34	1c	104	GLN
34	1c	176	HIS
35	1d	77	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	125	HIS
35	1d	129	ASN
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	56	GLN
38	1g	86	GLN
38	1g	110	GLN
40	1i	3	GLN
40	1i	58	HIS
41	1j	56	HIS
43	1l	99	HIS
48	1q	16	GLN
50	1s	23	ASN
50	1s	83	HIS
51	1t	16	HIS
53	1x	38	HIS
3	2D	126	GLN

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Mol	Chain	Res	Type
3	2D	143	HIS
3	2D	253	GLN
5	2F	69	HIS
5	2F	75	HIS
7	2H	74	ASN
8	2I	43	ASN
8	2I	104	GLN
9	2N	8	GLN
10	2O	90	GLN
15	2T	58	ASN
16	2U	81	HIS
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
20	2Y	92	ASN
21	2Z	73	GLN
22	20	70	GLN
25	23	32	GLN
26	24	46	GLN
27	25	23	HIS
31	29	29	ASN
33	2b	19	HIS
33	2b	37	ASN
33	2b	94	ASN
33	2b	135	GLN
34	2c	6	HIS
34	2c	162	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	161	ASN
36	2e	72	GLN
37	2f	73	ASN
37	2f	94	GLN
38	2g	28	ASN
38	2g	86	GLN
40	2i	3	GLN
40	2i	58	HIS
41	2j	69	ASN
42	2k	117	ASN
46	2o	28	GLN

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Mol	Chain	Res	Type
47	2p	76	GLN
48	2q	16	GLN
50	2s	14	HIS
50	2s	69	HIS
53	2x	19	HIS
53	2x	84	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	403 (14%)	58 (2%)
1	2A	2855/2915 (97%)	418 (14%)	51 (1%)
2	1B	119/120 (99%)	6 (5%)	0
2	2B	118/120 (98%)	8 (6%)	0
32	1a	1494/1521 (98%)	250 (16%)	0
32	2a	1498/1521 (98%)	249 (16%)	0
All	All	8948/9112 (98%)	1334 (14%)	109 (1%)

All (1334) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	60	G
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	155	C
1	1A	162	G
1	1A	170	A
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	202	A
1	1A	203	G
1	1A	204	G

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Mol	Chain	Res	Type
1	1A	205	A
1	1A	211	A
1	1A	218	A
1	1A	219	U
1	1A	222	A
1	1A	237	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	274	U
1	1A	288	U
1	1A	289	G
1	1A	303	C
1	1A	335	A
1	1A	351	G
1	1A	353	G
1	1A	354	A
1	1A	376	G
1	1A	386	U
1	1A	387	G
1	1A	413	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	448	U
1	1A	455	A
1	1A	474	U
1	1A	481	C
1	1A	482	C
1	1A	483	A
1	1A	505	A
1	1A	507	G
1	1A	530	A
1	1A	534	C
1	1A	543	G
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	574	G

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Mol	Chain	Res	Type
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	609	A
1	1A	615	G
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	633	G
1	1A	638	U
1	1A	639	G
1	1A	641	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	673	G
1	1A	697	C
1	1A	698	G
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	811	A
1	1A	812	G
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	839	G
1	1A	852	G
1	1A	859	C
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A
1	1A	927	G
1	1A	933	C
1	1A	934	A
1	1A	936	C
1	1A	937	A

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Mol	Chain	Res	Type
1	1A	938	G
1	1A	942	A
1	1A	956	A
1	1A	977	G
1	1A	983	G
1	1A	990	A
1	1A	991	G
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1019	G
1	1A	1020	C
1	1A	1021	G
1	1A	1029	A
1	1A	1042	A
1	1A	1051	C
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1079	U
1	1A	1088	G
1	1A	1089	C
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1099	C
1	1A	1100	A
1	1A	1106	U
1	1A	1107	U
1	1A	1108	G
1	1A	1109	G
1	1A	1110	C
1	1A	1111	U
1	1A	1113	A
1	1A	1114	G
1	1A	1115	A
1	1A	1116	A
1	1A	1117	G
1	1A	1119	A
1	1A	1122	C
1	1A	1123	A

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Mol	Chain	Res	Type
1	1A	1124	U
1	1A	1125	C
1	1A	1129	U
1	1A	1131	A
1	1A	1134	A
1	1A	1136	U
1	1A	1139	G
1	1A	1142	A
1	1A	1143	U
1	1A	1155	C
1	1A	1156	G
1	1A	1158	G
1	1A	1162	C
1	1A	1175	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1184	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1256	U
1	1A	1265	A
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1352	C
1	1A	1354	A
1	1A	1367	A
1	1A	1398	U
1	1A	1405	A
1	1A	1411	A
1	1A	1414	G
1	1A	1430	A

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Mol	Chain	Res	Type
1	1A	1431	G
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1500	A
1	1A	1514	C
1	1A	1518	A
1	1A	1529	G
1	1A	1539	C
1	1A	1540	A
1	1A	1554	A
1	1A	1555	C
1	1A	1571	G
1	1A	1578	C
1	1A	1589	A
1	1A	1594	C
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1626	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1695	C
1	1A	1700	G
1	1A	1701	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1767	A
1	1A	1776	G
1	1A	1781	G
1	1A	1787	G

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Mol	Chain	Res	Type
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1800	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1870	G
1	1A	1878	A
1	1A	1879	A
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1918	G
1	1A	1922	A
1	1A	1928	G
1	1A	1935	A
1	1A	1936	C
1	1A	1937	5MU
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2015	U
1	1A	2019	G
1	1A	2045	G
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C

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Mol	Chain	Res	Type
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2102	G
1	1A	2124	U
1	1A	2125	C
1	1A	2126	G
1	1A	2129	C
1	1A	2130	C
1	1A	2132	G
1	1A	2134	G
1	1A	2138	G
1	1A	2139	A
1	1A	2141	A
1	1A	2142	G
1	1A	2148	A
1	1A	2149	G
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2164	C
1	1A	2166	U
1	1A	2168	C
1	1A	2170	G
1	1A	2173	G
1	1A	2180	A
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2194	U
1	1A	2195	A
1	1A	2206	G
1	1A	2208	G
1	1A	2209	G
1	1A	2212	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G

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Mol	Chain	Res	Type
1	1A	2228	G
1	1A	2229	A
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2285	A
1	1A	2291	G
1	1A	2295	C
1	1A	2298	A
1	1A	2299	A
1	1A	2301	G
1	1A	2317	A
1	1A	2320	G
1	1A	2323	A
1	1A	2332	A
1	1A	2333	G
1	1A	2337	G
1	1A	2346	G
1	1A	2347	A
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2395	G
1	1A	2397	C
1	1A	2418	U
1	1A	2426	G
1	1A	2434	A
1	1A	2435	U
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2480	G
1	1A	2481	A
1	1A	2486	C
1	1A	2488	A
1	1A	2514	G

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Mol	Chain	Res	Type
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2532	C
1	1A	2541	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2597	U
1	1A	2598	C
1	1A	2613	C
1	1A	2614	A
1	1A	2615	G
1	1A	2623	U
1	1A	2624	C
1	1A	2642	G
1	1A	2666	A
1	1A	2675	G
1	1A	2694	U
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2770	A
1	1A	2771	A
1	1A	2774	G
1	1A	2778	A
1	1A	2779	G
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2813	G
1	1A	2828	G
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G

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Mol	Chain	Res	Type
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2903	G
1	1A	2906	U
2	1B	45	A
2	1B	51	G
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	101	A
32	1a	105	G
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	156	G
32	1a	159	G
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(E)	U
32	1a	189(F)	U
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G

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Mol	Chain	Res	Type
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	298	A
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	350	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	411	A
32	1a	412	A
32	1a	413	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	482	A
32	1a	484	G
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C

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Mol	Chain	Res	Type
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	564	C
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	592	G
32	1a	596	C
32	1a	618	C
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	633	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	672	U
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	733	A
32	1a	753	A
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	838	G
32	1a	840	C

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Mol	Chain	Res	Type
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	967	5MC
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	998	G
32	1a	999	C
32	1a	1002	G
32	1a	1004	A
32	1a	1005	A
32	1a	1006	C
32	1a	1020	U
32	1a	1022	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1031	G
32	1a	1032	G

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Mol	Chain	Res	Type
32	1a	1033	G
32	1a	1034	G
32	1a	1036	G
32	1a	1037	C
32	1a	1042	G
32	1a	1044	A
32	1a	1053	G
32	1a	1063	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1123	A
32	1a	1125	U
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1146	A
32	1a	1150	U
32	1a	1152	A
32	1a	1159	U
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1189	C
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1208	C
32	1a	1213	A
32	1a	1224	G
32	1a	1227	A
32	1a	1236	A

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Mol	Chain	Res	Type
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1261	A
32	1a	1270	C
32	1a	1273	G
32	1a	1278	U
32	1a	1280	A
32	1a	1282	C
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1312	G
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1378	C
32	1a	1397	C
32	1a	1409	C
32	1a	1419	G
32	1a	1441	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1457	G
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1497	G
32	1a	1499	A

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Mol	Chain	Res	Type
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
1	2A	10	G
1	2A	12	U
1	2A	34	C
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	157	U
1	2A	173	G
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	213	A
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G

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Mol	Chain	Res	Type
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	386	G
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	448	U
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	479	A
1	2A	481	G
1	2A	505	A
1	2A	509	C
1	2A	518	G
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	592	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	610	G
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	615	G
1	2A	627	A

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Mol	Chain	Res	Type
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	648	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	765	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	828	U
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	890	A
1	2A	896	A
1	2A	899	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G

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Mol	Chain	Res	Type
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1026	U
1	2A	1033	U
1	2A	1042	G
1	2A	1043	C
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1054	A
1	2A	1058	G
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A

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Mol	Chain	Res	Type
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1094	U
1	2A	1095	A
1	2A	1096	A
1	2A	1097	U
1	2A	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1171	G
1	2A	1211	U
1	2A	1218	C
1	2A	1220	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1306	C
1	2A	1308	A
1	2A	1321	A
1	2A	1352	U
1	2A	1359	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C

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Mol	Chain	Res	Type
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1452	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1525	G
1	2A	1531	C
1	2A	1533	G
1	2A	1542	A
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1579	A
1	2A	1581	G
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1722	A
1	2A	1746	G
1	2A	1750	G
1	2A	1756	G
1	2A	1762	A

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Mol	Chain	Res	Type
1	2A	1763	G
1	2A	1764	G
1	2A	1769	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1896	G
1	2A	1900	A
1	2A	1905	C
1	2A	1906	G
1	2A	1914	C
1	2A	1915	5MU
1	2A	1929	G
1	2A	1930	G
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2039	C

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Mol	Chain	Res	Type
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2080	G
1	2A	2102	U
1	2A	2103	C
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2110	G
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2138	C
1	2A	2142	C
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2158	A
1	2A	2159	G
1	2A	2160	G
1	2A	2172	U
1	2A	2173	A
1	2A	2178	C
1	2A	2184	G
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U

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Mol	Chain	Res	Type
1	2A	2190	G
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2273	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2286	A
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2320	A
1	2A	2321	G
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2414	G
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2468	G

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Mol	Chain	Res	Type
1	2A	2474	C
1	2A	2476	A
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2585	U
1	2A	2586	C
1	2A	2602	A
1	2A	2603	G
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2757	A
1	2A	2758	A
1	2A	2761	G
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A

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Mol	Chain	Res	Type
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C
1	2A	2894	G
1	2A	2896	C
1	2A	2897	U
2	2B	7	G
2	2B	8	U
2	2B	45	A
2	2B	51	G
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	110	G
32	2a	5	U
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	61	G
32	2a	66	G
32	2a	78	G
32	2a	96	U
32	2a	101	A
32	2a	105	G
32	2a	115	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	156	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	195	A

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Mol	Chain	Res	Type
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	298	A
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	411	A
32	2a	412	A
32	2a	413	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	482	A
32	2a	484	G
32	2a	485	G

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Mol	Chain	Res	Type
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	592	G
32	2a	596	C
32	2a	618	C
32	2a	619	U
32	2a	630	G
32	2a	632	A
32	2a	633	G
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	673	G
32	2a	687	A
32	2a	688	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	806	C

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Mol	Chain	Res	Type
32	2a	815	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	838	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	873	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	967	5MC
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	999	C
32	2a	1002	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1020	U

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Mol	Chain	Res	Type
32	2a	1024	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1031	G
32	2a	1032	G
32	2a	1041	A
32	2a	1044	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1113	C
32	2a	1117	G
32	2a	1123	A
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1147	C
32	2a	1150	U
32	2a	1152	A
32	2a	1158	C
32	2a	1159	U
32	2a	1168	A
32	2a	1183	A
32	2a	1184	G
32	2a	1189	C
32	2a	1196	U

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Mol	Chain	Res	Type
32	2a	1197	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1224	G
32	2a	1227	A
32	2a	1238	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1305	G
32	2a	1312	G
32	2a	1320	C
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1378	C
32	2a	1397	C
32	2a	1419	G
32	2a	1441	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1487	G
32	2a	1492	A

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Mol	Chain	Res	Type
32	2a	1493	A
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G

All (109) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	184	A
1	1A	185	A
1	1A	188	A
1	1A	238	C
1	1A	302	A
1	1A	334	A
1	1A	509	A
1	1A	572	A
1	1A	596	G
1	1A	732	A
1	1A	795	G
1	1A	811	A
1	1A	821	A
1	1A	823	G
1	1A	874	U
1	1A	913	A
1	1A	934	A
1	1A	935	C
1	1A	1019	G
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1099	C
1	1A	1115	A
1	1A	1116	A

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Mol	Chain	Res	Type
1	1A	1157	A
1	1A	1188	A
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1299	A
1	1A	1346	U
1	1A	1347	A
1	1A	1425	A
1	1A	1466	U
1	1A	1654	A
1	1A	1655	A
1	1A	1700	G
1	1A	1793	A
1	1A	2148	A
1	1A	2194	U
1	1A	2200	C
1	1A	2227	G
1	1A	2320	G
1	1A	2347	A
1	1A	2418	U
1	1A	2434	A
1	1A	2442	A
1	1A	2451	A
1	1A	2597	U
1	1A	2613	C
1	1A	2623	U
1	1A	2701	U
1	1A	2769	U
1	1A	2902	G
1	2A	195	A
1	2A	196	A
1	2A	199	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	310	A
1	2A	503	A
1	2A	532	A

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Mol	Chain	Res	Type
1	2A	573	G
1	2A	685	A
1	2A	752	A
1	2A	764	A
1	2A	774	A
1	2A	776	G
1	2A	827	U
1	2A	840	C
1	2A	887	A
1	2A	974	G
1	2A	1047	G
1	2A	1053	C
1	2A	1057	A
1	2A	1063	G
1	2A	1065	U
1	2A	1067	A
1	2A	1069	A
1	2A	1071	G
1	2A	1073	A
1	2A	1076	C
1	2A	1111	A
1	2A	1142(A)	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1608	A
1	2A	1992	G
1	2A	2126	A
1	2A	2158	A
1	2A	2288	A
1	2A	2308	G
1	2A	2335	A
1	2A	2406	U
1	2A	2422	A
1	2A	2439	A
1	2A	2585	U
1	2A	2611	U
1	2A	2689	U
1	2A	2756	U

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

48 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
1	2MA	1A	2515	55,1	17,25,26	1.60	3 (17%)	17,37,40	2.04	4 (23%)
1	5MU	2A	1939	55,1	19,22,23	1.02	1 (5%)	28,32,35	1.52	4 (14%)
32	MA6	1a	1519	32	19,26,27	1.14	2 (10%)	18,38,41	4.49	3 (16%)
32	5MC	2a	1407	32	18,22,23	1.03	1 (5%)	26,32,35	1.29	3 (11%)
32	2MG	2a	1207	32	18,26,27	1.90	4 (22%)	16,38,41	1.16	2 (12%)
32	5MC	1a	967	32	18,22,23	0.99	2 (11%)	26,32,35	1.30	4 (15%)
1	5MC	2A	1942	1	18,22,23	0.79	0	26,32,35	1.16	2 (7%)
1	PSU	1A	2617	1	18,21,22	1.45	4 (22%)	22,30,33	1.51	5 (22%)
1	PSU	1A	1939	55,1	18,21,22	1.22	1 (5%)	22,30,33	1.77	4 (18%)
1	PSU	1A	1933	1	18,21,22	1.19	3 (16%)	22,30,33	1.55	6 (27%)
32	UR3	2a	1498	32	19,22,23	1.74	3 (15%)	26,32,35	1.88	6 (23%)
32	M2G	2a	966	32	20,27,28	3.04	7 (35%)	22,40,43	1.88	4 (18%)
1	5MC	1A	1984	55,1	18,22,23	1.01	1 (5%)	26,32,35	1.56	5 (19%)
1	PSU	2A	1911	1	18,21,22	1.52	3 (16%)	22,30,33	1.47	5 (22%)
1	2MA	2A	2503	55,1	17,25,26	1.68	3 (17%)	17,37,40	1.53	3 (17%)
32	5MC	2a	1400	32	18,22,23	0.90	0	26,32,35	1.40	4 (15%)
32	MA6	1a	1518	32	19,26,27	0.94	2 (10%)	18,38,41	4.86	3 (16%)
1	5MC	2A	1962	55,1	18,22,23	1.48	2 (11%)	26,32,35	1.54	4 (15%)
1	OMG	2A	2251	55,1	18,26,27	1.77	5 (27%)	19,38,41	1.78	6 (31%)
32	7MG	2a	527	32	22,26,27	2.43	7 (31%)	29,39,42	1.87	7 (24%)
43	0TD	1l	92	43	7,9,10	2.25	2 (28%)	6,11,13	4.32	4 (66%)
1	5MU	1A	1961	55,1	19,22,23	1.04	2 (10%)	28,32,35	1.50	6 (21%)
32	PSU	2a	516	32	18,21,22	1.78	3 (16%)	22,30,33	2.23	5 (22%)
1	4OC	2A	1920	1	19,22,24	2.38	6 (31%)	26,31,35	1.14	3 (11%)
32	4OC	1a	1402	32	20,23,24	2.29	7 (35%)	26,32,35	1.00	2 (7%)
32	5MC	1a	1407	32	18,22,23	1.07	2 (11%)	26,32,35	1.43	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1A	1964	1	18,22,23	1.22	2 (11%)	26,32,35	1.39	3 (11%)
32	MA6	2a	1518	32	19,26,27	0.98	1 (5%)	18,38,41	4.55	3 (16%)
32	5MC	2a	967	32	18,22,23	0.98	1 (5%)	26,32,35	1.70	7 (26%)
32	PSU	1a	516	55,32	18,21,22	1.55	4 (22%)	22,30,33	2.19	5 (22%)
1	PSU	2A	1917	1	18,21,22	1.12	1 (5%)	22,30,33	1.60	5 (22%)
1	OMU	2A	2552	55,1	19,22,23	6.61	10 (52%)	26,31,34	2.30	7 (26%)
1	PSU	2A	2605	1	18,21,22	1.53	1 (5%)	22,30,33	1.66	2 (9%)
32	4OC	2a	1402	32	20,23,24	2.63	7 (35%)	26,32,35	1.39	4 (15%)
1	5MU	2A	1915	1	19,22,23	1.82	3 (15%)	28,32,35	1.67	6 (21%)
32	MA6	2a	1519	32	19,26,27	1.12	2 (10%)	18,38,41	4.99	3 (16%)
32	M2G	1a	966	32	20,27,28	2.90	5 (25%)	22,40,43	1.73	6 (27%)
32	2MG	1a	1207	55,32	18,26,27	1.96	4 (22%)	16,38,41	1.97	6 (37%)
32	5MC	2a	1404	32	18,22,23	0.96	1 (5%)	26,32,35	1.46	4 (15%)
32	UR3	1a	1498	32	19,22,23	1.78	4 (21%)	26,32,35	1.29	2 (7%)
1	OMU	1A	2564	55,1	19,22,23	6.27	10 (52%)	26,31,34	2.62	9 (34%)
32	5MC	1a	1400	32	18,22,23	0.98	1 (5%)	26,32,35	1.61	6 (23%)
32	5MC	1a	1404	32	18,22,23	1.01	1 (5%)	26,32,35	1.55	4 (15%)
1	OMG	1A	2263	55,1	18,26,27	1.83	6 (33%)	19,38,41	1.82	6 (31%)
43	0TD	2l	92	43	7,9,10	1.67	1 (14%)	6,11,13	3.27	4 (66%)
32	7MG	1a	527	55,32	22,26,27	2.06	6 (27%)	29,39,42	1.66	8 (27%)
1	4OC	1A	1942	55,1	19,22,24	2.12	5 (26%)	26,31,35	1.29	5 (19%)
1	5MU	1A	1937	1	19,22,23	1.56	3 (15%)	28,32,35	1.84	7 (25%)

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
1	2MA	1A	2515	55,1	-	1/3/25/26	0/3/3/3
1	5MU	2A	1939	55,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1939	55,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	1/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	5MC	1A	1984	55,1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	55,1	-	2/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	5MC	2A	1962	55,1	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
32	7MG	2a	527	32	-	2/7/37/38	0/3/3/3
43	0TD	1l	92	43	-	4/7/12/14	-
1	5MU	1A	1961	55,1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	2/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	55,32	-	1/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	55,1	-	0/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	5MU	2A	1915	1	-	4/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	6/7/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	2MG	1a	1207	55,32	-	2/5/27/28	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2564	55,1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	55,1	-	1/5/27/28	0/3/3/3
43	0TD	2l	92	43	-	3/7/12/14	-
32	7MG	1a	527	55,32	-	1/7/37/38	0/3/3/3
1	4OC	1A	1942	55,1	-	1/9/27/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1937	1	-	4/7/25/26	0/2/2/2

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	C4-N3	-15.55	1.10	1.38
1	1A	2564	OMU	C4-N3	-14.51	1.12	1.38
1	2A	2552	OMU	C5-C4	14.17	1.75	1.43
1	1A	2564	OMU	C5-C4	13.91	1.74	1.43
1	2A	2552	OMU	C6-C5	-10.28	1.11	1.35
32	1a	966	M2G	C2-N3	10.26	1.43	1.30
32	2a	966	M2G	C2-N3	10.26	1.43	1.30
1	1A	2564	OMU	C6-C5	-10.11	1.11	1.35
1	2A	2552	OMU	C3'-C2'	-8.65	1.33	1.52
1	2A	2552	OMU	C6-N1	8.14	1.57	1.38
1	1A	2564	OMU	C6-N1	8.10	1.57	1.38
1	1A	2564	OMU	C3'-C2'	-7.24	1.36	1.52
1	2A	2552	OMU	O4'-C4'	-7.03	1.29	1.45
1	2A	1915	5MU	C2-N1	6.41	1.48	1.38
32	2a	527	7MG	C8-N9	6.33	1.49	1.46
1	1A	2564	OMU	C1'-N1	-6.00	1.30	1.47
1	1A	2564	OMU	O4'-C1'	5.99	1.56	1.42
1	2A	2552	OMU	O4'-C1'	5.92	1.56	1.42
32	2a	1402	4OC	C4-N4	5.91	1.48	1.35
1	2A	1920	4OC	C4-N4	5.81	1.47	1.33
32	1a	527	7MG	C8-N9	5.70	1.49	1.46
1	2A	2552	OMU	C1'-N1	-5.57	1.31	1.47
32	2a	1402	4OC	C2-N3	5.54	1.47	1.36
1	1A	1937	5MU	C2-N1	5.43	1.47	1.38
32	2a	527	7MG	C5-N7	5.34	1.41	1.35
32	1a	1402	4OC	C4-N4	5.26	1.46	1.35
32	2a	516	PSU	C2-N1	5.26	1.43	1.36
32	2a	966	M2G	C2-N2	5.22	1.45	1.35
43	1l	92	0TD	CB-SB	-4.81	1.77	1.82
32	1a	966	M2G	C2-N2	4.80	1.44	1.35
1	1A	2564	OMU	O4'-C4'	-4.79	1.34	1.45
1	2A	2605	PSU	C2-N1	4.75	1.43	1.36
1	2A	1920	4OC	C6-C5	4.69	1.45	1.35
1	1A	1942	4OC	C4-N4	4.63	1.44	1.33
32	1a	1207	2MG	C2-N1	4.61	1.44	1.36
32	1a	1498	UR3	C6-C5	4.61	1.45	1.35
32	2a	1498	UR3	C6-C5	4.60	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1207	2MG	C2-N1	4.57	1.44	1.36
1	1A	1942	4OC	C2-N3	4.51	1.45	1.36
32	1a	1207	2MG	C2-N2	4.48	1.43	1.33
32	2a	1402	4OC	C6-C5	4.45	1.45	1.35
1	1A	2564	OMU	C3'-C4'	4.33	1.64	1.53
32	2a	1498	UR3	C2-N3	4.32	1.47	1.39
32	2a	1207	2MG	C2-N2	4.30	1.42	1.33
32	2a	1402	4OC	C4-N3	4.25	1.40	1.32
1	2A	1911	PSU	C2-N1	4.21	1.42	1.36
1	2A	2503	2MA	C2-N3	4.20	1.40	1.31
32	1a	1498	UR3	C2-N1	4.15	1.44	1.38
1	2A	1920	4OC	C2-N3	4.15	1.44	1.36
32	2a	527	7MG	C4-N3	4.14	1.44	1.34
32	2a	527	7MG	C2-N3	4.13	1.43	1.33
1	1A	2263	OMG	C5-C4	-4.08	1.32	1.43
32	1a	1402	4OC	O2-C2	-4.04	1.16	1.23
32	1a	1402	4OC	C6-C5	4.01	1.44	1.35
1	2A	1962	5MC	C2-N3	4.00	1.44	1.36
1	1A	2515	2MA	C5-C4	-3.91	1.33	1.43
32	1a	527	7MG	C4-N3	3.90	1.43	1.34
32	1a	527	7MG	C5-N7	3.83	1.40	1.35
1	1A	1942	4OC	C6-C5	3.83	1.43	1.35
32	1a	527	7MG	C2-N3	3.69	1.42	1.33
1	2A	2503	2MA	C5-C4	-3.61	1.33	1.43
32	2a	1402	4OC	C5-C4	3.54	1.48	1.40
32	1a	516	PSU	C2-N1	3.52	1.41	1.36
32	1a	1402	4OC	C5-C4	3.48	1.48	1.40
32	2a	1402	4OC	O2-C2	-3.47	1.17	1.23
1	2A	2251	OMG	C5-C4	-3.45	1.34	1.43
1	2A	1920	4OC	O2-C2	-3.44	1.17	1.23
1	2A	2251	OMG	C2-N3	3.44	1.41	1.33
1	2A	1917	PSU	C2-N1	3.43	1.41	1.36
1	2A	2552	OMU	C3'-C4'	3.40	1.61	1.53
32	1a	516	PSU	C6-N1	3.38	1.41	1.36
32	1a	966	M2G	C5-C4	-3.29	1.34	1.43
1	1A	1939	PSU	C2-N1	3.26	1.41	1.36
1	2A	1920	4OC	C2-N1	3.20	1.46	1.40
32	2a	966	M2G	C4-N3	3.19	1.45	1.37
1	1A	1942	4OC	C2-N1	3.19	1.46	1.40
32	2a	1207	2MG	C4-N3	3.19	1.45	1.37
32	1a	1402	4OC	C4-N3	3.17	1.38	1.32
43	2l	92	0TD	CB-SB	-3.15	1.79	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	516	PSU	C6-N1	3.14	1.41	1.36
32	2a	1519	MA6	C2-N3	3.12	1.37	1.32
32	1a	1402	4OC	C2-N3	3.12	1.42	1.36
32	2a	966	M2G	C2-N1	3.11	1.44	1.36
1	1A	1942	4OC	O2-C2	-3.10	1.18	1.23
32	2a	516	PSU	O4'-C1'	-3.10	1.39	1.43
32	1a	1519	MA6	C2-N3	3.09	1.37	1.32
1	2A	1911	PSU	C6-N1	3.07	1.41	1.36
32	1a	1498	UR3	C2-N3	3.03	1.44	1.39
1	2A	2251	OMG	C6-N1	3.00	1.42	1.37
1	1A	2515	2MA	C2-N3	2.99	1.37	1.31
1	1A	2263	OMG	C2-N3	2.98	1.40	1.33
1	2A	1915	5MU	C2-N3	2.98	1.43	1.38
32	1a	1207	2MG	C4-N3	2.95	1.44	1.37
1	2A	1962	5MC	CM5-C5	-2.94	1.43	1.50
1	1A	2263	OMG	C4-N3	2.93	1.44	1.37
1	1A	2263	OMG	O6-C6	-2.92	1.17	1.23
32	1a	966	M2G	C4-N3	2.88	1.44	1.37
32	2a	527	7MG	C2-N2	2.83	1.40	1.34
32	2a	966	M2G	C5-C4	-2.80	1.35	1.43
32	1a	1407	5MC	C2-N1	2.79	1.46	1.40
1	1A	1933	PSU	C4-N3	2.78	1.44	1.38
1	2A	1939	5MU	C5M-C5	-2.77	1.43	1.50
1	1A	1984	5MC	CM5-C5	-2.76	1.43	1.50
1	2A	2251	OMG	C4-N3	2.75	1.44	1.37
32	2a	966	M2G	C5-C6	2.69	1.52	1.47
1	2A	1911	PSU	C4-N3	2.68	1.43	1.38
32	2a	1207	2MG	CM2-N2	-2.66	1.40	1.45
32	2a	527	7MG	C5-C6	2.66	1.50	1.43
1	2A	1920	4OC	C5-C4	2.62	1.48	1.42
32	2a	966	M2G	C6-N1	2.61	1.41	1.37
32	1a	1400	5MC	C2-N1	2.59	1.45	1.40
32	1a	966	M2G	C2-N1	2.57	1.43	1.36
32	2a	1407	5MC	C2-N1	2.51	1.45	1.40
32	1a	1404	5MC	CM5-C5	-2.50	1.44	1.50
32	2a	967	5MC	C6-C5	2.47	1.38	1.34
1	1A	1964	5MC	C2-N1	-2.44	1.34	1.40
1	1A	1961	5MU	C4-C5	-2.44	1.40	1.44
32	1a	1402	4OC	CM4-N4	-2.43	1.41	1.45
1	1A	1937	5MU	C2-N3	2.42	1.42	1.38
32	2a	1498	UR3	C2-N1	2.42	1.42	1.38
1	1A	2617	PSU	C6-N1	2.42	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	516	PSU	O4'-C1'	-2.38	1.40	1.43
32	2a	1402	4OC	C2-N1	2.36	1.45	1.40
32	2a	1519	MA6	C5-C4	-2.35	1.34	1.40
1	1A	1933	PSU	C2-N1	2.34	1.39	1.36
32	1a	1518	MA6	C5-C4	-2.29	1.34	1.40
32	1a	1519	MA6	C5-C4	-2.29	1.34	1.40
32	1a	1407	5MC	CM5-C5	-2.25	1.45	1.50
32	1a	1518	MA6	C2-N3	2.24	1.35	1.32
32	1a	527	7MG	C2-N2	2.22	1.39	1.34
32	1a	1498	UR3	C3U-N3	-2.22	1.43	1.47
32	2a	1404	5MC	C2-N3	2.22	1.40	1.36
1	1A	2617	PSU	C6-C5	-2.21	1.32	1.35
1	2A	2552	OMU	O2'-C2'	2.21	1.48	1.42
1	1A	2564	OMU	O2'-C2'	2.19	1.48	1.42
1	1A	2617	PSU	O4'-C1'	-2.17	1.40	1.43
1	1A	1933	PSU	C6-N1	2.17	1.39	1.36
32	2a	1518	MA6	C2-N3	2.17	1.35	1.32
1	1A	1937	5MU	C4-C5	2.17	1.48	1.44
1	1A	2263	OMG	C8-N7	2.16	1.38	1.35
32	1a	967	5MC	C2-N1	2.12	1.44	1.40
32	2a	527	7MG	C2-N1	2.10	1.42	1.37
1	1A	2617	PSU	O4-C4	-2.09	1.19	1.23
32	1a	516	PSU	O4-C4	-2.09	1.19	1.23
43	1l	92	0TD	CA-N	-2.08	1.41	1.47
32	1a	967	5MC	C6-C5	2.08	1.38	1.34
1	2A	2503	2MA	C2-N1	2.06	1.43	1.36
1	1A	1964	5MC	C6-C5	2.05	1.38	1.34
1	1A	1961	5MU	C2-N3	2.05	1.41	1.38
32	1a	527	7MG	C2-N1	2.04	1.42	1.37
1	2A	2251	OMG	C2-N1	2.04	1.42	1.37
1	1A	2263	OMG	O5'-C5'	-2.03	1.39	1.44
1	1A	2515	2MA	C2-N1	2.03	1.42	1.36
32	1a	1207	2MG	C5-C4	-2.03	1.37	1.43
1	2A	1915	5MU	C4-N3	2.02	1.42	1.38

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1519	MA6	N1-C6-N6	-20.27	95.72	117.06
32	1a	1518	MA6	N1-C6-N6	-18.93	97.13	117.06
32	1a	1519	MA6	N1-C6-N6	-17.94	98.18	117.06
32	2a	1518	MA6	N1-C6-N6	-17.87	98.25	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	516	PSU	C6-C5-C4	8.05	123.83	118.20
43	1l	92	0TD	CSB-SB-CB	7.94	116.81	102.44
32	1a	516	PSU	C6-C5-C4	7.71	123.59	118.20
1	1A	2564	OMU	C5-C4-N3	6.92	125.18	114.84
32	2a	966	M2G	N1-C2-N2	6.51	123.58	118.04
32	1a	1518	MA6	C1'-N9-C4	-6.37	115.45	126.64
1	2A	2605	PSU	C6-C5-C4	5.93	122.35	118.20
1	2A	2552	OMU	C5-C4-N3	5.91	123.68	114.84
1	1A	2515	2MA	CM2-C2-N1	5.78	129.09	116.23
43	2l	92	0TD	CSB-SB-CB	5.75	112.84	102.44
32	2a	1498	UR3	C4-N3-C2	-5.68	119.21	124.56
1	1A	1939	PSU	C6-C5-C4	5.41	121.98	118.20
32	2a	1518	MA6	C1'-N9-C4	-5.39	117.18	126.64
32	2a	967	5MC	C5-C6-N1	-5.07	118.12	123.34
1	1A	2564	OMU	C4-N3-C2	-4.89	120.13	126.58
43	1l	92	0TD	CB-CA-N	-4.86	98.74	109.10
32	1a	1518	MA6	N3-C2-N1	-4.85	121.10	128.68
1	1A	2564	OMU	O4-C4-C5	-4.82	116.69	125.16
32	2a	527	7MG	C5-C6-N1	4.77	119.39	110.99
1	1A	2564	OMU	O2'-C2'-C1'	-4.75	99.81	109.08
32	1a	1519	MA6	N3-C2-N1	-4.74	121.26	128.68
1	2A	1962	5MC	C4-N3-C2	-4.54	114.55	120.69
32	1a	1404	5MC	C5-C6-N1	-4.49	118.71	123.34
32	2a	1402	4OC	C6-C5-C4	4.35	122.28	116.96
32	1a	966	M2G	N1-C2-N2	4.34	121.73	118.04
32	1a	527	7MG	C5-C6-N1	4.28	118.52	110.99
1	2A	1939	5MU	C4-N3-C2	-4.25	121.85	127.35
1	2A	2552	OMU	O2-C2-N1	-4.24	117.15	122.79
32	2a	1519	MA6	N3-C2-N1	-4.24	122.05	128.68
1	2A	1917	PSU	C6-C5-C4	4.21	121.14	118.20
1	1A	1964	5MC	C5-C6-N1	-4.19	119.03	123.34
32	2a	1518	MA6	N3-C2-N1	-4.19	122.14	128.68
1	2A	2552	OMU	N3-C2-N1	4.18	120.44	114.89
32	2a	1400	5MC	C5-C6-N1	-4.10	119.12	123.34
1	1A	1984	5MC	C5-C4-N3	4.09	126.08	121.67
1	2A	1911	PSU	C6-C5-C4	4.03	121.02	118.20
1	1A	1961	5MU	C4-N3-C2	-3.98	122.19	127.35
32	1a	1404	5MC	C4-N3-C2	-3.98	115.31	120.69
32	2a	1498	UR3	O2-C2-N3	3.97	126.93	121.34
1	1A	2263	OMG	O6-C6-N1	-3.96	115.97	120.65
32	2a	527	7MG	C2-N3-C4	3.94	119.33	112.30
1	1A	1937	5MU	C1'-N1-C2	3.93	124.69	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2564	OMU	N3-C2-N1	3.93	120.10	114.89
1	1A	2263	OMG	C8-N7-C5	3.87	110.36	102.99
32	2a	1404	5MC	C5-C6-N1	-3.83	119.40	123.34
32	1a	1400	5MC	C5-C6-N1	-3.81	119.42	123.34
43	2l	92	0TD	OD2-CG-CB	3.80	121.36	113.15
1	2A	2552	OMU	C4-N3-C2	-3.80	121.57	126.58
43	1l	92	0TD	OD2-CG-CB	3.79	121.33	113.15
1	1A	2515	2MA	C5-C6-N1	3.78	120.55	114.02
32	1a	1400	5MC	C5-C4-N3	3.77	125.74	121.67
32	2a	527	7MG	C5-C4-N3	-3.73	121.03	128.13
1	1A	1933	PSU	C6-C5-C4	3.72	120.80	118.20
1	2A	2552	OMU	C6-C5-C4	-3.72	114.44	119.52
1	1A	2564	OMU	C6-C5-C4	-3.71	114.44	119.52
1	1A	1961	5MU	C6-C5-C4	3.71	121.13	118.03
32	1a	1407	5MC	C5-C4-N3	3.70	125.67	121.67
32	2a	1519	MA6	C1'-N9-C4	-3.69	120.15	126.64
32	1a	1498	UR3	C4-N3-C2	-3.68	121.09	124.56
1	1A	1984	5MC	C5-C6-N1	-3.68	119.55	123.34
32	1a	516	PSU	C6-N1-C2	-3.68	118.92	122.68
1	2A	1915	5MU	C1'-N1-C2	3.67	124.22	117.57
1	1A	1937	5MU	C1'-N1-C6	-3.66	115.04	121.12
32	2a	527	7MG	C5-C4-N9	3.57	110.98	106.35
32	1a	527	7MG	C4-C5-N7	3.57	110.49	105.53
1	1A	2617	PSU	C6-C5-C4	3.55	120.68	118.20
32	2a	1404	5MC	C4-N3-C2	-3.55	115.90	120.69
1	2A	2251	OMG	C8-N7-C5	3.53	109.72	102.99
32	2a	1498	UR3	O2-C2-N1	-3.53	114.46	122.72
1	1A	2263	OMG	C5-C6-N1	3.52	120.18	113.95
1	2A	1939	5MU	C5-C4-N3	3.51	118.30	115.31
1	1A	2515	2MA	CM2-C2-N3	-3.50	109.12	119.47
1	2A	2503	2MA	C5-C6-N1	3.50	120.06	114.02
32	2a	1404	5MC	C5-C4-N3	3.48	125.43	121.67
32	1a	967	5MC	C5-C6-N1	-3.46	119.78	123.34
1	1A	1937	5MU	C4-N3-C2	-3.44	122.89	127.35
32	1a	1207	2MG	C8-N7-C5	3.44	109.54	102.99
32	1a	966	M2G	C5-C6-N1	3.44	120.02	113.95
1	2A	1939	5MU	C6-C5-C4	3.43	120.90	118.03
32	1a	967	5MC	C5-C4-N3	3.42	125.37	121.67
1	2A	2251	OMG	C2-N1-C6	-3.42	118.79	125.10
1	1A	1984	5MC	C4-N3-C2	-3.41	116.08	120.69
32	1a	966	M2G	C2-N1-C6	-3.40	118.07	123.71
32	2a	1407	5MC	C5-C4-N3	3.39	125.33	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1519	MA6	C1'-N9-C4	-3.38	120.70	126.64
1	2A	1962	5MC	C5-C6-N1	-3.36	119.89	123.34
32	1a	1407	5MC	N4-C4-N3	-3.25	112.54	118.48
43	1l	92	0TD	OD2-CG-OD1	-3.22	116.78	124.09
1	1A	1937	5MU	C5M-C5-C6	-3.21	118.56	122.85
32	2a	1400	5MC	C5-C4-N3	3.20	125.12	121.67
32	1a	1498	UR3	C1'-N1-C2	3.18	122.36	116.99
1	2A	1915	5MU	C4-N3-C2	-3.16	123.25	127.35
1	2A	1942	5MC	C5-C6-N1	-3.14	120.10	123.34
1	2A	2251	OMG	C5-C6-N1	3.13	119.47	113.95
32	2a	967	5MC	C4-N3-C2	-3.12	116.47	120.69
32	2a	967	5MC	N4-C4-N3	-3.11	112.80	118.48
32	1a	516	PSU	N1-C2-N3	3.10	118.65	115.13
32	2a	967	5MC	C5-C4-N3	3.06	124.97	121.67
1	1A	2617	PSU	O4-C4-N3	-3.03	114.31	120.12
32	1a	1404	5MC	C5-C4-N3	3.03	124.94	121.67
32	2a	527	7MG	C4-C5-N7	3.03	109.73	105.53
1	2A	1942	5MC	C5-C4-N3	3.02	124.93	121.67
1	2A	1915	5MU	C1'-N1-C6	-3.02	116.10	121.12
1	1A	1939	PSU	O2-C2-N1	-3.02	119.47	122.79
1	2A	2251	OMG	CM2-O2'-C2'	-3.00	106.65	114.52
1	2A	1920	4OC	O2-C2-N3	-2.99	117.47	122.33
1	1A	1964	5MC	C4-N3-C2	-2.98	116.66	120.69
43	2l	92	0TD	CB-CA-N	-2.95	102.81	109.10
1	2A	2552	OMU	O4-C4-C5	-2.94	119.98	125.16
1	2A	1939	5MU	C5-C6-N1	-2.93	120.33	123.34
32	1a	1207	2MG	O3'-C3'-C2'	2.92	121.28	111.82
32	2a	516	PSU	C6-N1-C2	-2.92	119.70	122.68
32	1a	1207	2MG	O3'-C3'-C4'	2.91	119.47	111.05
32	1a	1400	5MC	C1'-N1-C6	-2.90	116.30	121.12
1	2A	1915	5MU	C6-C5-C4	2.89	120.45	118.03
32	2a	966	M2G	C5-C6-N1	2.87	119.02	113.95
32	2a	966	M2G	C8-N7-C5	2.87	108.45	102.99
32	1a	527	7MG	C5-C4-N9	2.86	110.06	106.35
32	1a	1400	5MC	C4-N3-C2	-2.85	116.83	120.69
1	1A	1933	PSU	O2-C2-N1	-2.85	119.65	122.79
32	1a	1207	2MG	O6-C6-N1	-2.84	117.30	120.65
1	1A	1961	5MU	O4-C4-C5	-2.82	121.63	124.90
1	2A	2503	2MA	CM2-C2-N1	2.79	122.44	116.23
32	1a	1207	2MG	C5-C6-N1	2.77	118.85	113.95
1	2A	1917	PSU	O2-C2-N1	-2.77	119.75	122.79
32	2a	516	PSU	N1-C2-N3	2.76	118.26	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	967	5MC	C4-N3-C2	-2.69	117.05	120.69
32	1a	1407	5MC	C5-C6-N1	-2.69	120.57	123.34
1	1A	1942	4OC	CM2-O2'-C2'	-2.65	107.58	114.52
32	2a	1402	4OC	C5-C4-N3	-2.64	118.34	122.59
32	2a	1207	2MG	C8-N7-C5	2.61	107.96	102.99
1	2A	1962	5MC	CM5-C5-C6	-2.61	119.36	122.85
1	1A	1937	5MU	C5M-C5-C4	2.60	121.63	118.77
1	1A	1933	PSU	N1-C2-N3	2.59	118.06	115.13
32	1a	527	7MG	C2-N3-C4	2.58	116.90	112.30
1	1A	2564	OMU	O2-C2-N1	-2.57	119.37	122.79
1	1A	1939	PSU	N1-C2-N3	2.57	118.04	115.13
1	1A	1961	5MU	C5-C4-N3	2.51	117.46	115.31
32	1a	516	PSU	O4'-C1'-C2'	2.51	108.68	105.14
1	2A	1962	5MC	C5-C4-N3	2.51	124.38	121.67
32	2a	1400	5MC	C4-N3-C2	-2.50	117.31	120.69
32	1a	1207	2MG	C3'-C2'-C1'	-2.50	97.21	100.98
1	1A	2564	OMU	C3'-C2'-C1'	2.50	107.58	102.89
32	2a	1407	5MC	C5-C6-N1	-2.49	120.78	123.34
32	1a	966	M2G	C8-N7-C5	2.47	107.69	102.99
32	1a	967	5MC	N4-C4-N3	-2.47	113.98	118.48
32	2a	1402	4OC	O2-C2-N1	-2.45	113.83	118.89
32	1a	527	7MG	C5-C4-N3	-2.45	123.47	128.13
32	1a	1407	5MC	C4-N3-C2	-2.45	117.38	120.69
32	2a	516	PSU	O4'-C1'-C2'	2.44	108.58	105.14
1	1A	1937	5MU	C5-C4-N3	2.44	117.39	115.31
43	2l	92	0TD	OD2-CG-OD1	-2.43	118.56	124.09
1	1A	1964	5MC	C5-C4-N3	2.43	124.30	121.67
1	1A	1984	5MC	CM5-C5-C6	-2.41	119.63	122.85
1	1A	2617	PSU	C6-N1-C2	-2.39	120.23	122.68
32	1a	527	7MG	O6-C6-C5	-2.39	121.67	127.54
1	2A	1915	5MU	C5M-C5-C6	-2.39	119.66	122.85
32	1a	1402	4OC	CM4-N4-C4	-2.39	117.79	122.45
32	2a	1498	UR3	C5-C6-N1	-2.39	117.81	121.81
1	2A	1917	PSU	O4-C4-N3	-2.38	115.55	120.12
1	1A	1942	4OC	C5-C4-N4	-2.38	116.83	120.57
32	1a	966	M2G	O6-C6-C5	-2.38	119.73	124.37
1	2A	2503	2MA	C8-N7-C5	2.37	107.51	102.99
32	2a	966	M2G	C2-N1-C6	-2.37	119.78	123.71
32	1a	966	M2G	CM2-N2-CM1	2.35	123.03	115.77
32	2a	1404	5MC	CM5-C5-C6	-2.35	119.72	122.85
32	2a	1498	UR3	O4-C4-C5	-2.34	117.34	124.37
1	2A	2251	OMG	O6-C6-C5	-2.34	119.81	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	516	PSU	C5-C6-N1	-2.33	118.61	122.11
32	1a	1400	5MC	CM5-C5-C6	-2.33	119.74	122.85
1	2A	2605	PSU	C4-N3-C2	-2.32	122.99	126.34
32	1a	1407	5MC	CM5-C5-C6	-2.32	119.74	122.85
32	2a	527	7MG	C2-N1-C6	-2.32	120.86	125.10
1	2A	2251	OMG	N2-C2-N1	2.30	121.61	116.71
32	1a	1402	4OC	CM2-O2'-C2'	2.28	120.51	114.52
32	2a	1407	5MC	C4-N3-C2	-2.28	117.61	120.69
1	1A	1984	5MC	N4-C4-N3	-2.28	114.33	118.48
32	1a	1400	5MC	N4-C4-N3	-2.27	114.34	118.48
1	1A	1961	5MU	C5-C6-N1	-2.26	121.02	123.34
1	1A	2263	OMG	N1-C2-N3	-2.25	119.12	123.32
1	1A	1942	4OC	C2'-C1'-N1	-2.25	109.86	114.22
32	2a	527	7MG	O6-C6-C5	-2.23	122.06	127.54
32	2a	967	5MC	C1'-N1-C2	-2.23	113.45	118.42
1	2A	1920	4OC	C6-C5-C4	2.22	121.09	117.50
1	1A	2617	PSU	O2'-C2'-C1'	-2.22	105.95	111.23
1	2A	1911	PSU	O4-C4-N3	-2.20	115.90	120.12
1	2A	1917	PSU	N1-C2-N3	2.18	117.59	115.13
32	2a	1400	5MC	N4-C4-N3	-2.17	114.51	118.48
32	2a	1207	2MG	C5-C6-N1	2.17	117.79	113.95
1	2A	1911	PSU	O2-C2-N1	-2.15	120.42	122.79
1	1A	1942	4OC	N4-C4-N3	2.13	121.71	117.97
1	1A	1937	5MU	C6-C5-C4	2.13	119.81	118.03
1	1A	2263	OMG	C2-N1-C6	-2.12	121.19	125.10
1	1A	1933	PSU	O4'-C1'-C2'	2.11	108.12	105.14
1	2A	1911	PSU	O4'-C1'-C2'	2.11	108.11	105.14
1	1A	1933	PSU	O4-C4-C5	2.10	129.56	124.05
1	1A	1933	PSU	O4-C4-N3	-2.10	116.09	120.12
1	2A	1911	PSU	N1-C2-N3	2.10	117.51	115.13
1	1A	1961	5MU	C5M-C5-C4	-2.10	116.46	118.77
1	1A	2263	OMG	N2-C2-N1	2.09	121.17	116.71
1	2A	1917	PSU	C4-N3-C2	-2.09	123.32	126.34
1	1A	2515	2MA	C8-N7-C5	2.09	106.97	102.99
32	2a	1402	4OC	N1-C2-N3	2.09	122.61	118.81
32	1a	527	7MG	C6-C5-C4	-2.08	118.33	122.62
1	2A	1920	4OC	C2'-C1'-N1	-2.07	110.20	114.22
32	2a	967	5MC	CM5-C5-C6	-2.07	120.08	122.85
1	1A	1942	4OC	C1'-N1-C6	-2.07	116.33	120.84
1	1A	2564	OMU	CM2-O2'-C2'	-2.06	109.12	114.52
32	1a	527	7MG	C2-N1-C6	-2.06	121.35	125.10
1	2A	1915	5MU	O4'-C1'-N1	2.05	113.05	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1404	5MC	CM5-C5-C6	-2.05	120.11	122.85
1	1A	1939	PSU	O4-C4-N3	-2.04	116.21	120.12
32	2a	967	5MC	C6-N1-C2	2.03	123.69	120.87
1	2A	2552	OMU	O4-C4-N3	-2.03	116.33	119.31
32	2a	1498	UR3	C6-N1-C2	2.02	123.60	121.79
32	1a	516	PSU	C4-N3-C2	-2.01	123.44	126.34
1	1A	2617	PSU	O4-C4-C5	2.01	129.30	124.05

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C1'-N1-C2
1	1A	1937	5MU	O4'-C1'-N1-C6
1	1A	1937	5MU	O4'-C4'-C5'-O5'
1	1A	2263	OMG	C1'-C2'-O2'-CM2
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD2
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C9
32	2a	1519	MA6	C5-C6-N6-C10
43	2l	92	0TD	SB-CB-CG-OD2
1	1A	1937	5MU	C3'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	N1-C6-N6-C10
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C9
1	2A	1915	5MU	O4'-C4'-C5'-O5'
32	1a	1207	2MG	O4'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1207	2MG	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB

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Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	CG-CB-SB-CSB
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
1	2A	2503	2MA	C4'-C5'-O5'-P
32	1a	516	PSU	O4'-C1'-C5-C4
32	2a	516	PSU	O4'-C1'-C5-C4
43	1l	92	0TD	CA-CB-SB-CSB
1	2A	1920	4OC	C2'-C1'-N1-C2
1	1A	2515	2MA	O4'-C4'-C5'-O5'
32	2a	1498	UR3	O4'-C4'-C5'-O5'
32	2a	516	PSU	O4'-C1'-C5-C6
1	1A	1942	4OC	C2'-C1'-N1-C2
32	1a	527	7MG	C3'-C4'-C5'-O5'
1	2A	1915	5MU	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
1	2A	1962	5MC	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6

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 2435 ligands modelled in this entry, 2431 are monoatomic and 2 are modelled with single atom - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	2d	501	35	0,12,12	-	-	-		
58	SF4	1d	501	35	0,12,12	-	-	-		

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
58	SF4	2d	501	35	-	-	0/6/5/5
58	SF4	1d	501	35	-	-	0/6/5/5

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2A	2801(A):A	O3'	2802:G	P	3.50

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2861/2915 (98%)	0.04	136 (4%) 30 27	16, 34, 100, 113	0
1	2A	2856/2915 (97%)	0.02	141 (4%) 29 26	31, 56, 101, 114	0
2	1B	120/120 (100%)	-0.45	0 100 100	27, 51, 64, 93	0
2	2B	120/120 (100%)	-0.34	0 100 100	60, 79, 88, 96	0
3	1D	275/275 (100%)	-0.40	0 100 100	17, 34, 49, 74	0
3	2D	275/275 (100%)	-0.25	0 100 100	27, 49, 64, 83	0
4	1E	204/204 (100%)	-0.40	0 100 100	16, 37, 58, 73	0
4	2E	204/204 (100%)	-0.20	1 (0%) 91 91	31, 57, 73, 83	0
5	1F	203/203 (100%)	-0.29	1 (0%) 91 91	16, 38, 68, 92	0
5	2F	203/203 (100%)	-0.25	0 100 100	33, 66, 82, 91	0
6	1G	181/181 (100%)	-0.35	2 (1%) 80 80	47, 66, 83, 95	0
6	2G	181/181 (100%)	0.48	12 (6%) 18 14	76, 85, 92, 98	0
7	1H	174/174 (100%)	-0.42	1 (0%) 89 89	36, 51, 65, 70	0
7	2H	173/174 (99%)	0.77	28 (16%) 1 1	66, 85, 94, 98	0
8	1I	147/147 (100%)	-0.19	0 100 100	40, 71, 82, 87	0
8	2I	146/147 (99%)	0.35	7 (4%) 30 27	53, 80, 91, 97	0
9	1N	140/140 (100%)	-0.39	0 100 100	19, 33, 57, 73	0
9	2N	140/140 (100%)	-0.13	1 (0%) 87 87	46, 64, 76, 88	0
10	1O	122/122 (100%)	-0.40	0 100 100	26, 38, 55, 65	0
10	2O	122/122 (100%)	-0.36	0 100 100	41, 54, 68, 76	0
11	1P	149/149 (100%)	-0.27	0 100 100	17, 43, 64, 79	0
11	2P	149/149 (100%)	0.22	3 (2%) 65 63	38, 66, 83, 91	0
12	1Q	141/141 (100%)	-0.29	0 100 100	25, 38, 53, 68	0
12	2Q	141/141 (100%)	-0.30	1 (0%) 87 87	46, 63, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.35	0 100 100	21, 32, 51, 61	0
13	2R	118/118 (100%)	-0.10	0 100 100	39, 53, 63, 76	0
14	1S	110/110 (100%)	-0.32	0 100 100	37, 51, 66, 69	0
14	2S	110/110 (100%)	0.31	5 (4%) 33 29	63, 75, 84, 86	0
15	1T	131/131 (100%)	-0.39	1 (0%) 86 86	32, 43, 70, 84	0
15	2T	131/131 (100%)	-0.31	0 100 100	48, 59, 79, 86	0
16	1U	116/116 (100%)	-0.46	0 100 100	19, 27, 42, 62	0
16	2U	116/116 (100%)	-0.15	0 100 100	41, 61, 77, 86	0
17	1V	101/101 (100%)	-0.39	0 100 100	17, 36, 54, 69	0
17	2V	101/101 (100%)	-0.11	1 (0%) 82 82	39, 72, 81, 89	0
18	1W	112/112 (100%)	-0.45	1 (0%) 84 84	19, 27, 50, 92	0
18	2W	112/112 (100%)	-0.25	0 100 100	38, 48, 67, 87	0
19	1X	95/95 (100%)	-0.37	0 100 100	22, 35, 62, 71	0
19	2X	95/95 (100%)	-0.06	1 (1%) 80 80	45, 61, 74, 78	0
20	1Y	107/107 (100%)	-0.32	1 (0%) 84 84	32, 47, 68, 78	0
20	2Y	107/107 (100%)	0.62	16 (14%) 2 1	55, 72, 84, 94	0
21	1Z	203/203 (100%)	-0.36	2 (0%) 82 82	40, 58, 77, 88	0
21	2Z	201/203 (99%)	0.18	7 (3%) 44 38	64, 79, 88, 95	0
22	10	77/77 (100%)	-0.29	1 (1%) 77 77	26, 35, 58, 65	0
22	20	77/77 (100%)	0.33	5 (6%) 18 14	53, 62, 74, 78	0
23	11	97/97 (100%)	-0.05	1 (1%) 82 82	25, 39, 67, 80	0
23	21	97/97 (100%)	-0.06	1 (1%) 82 82	40, 57, 79, 88	0
24	12	70/70 (100%)	-0.37	0 100 100	33, 47, 62, 82	0
24	22	70/70 (100%)	0.06	0 100 100	61, 71, 81, 83	0
25	13	59/59 (100%)	-0.35	0 100 100	21, 32, 58, 77	0
25	23	59/59 (100%)	0.62	6 (10%) 6 5	48, 62, 77, 82	0
26	14	69/69 (100%)	0.17	10 (14%) 2 1	63, 82, 96, 98	0
26	24	69/69 (100%)	1.04	17 (24%) 0 0	80, 92, 99, 100	0
27	15	59/59 (100%)	-0.41	0 100 100	15, 32, 48, 62	0
27	25	59/59 (100%)	-0.37	0 100 100	35, 52, 70, 76	0
28	16	53/53 (100%)	-0.40	0 100 100	32, 40, 55, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/53 (100%)	-0.24	0 100 100	52, 62, 69, 76	0
29	17	48/48 (100%)	-0.20	1 (2%) 63 61	18, 24, 58, 65	0
29	27	48/48 (100%)	-0.12	0 100 100	32, 40, 66, 79	0
30	18	64/64 (100%)	-0.33	0 100 100	23, 30, 39, 48	0
30	28	64/64 (100%)	-0.02	0 100 100	41, 54, 64, 72	0
31	19	37/37 (100%)	-0.10	0 100 100	30, 40, 59, 71	0
31	29	37/37 (100%)	0.52	2 (5%) 25 22	61, 68, 79, 82	0
32	1a	1488/1521 (97%)	-0.02	48 (3%) 47 43	31, 74, 100, 114	0
32	2a	1492/1521 (98%)	-0.04	54 (3%) 42 37	41, 76, 100, 112	0
33	1b	231/231 (100%)	0.16	16 (6%) 16 13	67, 82, 92, 101	0
33	2b	231/231 (100%)	0.31	18 (7%) 13 10	68, 85, 94, 98	0
34	1c	206/206 (100%)	0.20	12 (5%) 23 19	70, 83, 92, 97	0
34	2c	206/206 (100%)	0.30	7 (3%) 45 40	77, 86, 93, 99	0
35	1d	208/208 (100%)	-0.06	5 (2%) 59 56	59, 76, 87, 91	0
35	2d	208/208 (100%)	-0.03	1 (0%) 91 91	61, 73, 84, 88	0
36	1e	148/148 (100%)	-0.14	1 (0%) 87 87	48, 69, 79, 96	0
36	2e	148/148 (100%)	-0.20	0 100 100	58, 71, 81, 89	0
37	1f	100/100 (100%)	-0.30	1 (1%) 82 82	53, 73, 80, 84	0
37	2f	100/100 (100%)	-0.44	0 100 100	57, 70, 82, 87	0
38	1g	155/155 (100%)	0.10	6 (3%) 39 35	67, 77, 86, 90	0
38	2g	155/155 (100%)	0.41	13 (8%) 11 8	73, 81, 89, 95	0
39	1h	137/137 (100%)	0.00	1 (0%) 87 87	55, 69, 77, 89	0
39	2h	137/137 (100%)	-0.12	1 (0%) 87 87	60, 72, 80, 87	0
40	1i	127/127 (100%)	0.56	11 (8%) 10 7	68, 86, 93, 97	0
40	2i	126/127 (99%)	1.03	22 (17%) 1 1	74, 88, 94, 97	0
41	1j	97/97 (100%)	1.13	21 (21%) 0 0	70, 87, 95, 98	0
41	2j	96/97 (98%)	1.08	20 (20%) 1 0	75, 89, 95, 97	0
42	1k	114/114 (100%)	-0.25	1 (0%) 84 84	40, 65, 81, 87	0
42	2k	114/114 (100%)	-0.06	1 (0%) 84 84	54, 71, 85, 91	0
43	1l	121/122 (99%)	-0.14	2 (1%) 70 69	47, 63, 75, 78	0
43	2l	121/122 (99%)	-0.14	0 100 100	54, 66, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/116 (100%)	0.31	7 (6%) 21 18	71, 81, 88, 91	0
44	2m	114/116 (98%)	0.39	8 (7%) 16 12	76, 88, 93, 95	0
45	1n	60/60 (100%)	0.38	1 (1%) 70 69	71, 80, 88, 89	0
45	2n	60/60 (100%)	0.90	11 (18%) 1 0	76, 88, 92, 95	0
46	1o	88/88 (100%)	0.05	3 (3%) 45 40	46, 68, 80, 84	0
46	2o	88/88 (100%)	-0.10	0 100 100	55, 71, 83, 86	0
47	1p	82/82 (100%)	0.41	6 (7%) 15 11	64, 77, 86, 90	0
47	2p	82/82 (100%)	0.20	3 (3%) 41 37	58, 70, 79, 86	0
48	1q	99/99 (100%)	-0.04	1 (1%) 82 82	53, 68, 80, 84	0
48	2q	99/99 (100%)	-0.13	1 (1%) 82 82	57, 70, 79, 83	0
49	1r	68/68 (100%)	0.27	3 (4%) 34 30	55, 67, 80, 86	0
49	2r	68/68 (100%)	0.13	3 (4%) 34 30	61, 71, 82, 86	0
50	1s	83/83 (100%)	0.73	10 (12%) 4 3	76, 84, 91, 94	0
50	2s	83/83 (100%)	1.81	35 (42%) 0 0	84, 90, 97, 99	0
51	1t	96/98 (97%)	0.33	3 (3%) 49 44	64, 75, 86, 92	0
51	2t	98/98 (100%)	0.12	1 (1%) 82 82	56, 69, 83, 85	0
52	1u	23/23 (100%)	1.17	5 (21%) 0 0	72, 77, 83, 85	0
52	2u	23/23 (100%)	1.76	10 (43%) 0 0	79, 86, 89, 90	0
53	1x	97/97 (100%)	0.07	2 (2%) 63 61	52, 67, 81, 86	0
53	2x	96/97 (98%)	1.95	45 (46%) 0 0	72, 82, 93, 96	0
54	1y	10/10 (100%)	-0.26	0 100 100	30, 33, 40, 40	0
54	2y	10/10 (100%)	-0.13	0 100 100	43, 47, 58, 58	0
All	All	20786/20974 (99%)	0.01	833 (4%) 38 33	15, 64, 93, 114	0

All (833) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1133	G	17.7
1	1A	1118	C	12.5
1	1A	1135	G	12.5
1	1A	1137	G	12.0
1	1A	1121	C	11.6
1	1A	1132	A	11.4
1	1A	1109	G	11.2

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Mol	Chain	Res	Type	RSRZ
1	1A	1123	A	11.0
1	1A	1134	A	10.6
1	1A	1120	G	10.4
1	1A	1122	C	10.3
1	1A	1136	U	10.3
1	1A	1110	C	10.2
1	1A	1149	A	10.0
1	1A	1125	C	9.6
1	1A	1113	A	9.2
1	1A	1126	C	9.0
1	1A	1127	U	9.0
1	1A	1124	U	8.9
1	1A	1139	G	8.9
1	2A	2802	G	8.5
1	1A	1112	U	8.3
1	2A	2125	G	8.1
38	2g	156	TRP	8.1
1	1A	1128	U	7.9
32	1a	1030(B)	C	7.8
32	2a	1001(A)	G	7.8
32	1a	1036	G	7.8
1	2A	2147	G	7.8
44	1m	115	LYS	7.6
1	1A	1129	U	7.6
53	2x	9	GLN	7.4
1	1A	1148	C	7.4
32	2a	1030(A)	G	7.4
1	2A	2169	A	7.4
1	1A	1119	A	7.3
1	2A	2123	G	7.3
32	2a	1030(B)	C	7.2
1	2A	2139	C	7.1
26	14	52	THR	7.0
1	1A	2139	A	6.9
1	1A	2138	G	6.9
1	1A	2166	U	6.7
1	1A	1138	C	6.6
53	2x	42	SER	6.6
1	1A	1117	G	6.6
1	2A	1046	A	6.5
1	2A	2126	A	6.5
1	2A	2162	G	6.5

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Mol	Chain	Res	Type	RSRZ
32	1a	1030(C)	G	6.3
1	2A	2124	G	6.3
1	2A	2168	G	6.3
32	2a	1001	A	6.2
1	1A	1131	A	6.1
1	1A	1150	C	6.1
32	2a	1036	G	6.1
20	2Y	1	MET	6.1
1	2A	2118	U	6.0
1	1A	2145	G	5.9
32	1a	1002	G	5.9
1	1A	1111	U	5.8
1	2A	2148	G	5.8
1	1A	1103	A	5.8
1	1A	1114	G	5.8
53	2x	73	ALA	5.7
34	1c	193	TYR	5.7
32	1a	1031	G	5.6
41	2j	6	ILE	5.6
1	2A	2155	G	5.5
1	2A	2173	A	5.5
53	2x	75	ASN	5.4
32	2a	1257	U	5.4
1	2A	2152	G	5.4
1	2A	2154	G	5.4
1	1A	2195	A	5.4
53	2x	45	PRO	5.4
32	1a	1001	A	5.4
1	2A	2133	G	5.3
1	1A	2169	G	5.3
32	1a	1037	C	5.3
23	21	2	SER	5.3
1	2A	2174	C	5.2
53	2x	41	LEU	5.2
1	2A	1085	A	5.2
53	2x	38	HIS	5.2
32	1a	1035	A	5.1
1	1A	1108	G	5.1
32	1a	1034	G	5.1
1	2A	1083	U	5.1
1	2A	2896	C	5.1
1	1A	1555	C	5.1

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Mol	Chain	Res	Type	RSRZ
32	1a	1001(A)	G	5.1
1	2A	2803	C	5.1
1	2A	2113	U	5.0
41	2j	74	ILE	5.0
1	1A	2183	C	5.0
1	2A	2153	G	5.0
1	2A	2138	C	5.0
32	2a	1030(C)	G	5.0
1	2A	2141	G	4.9
32	1a	1030	C	4.9
26	24	49	PHE	4.9
1	2A	2107	C	4.9
1	2A	2146	C	4.9
50	2s	12	ASP	4.9
50	2s	53	ASN	4.9
53	2x	64	SER	4.9
32	1a	1003	G	4.8
1	2A	888	C	4.8
1	2A	2132	U	4.8
1	2A	1095	A	4.8
1	2A	2131	G	4.8
1	2A	1082	U	4.8
50	2s	71	LEU	4.8
1	2A	2897	U	4.7
1	2A	2170	A	4.7
1	2A	2157	G	4.7
1	2A	229	A	4.7
33	2b	232	PRO	4.7
1	2A	2801(A)	A	4.7
1	2A	2145	C	4.7
1	1A	2161	C	4.7
41	2j	72	VAL	4.6
41	1j	10	GLY	4.6
1	2A	2176	A	4.6
32	1a	1026	G	4.6
1	2A	2110	G	4.6
32	1a	202	U	4.6
26	24	69	LYS	4.5
1	2A	2112	G	4.5
38	2g	154	TYR	4.4
1	1A	1130	A	4.4
1	1A	2137	G	4.4

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Mol	Chain	Res	Type	RSRZ
1	1A	2188	G	4.4
1	2A	2127	G	4.4
32	2a	1030	C	4.4
41	1j	100	THR	4.4
32	2a	1034	G	4.4
1	2A	2136	C	4.4
1	2A	2140	C	4.4
1	2A	2137	C	4.3
1	1A	1141	A	4.3
1	1A	2154	U	4.3
1	2A	1509	C	4.3
1	2A	2128	C	4.3
50	1s	40	ILE	4.3
40	1i	15	ALA	4.3
1	2A	2122	U	4.3
6	2G	62	LEU	4.3
33	1b	129	GLU	4.2
1	2A	6	A	4.2
32	2a	1030(D)	A	4.2
1	1A	2148	A	4.2
32	2a	1035	A	4.2
1	1A	2814	C	4.2
7	2H	103	LEU	4.2
1	2A	2167	U	4.2
52	1u	18	TYR	4.2
32	1a	1030(A)	G	4.1
53	2x	8	LYS	4.1
1	2A	2165	G	4.1
18	1W	111	HIS	4.1
32	1a	1030(D)	A	4.1
53	2x	48	PHE	4.1
41	2j	71	LEU	4.1
1	1A	2165	C	4.1
1	2A	2108	C	4.1
53	2x	65	GLY	4.1
1	2A	2143	C	4.1
32	1a	1039	C	4.1
1	2A	2119	A	4.1
1	1A	2194	U	4.1
32	1a	204	U	4.1
42	2k	13	GLN	4.1
50	2s	16	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	2A	1064	C	4.0
1	2A	2179	C	4.0
41	1j	8	LEU	4.0
53	2x	77	LEU	4.0
1	2A	2793	G	4.0
1	2A	2142	C	4.0
6	2G	2	PRO	4.0
32	1a	1257	U	4.0
1	1A	2177	G	4.0
1	2A	2121	G	4.0
32	1a	1027	C	4.0
32	2a	1026	G	4.0
1	2A	2109	U	4.0
1	1A	2807	C	4.0
1	1A	935	C	3.9
41	1j	98	ILE	3.9
1	2A	2166	G	3.9
40	2i	102	LEU	3.9
1	1A	2147	G	3.9
1	1A	2175	G	3.9
1	2A	2120	G	3.9
53	2x	10	MET	3.9
1	2A	2159	G	3.9
32	2a	1003	G	3.9
32	2a	1031	G	3.9
26	24	45	GLY	3.9
1	1A	2130	C	3.9
1	1A	2162	C	3.9
1	2A	2164	C	3.9
32	2a	723	U	3.9
32	2a	1002	G	3.9
1	2A	652(B)	A	3.9
1	1A	2168	C	3.8
1	2A	2171	A	3.8
1	1A	2191	A	3.8
1	2A	1067	A	3.8
45	2n	13	THR	3.8
32	1a	1006	C	3.8
14	2S	58	LEU	3.8
1	1A	2181	G	3.8
1	1A	2182	G	3.8
1	2A	2175	C	3.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2178	C	3.8
31	29	37	GLY	3.8
52	2u	6	ARG	3.8
41	1j	35	SER	3.8
1	1A	1104	G	3.8
1	1A	2189	U	3.8
53	2x	39	ILE	3.8
41	1j	7	LYS	3.8
1	2A	2111	C	3.8
1	2A	2804	C	3.8
1	1A	2163	G	3.7
1	1A	2187	G	3.7
46	1o	89	GLY	3.7
33	1b	232	PRO	3.7
1	1A	2816	G	3.7
1	1A	2140	U	3.7
1	1A	2151	C	3.7
1	1A	2164	C	3.7
1	1A	2180	A	3.7
1	2A	2151	G	3.7
38	1g	156	TRP	3.7
1	1A	2198	A	3.7
1	1A	2155	G	3.7
26	24	68	ARG	3.6
53	2x	50	ALA	3.6
20	2Y	5	MET	3.6
1	2A	2144	U	3.6
1	2A	2177	C	3.6
21	2Z	199	LYS	3.6
33	1b	136	VAL	3.6
1	1A	2190	G	3.6
1	2A	2106	G	3.6
1	2A	2116	G	3.6
26	24	63	TYR	3.6
1	2A	2114	A	3.6
52	1u	19	GLY	3.6
1	1A	2815	C	3.5
1	1A	2806	G	3.5
40	2i	7	THR	3.5
1	1A	2178	G	3.5
1	2A	1080	C	3.5
1	2A	2163	C	3.5

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Mol	Chain	Res	Type	RSRZ
44	1m	2	ALA	3.5
41	1j	72	VAL	3.5
33	1b	133	LYS	3.5
32	1a	1024	G	3.5
32	2a	1021	G	3.5
45	2n	2	ALA	3.5
32	2a	202	U	3.5
1	2A	1076	C	3.5
7	2H	113	VAL	3.5
7	2H	169	VAL	3.5
14	2S	35	ILE	3.5
1	2A	2805	G	3.5
32	1a	1033	G	3.5
7	2H	48	GLY	3.5
53	2x	68	GLU	3.5
53	2x	12	ILE	3.5
1	1A	2186	C	3.5
53	2x	20	VAL	3.4
1	1A	2129	C	3.4
1	1A	2141	A	3.4
1	2A	1088	A	3.4
23	11	2	SER	3.4
34	2c	190	ARG	3.4
32	2a	1037	C	3.4
1	2A	2134	A	3.4
25	23	26	LEU	3.4
1	1A	2134	G	3.4
33	2b	122	PHE	3.4
40	1i	106	ALA	3.4
1	1A	2146	G	3.4
53	2x	71	TYR	3.4
1	1A	2167	C	3.4
45	2n	11	LYS	3.4
41	2j	36	GLY	3.4
53	2x	92	GLY	3.4
26	14	68	ARG	3.4
32	1a	1032	G	3.4
1	1A	2160	C	3.4
22	20	9	SER	3.4
52	2u	11	GLY	3.4
41	2j	85	LEU	3.4
45	2n	12	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
53	2x	46	GLN	3.4
1	2A	1079	C	3.4
33	2b	136	VAL	3.3
32	1a	1038	C	3.3
50	2s	80	TYR	3.3
1	2A	2156	G	3.3
1	2A	2150	U	3.3
33	1b	130	ARG	3.3
1	2A	2794	C	3.3
32	1a	1029	C	3.3
50	2s	13	ASP	3.3
32	1a	1005	A	3.3
53	2x	11	GLU	3.3
32	2a	1040	U	3.3
1	1A	218	A	3.3
32	2a	1027	C	3.3
52	2u	18	TYR	3.3
45	2n	10	ALA	3.3
6	2G	49	ASP	3.3
32	2a	1286	A	3.3
32	2a	80	G	3.3
32	1a	203	U	3.3
50	2s	74	PHE	3.3
20	2Y	90	LEU	3.3
45	2n	38	GLY	3.3
38	2g	32	ARG	3.2
40	2i	8	GLY	3.2
50	2s	48	THR	3.2
34	2c	158	GLY	3.2
32	2a	1032	G	3.2
47	1p	19	ILE	3.2
52	2u	10	ARG	3.2
33	1b	214	ILE	3.2
20	2Y	45	VAL	3.2
1	2A	2105	C	3.2
22	20	8	GLY	3.2
32	1a	1004	A	3.2
41	1j	96	ILE	3.2
7	2H	105	LEU	3.2
53	2x	70	MET	3.2
52	1u	9	ARG	3.2
53	2x	49	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	2A	889	C	3.2
41	2j	34	VAL	3.1
50	2s	45	VAL	3.1
7	2H	13	LYS	3.1
26	14	54	GLY	3.1
32	1a	1286	A	3.1
1	2A	2807	G	3.1
7	2H	159	GLU	3.1
26	14	56	VAL	3.1
53	2x	67	HIS	3.1
51	1t	9	ASN	3.1
39	2h	122	ARG	3.1
41	1j	34	VAL	3.1
33	1b	131	PRO	3.1
1	1A	2202	U	3.1
1	2A	2172	U	3.1
41	1j	73	ASP	3.1
7	2H	82	GLY	3.1
44	1m	117	VAL	3.1
1	1A	2170	G	3.1
6	2G	75	LYS	3.1
32	1a	841	U	3.1
32	2a	204	U	3.1
40	2i	19	LEU	3.1
40	2i	127	LYS	3.1
52	1u	22	ARG	3.1
26	24	67	TYR	3.1
32	2a	1042	G	3.1
41	2j	47	PHE	3.1
20	1Y	1	MET	3.1
32	2a	1029	C	3.1
44	1m	94	ARG	3.1
1	1A	2171	G	3.1
32	2a	1033	G	3.1
46	1o	87	ILE	3.1
1	2A	2135	A	3.0
1	1A	696	C	3.0
1	2A	2129	C	3.0
38	2g	42	ILE	3.0
1	2A	2792	G	3.0
14	2S	20	ARG	3.0
6	1G	49	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
7	2H	112	PRO	3.0
1	1A	1143	U	3.0
1	1A	2144	U	3.0
7	2H	47	GLU	3.0
50	1s	66	MET	3.0
8	2I	12	LEU	3.0
1	2A	10	G	3.0
1	2A	2894	G	3.0
50	2s	52	TYR	3.0
38	2g	16	LEU	3.0
6	2G	26	GLN	3.0
50	2s	56	GLN	3.0
1	2A	2160	G	3.0
1	1A	1151	U	3.0
1	2A	2149	G	3.0
41	1j	75	ILE	3.0
11	2P	91	PHE	3.0
32	1a	1007	C	3.0
50	2s	9	VAL	3.0
40	1i	47	LEU	2.9
49	1r	29	PHE	2.9
26	14	59	PHE	2.9
32	1a	1028	C	2.9
33	2b	135	GLN	2.9
19	2X	68	ARG	2.9
1	1A	2152	U	2.9
34	2c	206	GLU	2.9
53	2x	5	ILE	2.9
40	2i	59	PHE	2.9
20	2Y	58	GLY	2.9
1	1A	2153	G	2.9
32	1a	1000	U	2.9
32	2a	1041	A	2.9
53	2x	95	ARG	2.9
4	2E	1	MET	2.9
8	2I	3	VAL	2.9
26	24	50	VAL	2.9
29	17	48	LYS	2.9
20	2Y	57	GLN	2.9
38	2g	78	ARG	2.9
33	1b	228	GLY	2.9
44	2m	116	THR	2.9

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Mol	Chain	Res	Type	RSRZ
46	1o	88	ARG	2.9
50	2s	14	HIS	2.9
1	1A	2813	G	2.9
1	2A	1044	G	2.9
7	2H	50	VAL	2.9
20	2Y	89	PHE	2.9
26	24	59	PHE	2.9
33	1b	126	GLU	2.9
33	2b	124	SER	2.9
26	24	52	THR	2.9
38	1g	16	LEU	2.9
1	1A	2150	C	2.8
33	1b	128	GLU	2.8
40	2i	42	ARG	2.8
32	2a	1004	A	2.8
40	1i	19	LEU	2.8
32	2a	90	U	2.8
52	2u	14	TRP	2.8
33	1b	122	PHE	2.8
33	2b	132	LYS	2.8
1	1A	1140	U	2.8
53	1x	95	ARG	2.8
1	1A	1099	C	2.8
32	2a	998	G	2.8
41	2j	63	PHE	2.8
48	2q	100	LYS	2.8
50	1s	49	ILE	2.8
32	2a	89	C	2.8
49	1r	43	PHE	2.8
1	1A	1221	G	2.8
44	1m	87	TYR	2.8
50	2s	30	LEU	2.8
1	2A	2180	U	2.8
7	2H	100	GLY	2.8
5	1F	15	SER	2.8
44	2m	102	ARG	2.8
52	2u	9	ARG	2.8
47	2p	48	TRP	2.8
1	1A	1105	G	2.8
50	2s	49	ILE	2.8
34	1c	87	LEU	2.8
8	2I	74	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
41	1j	5	ARG	2.7
52	2u	24	ARG	2.7
41	1j	71	LEU	2.7
21	2Z	188	ALA	2.7
1	2A	2892	A	2.7
41	2j	29	ARG	2.7
53	2x	80	LYS	2.7
1	1A	2128	G	2.7
38	1g	154	TYR	2.7
1	1A	2193	A	2.7
52	2u	17	THR	2.7
51	1t	55	ILE	2.7
20	2Y	50	ARG	2.7
1	1A	1147	U	2.7
7	2H	29	PRO	2.7
38	2g	79	ARG	2.7
53	2x	7	SER	2.7
32	2a	1000	U	2.7
1	1A	2179	G	2.7
1	1A	2184	G	2.7
41	1j	40	LEU	2.7
41	2j	40	LEU	2.7
1	2A	1057	A	2.7
50	2s	44	MET	2.7
38	2g	155	ARG	2.7
1	2A	2161	C	2.7
1	2A	1062	G	2.7
50	2s	35	SER	2.6
51	2t	55	ILE	2.6
25	23	60	GLU	2.6
50	2s	64	GLU	2.6
34	1c	101	LEU	2.6
53	2x	69	ASP	2.6
34	1c	194	GLY	2.6
32	2a	1039	C	2.6
50	2s	10	PHE	2.6
41	2j	98	ILE	2.6
6	2G	35	GLU	2.6
1	1A	2812	A	2.6
25	23	47	VAL	2.6
1	2A	1104	C	2.6
1	1A	2906	U	2.6

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Mol	Chain	Res	Type	RSRZ
44	1m	90	LEU	2.6
43	1l	64	TYR	2.6
1	2A	1086	A	2.6
50	2s	32	LYS	2.6
50	2s	83	HIS	2.6
53	2x	76	GLU	2.6
34	1c	2	GLY	2.6
35	2d	183	GLY	2.6
26	24	44	THR	2.6
49	2r	58	LEU	2.6
1	1A	2176	G	2.6
1	1A	2201	C	2.6
26	24	43	TYR	2.6
40	2i	33	PHE	2.6
7	2H	115	VAL	2.5
1	2A	1042	G	2.5
32	1a	216	G	2.5
33	2b	137	ARG	2.5
45	2n	25	VAL	2.5
49	1r	24	ALA	2.5
38	2g	82	GLY	2.5
41	2j	65	LEU	2.5
50	2s	15	LEU	2.5
1	1A	2131	U	2.5
1	2A	652(V)	C	2.5
1	2A	2158	A	2.5
32	2a	848	C	2.5
41	1j	27	ALA	2.5
20	2Y	91	GLU	2.5
1	2A	1081	U	2.5
32	1a	1025	U	2.5
40	2i	37	PHE	2.5
7	2H	128	PRO	2.5
50	1s	56	GLN	2.5
1	2A	2181	G	2.5
21	2Z	200	GLY	2.5
33	2b	201	ILE	2.5
6	1G	80	PHE	2.5
20	2Y	4	LYS	2.5
32	2a	1019	C	2.5
1	1A	2157	A	2.5
26	24	66	SER	2.5

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Mol	Chain	Res	Type	RSRZ
32	1a	161	A	2.5
32	1a	344	A	2.5
35	1d	2	GLY	2.5
20	2Y	75	ILE	2.5
1	1A	2203	G	2.5
1	2A	1087	G	2.5
1	2A	2130	U	2.5
6	2G	41	GLN	2.5
1	1A	1116	A	2.5
32	2a	1531	A	2.5
53	2x	40	ILE	2.5
47	2p	59	TRP	2.5
47	1p	45	THR	2.5
53	2x	63	ALA	2.5
41	2j	10	GLY	2.5
1	1A	2196	C	2.5
1	2A	1536	C	2.5
15	1T	38	ASN	2.5
32	2a	1020	U	2.5
12	2Q	59	ARG	2.5
1	1A	2149	G	2.5
40	2i	4	TYR	2.5
32	2a	91	C	2.5
44	2m	93	ARG	2.5
53	2x	58	ASN	2.5
1	1A	2803	A	2.5
20	2Y	88	LYS	2.5
1	2A	2187	G	2.5
35	1d	135	LEU	2.5
7	2H	95	ARG	2.4
6	2G	67	LYS	2.4
34	2c	100	ALA	2.4
33	1b	137	ARG	2.4
41	1j	70	ARG	2.4
1	2A	652(U)	G	2.4
32	2a	1024	G	2.4
44	2m	106	ASN	2.4
7	2H	102	ALA	2.4
36	1e	95	ALA	2.4
7	2H	94	TYR	2.4
8	2I	81	VAL	2.4
32	1a	65	U	2.4

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Mol	Chain	Res	Type	RSRZ
32	2a	1028	C	2.4
33	1b	135	GLN	2.4
50	2s	31	ILE	2.4
7	1H	2	SER	2.4
1	1A	2185	C	2.4
38	2g	6	ARG	2.4
50	2s	36	ARG	2.4
34	2c	124	ILE	2.4
40	2i	62	TYR	2.4
11	2P	15	ARG	2.4
50	2s	68	GLY	2.4
32	1a	345	C	2.4
1	1A	2174	G	2.4
50	2s	40	ILE	2.4
7	2H	45	VAL	2.4
26	14	45	GLY	2.4
35	1d	3	ARG	2.4
40	2i	5	TYR	2.4
40	2i	88	TYR	2.4
32	1a	723	U	2.4
40	2i	110	GLU	2.4
53	2x	24	LEU	2.4
26	24	56	VAL	2.4
40	1i	78	LYS	2.4
6	2G	48	GLU	2.4
33	2b	81	VAL	2.4
44	2m	60	VAL	2.4
1	1A	2126	G	2.4
22	20	70	GLN	2.4
26	14	65	ASP	2.4
32	1a	1532	U	2.4
41	1j	33	GLN	2.4
31	29	5	ALA	2.4
45	2n	39	LEU	2.4
50	2s	11	VAL	2.3
35	1d	138	TYR	2.3
44	2m	87	TYR	2.3
47	1p	57	ARG	2.3
50	1s	50	ALA	2.3
32	2a	994	A	2.3
33	2b	70	PHE	2.3
44	2m	92	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
9	2N	140	VAL	2.3
6	2G	25	TYR	2.3
45	2n	15	LYS	2.3
50	1s	59	PRO	2.3
7	2H	89	ILE	2.3
34	1c	90	GLU	2.3
40	2i	126	SER	2.3
45	2n	8	GLU	2.3
1	1A	1115	A	2.3
20	2Y	60	PHE	2.3
1	1A	2210	C	2.3
14	2S	57	LYS	2.3
32	2a	999	C	2.3
34	1c	76	VAL	2.3
41	2j	68	HIS	2.3
40	2i	90	PRO	2.3
40	1i	46	ALA	2.3
53	2x	94	ALA	2.3
6	2G	19	LEU	2.3
7	2H	148	ILE	2.3
34	1c	204	LEU	2.3
32	2a	1023	G	2.3
32	2a	1044	A	2.3
1	1A	2159	C	2.3
32	1a	201	C	2.3
38	2g	120	ILE	2.3
1	1A	697	C	2.3
22	20	75	LEU	2.3
1	1A	2905	C	2.3
40	2i	36	TYR	2.3
7	2H	161	GLY	2.3
22	10	8	GLY	2.3
47	2p	19	ILE	2.3
22	20	45	PHE	2.3
41	2j	100	THR	2.3
20	2Y	51	VAL	2.3
26	14	50	VAL	2.3
41	1j	85	LEU	2.3
44	2m	114	ARG	2.3
1	1A	2204	G	2.3
40	2i	30	GLY	2.3
7	2H	106	THR	2.3

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Mol	Chain	Res	Type	RSRZ
21	1Z	193	GLU	2.3
50	1s	19	VAL	2.3
1	1A	1106	U	2.3
1	2A	887	A	2.3
1	2A	1054	A	2.3
1	2A	2117	A	2.3
38	2g	80	VAL	2.2
38	2g	76	ARG	2.2
1	2A	1065	U	2.2
21	2Z	201	LYS	2.2
26	24	9	LEU	2.2
38	1g	130	GLY	2.2
53	2x	34	LEU	2.2
51	1t	79	ARG	2.2
1	2A	614(A)	U	2.2
33	2b	214	ILE	2.2
45	2n	34	TYR	2.2
1	2A	34	C	2.2
26	24	46	GLN	2.2
52	2u	15	ARG	2.2
32	2a	1447	A	2.2
53	2x	79	ASN	2.2
1	2A	11	G	2.2
1	2A	1056	G	2.2
33	2b	215	LEU	2.2
1	2A	645	C	2.2
1	2A	652(T)	C	2.2
21	2Z	198	LYS	2.2
32	2a	1018	C	2.2
1	1A	2614	A	2.2
34	2c	154	SER	2.2
33	1b	231	GLU	2.2
41	1j	91	PRO	2.2
50	2s	75	ALA	2.2
40	2i	9	ARG	2.2
1	1A	1072	U	2.2
45	1n	11	LYS	2.2
53	2x	74	ILE	2.2
1	2A	1059	G	2.2
1	2A	2893	G	2.2
33	2b	130	ARG	2.2
41	2j	7	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
50	1s	30	LEU	2.2
50	2s	81	ARG	2.2
26	14	66	SER	2.2
48	1q	99	SER	2.2
7	2H	41	MET	2.2
47	1p	39	TYR	2.2
52	2u	21	TYR	2.2
1	2A	1533	G	2.2
14	2S	111	GLU	2.2
40	2i	105	ASP	2.2
40	1i	7	THR	2.2
50	2s	63	THR	2.2
7	2H	114	VAL	2.2
40	2i	72	GLY	2.2
1	1A	694	G	2.2
1	2A	2115	G	2.2
1	2A	2186	G	2.2
53	2x	88	LEU	2.2
53	2x	15	ALA	2.2
21	2Z	1	MET	2.2
47	1p	46	PRO	2.2
34	1c	89	GLU	2.2
35	1d	112	VAL	2.2
50	2s	41	VAL	2.2
1	2A	1075	C	2.1
34	1c	126	ARG	2.1
8	2I	77	LEU	2.1
50	1s	74	PHE	2.1
42	1k	42	TRP	2.1
8	2I	99	GLU	2.1
25	23	29	ARG	2.1
38	1g	155	ARG	2.1
8	2I	19	VAL	2.1
17	2V	42	GLY	2.1
26	24	64	GLY	2.1
38	1g	85	TYR	2.1
37	1f	98	LEU	2.1
47	1p	50	LYS	2.1
33	2b	97	TRP	2.1
7	2H	43	VAL	2.1
34	1c	81	GLY	2.1
50	2s	47	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
50	2s	51	VAL	2.1
1	2A	2100	G	2.1
25	23	3	ARG	2.1
40	1i	18	PHE	2.1
41	2j	46	ARG	2.1
32	1a	1040	U	2.1
21	2Z	143	GLY	2.1
26	24	7	PRO	2.1
50	2s	57	HIS	2.1
50	1s	71	LEU	2.1
21	1Z	192	ALA	2.1
53	1x	91	LYS	2.1
32	1a	1137	C	2.1
41	1j	9	ARG	2.1
52	1u	24	ARG	2.1
43	1l	61	THR	2.1
1	1A	1145	G	2.1
1	2A	652(C)	G	2.1
40	1i	8	GLY	2.1
1	1A	1144	A	2.1
7	2H	101	ARG	2.1
34	2c	198	VAL	2.1
1	2A	886	C	2.1
32	2a	1038	C	2.1
33	1b	210	SER	2.1
34	1c	196	LEU	2.1
1	1A	2172	U	2.1
32	1a	1212	U	2.1
53	2x	47	GLY	2.1
25	23	59	VAL	2.1
32	1a	77	G	2.1
32	2a	79	G	2.1
1	2A	2602	A	2.1
32	2a	1006	C	2.1
32	2a	1045	C	2.1
41	2j	20	ALA	2.1
44	1m	93	ARG	2.1
6	2G	86	MET	2.1
41	2j	86	MET	2.1
50	2s	27	GLU	2.1
33	2b	133	LYS	2.1
1	2A	2104	G	2.1

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Mol	Chain	Res	Type	RSRZ
49	2r	24	ALA	2.0
53	2x	52	ALA	2.0
20	2Y	93	GLY	2.0
7	2H	32	GLU	2.0
33	2b	131	PRO	2.0
33	1b	187	LEU	2.0
40	1i	33	PHE	2.0
1	1A	1101	G	2.0
1	1A	2173	G	2.0
41	1j	89	ASP	2.0
1	1A	934	A	2.0
1	1A	2199	C	2.0
20	2Y	55	TYR	2.0
33	2b	123	ALA	2.0
26	14	49	PHE	2.0
40	1i	20	ARG	2.0
49	2r	54	ARG	2.0
53	2x	87	LYS	2.0
1	2A	1043	C	2.0
1	2A	2895	U	2.0
32	1a	217	C	2.0
32	2a	841	U	2.0
53	2x	72	THR	2.0
11	2P	122	PRO	2.0
40	2i	21	PRO	2.0
33	2b	127	ILE	2.0
39	1h	58	TYR	2.0
32	2a	1022	G	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	1A	1939	20/21	0.92	0.20	62,78,87,88	0
1	PSU	2A	1917	20/21	0.92	0.14	72,79,85,102	0
1	5MU	1A	1937	21/22	0.93	0.22	79,86,100,113	0
1	5MU	2A	1915	21/22	0.94	0.16	79,87,92,108	0
32	PSU	2a	516	20/21	0.94	0.16	72,83,88,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	2MG	2a	1207	24/25	0.94	0.17	81,90,95,99	0
32	5MC	2a	967	21/22	0.95	0.15	67,73,82,90	0
32	PSU	1a	516	20/21	0.95	0.15	66,74,77,77	0
1	PSU	2A	1911	20/21	0.96	0.11	65,73,80,81	0
32	M2G	1a	966	25/26	0.96	0.14	52,62,74,77	0
32	5MC	1a	967	21/22	0.96	0.14	57,65,75,83	0
32	2MG	1a	1207	24/25	0.96	0.12	76,81,85,85	0
32	7MG	2a	527	24/25	0.96	0.17	69,74,77,79	0
32	M2G	2a	966	25/26	0.96	0.14	67,71,86,94	0
32	5MC	1a	1407	21/22	0.96	0.14	44,53,58,61	0
43	0TD	1l	92	10/11	0.96	0.14	63,65,74,80	0
32	5MC	2a	1400	21/22	0.96	0.20	65,74,78,83	0
32	4OC	2a	1402	22/23	0.96	0.16	52,60,65,67	0
32	5MC	2a	1404	21/22	0.96	0.14	49,53,60,64	0
43	0TD	2l	92	10/11	0.96	0.15	71,73,77,92	0
1	PSU	2A	2605	20/21	0.97	0.17	33,35,41,41	0
1	4OC	1A	1942	21/23	0.97	0.16	47,59,64,65	0
32	UR3	1a	1498	21/22	0.97	0.19	41,50,56,59	0
1	PSU	1A	1933	20/21	0.97	0.15	57,70,74,76	0
32	7MG	1a	527	24/25	0.97	0.16	50,63,66,71	0
32	4OC	1a	1402	22/23	0.97	0.17	45,52,58,61	0
32	5MC	1a	1404	21/22	0.97	0.15	44,48,55,59	0
1	4OC	2A	1920	21/23	0.97	0.16	54,65,70,72	0
1	5MC	2A	1942	21/22	0.97	0.17	46,53,57,61	0
32	5MC	2a	1407	21/22	0.97	0.14	50,59,63,65	0
32	UR3	2a	1498	21/22	0.97	0.15	47,56,64,66	0
1	2MA	2A	2503	23/24	0.97	0.21	30,35,40,48	0
32	MA6	1a	1518	24/25	0.98	0.17	38,49,52,57	0
32	MA6	1a	1519	24/25	0.98	0.17	41,50,55,58	0
1	2MA	1A	2515	23/24	0.98	0.19	16,20,24,25	0
1	OMU	1A	2564	21/22	0.98	0.18	21,26,29,32	0
32	5MC	1a	1400	21/22	0.98	0.16	54,59,64,67	0
1	PSU	1A	2617	20/21	0.98	0.18	20,24,30,33	0
1	5MU	1A	1961	21/22	0.98	0.15	20,26,29,33	0
1	5MU	2A	1939	21/22	0.98	0.15	30,36,42,44	0
1	5MC	1A	1964	21/22	0.98	0.13	25,36,39,42	0
1	5MC	2A	1962	21/22	0.98	0.13	34,44,51,60	0
1	OMG	2A	2251	24/25	0.98	0.17	35,39,44,46	0
32	MA6	2a	1518	24/25	0.98	0.17	50,59,65,66	0
32	MA6	2a	1519	24/25	0.98	0.19	52,58,64,69	0
1	5MC	1A	1984	21/22	0.98	0.14	30,32,36,41	0
1	OMG	1A	2263	24/25	0.99	0.16	16,22,25,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	OMU	2A	2552	21/22	0.99	0.15	30,36,40,42	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3533	1/1	0.04	0.39	99,99,99,99	0
55	MG	2A	3768	1/1	0.23	0.36	95,95,95,95	0
55	MG	2A	3606	1/1	0.32	0.27	68,68,68,68	0
55	MG	1P	203	1/1	0.34	0.20	90,90,90,90	0
55	MG	2A	3090	1/1	0.38	0.41	76,76,76,76	0
55	MG	1a	3161	1/1	0.41	0.82	77,77,77,77	0
55	MG	1a	3005	1/1	0.41	0.19	81,81,81,81	0
55	MG	2A	3455	1/1	0.41	0.58	59,59,59,59	0
55	MG	2A	3792	1/1	0.41	1.02	79,79,79,79	0
55	MG	2A	3010	1/1	0.42	0.32	63,63,63,63	0
55	MG	1A	3246	1/1	0.45	0.19	78,78,78,78	0
55	MG	1A	3861	1/1	0.45	0.08	82,82,82,82	0
55	MG	2A	3800	1/1	0.45	0.27	112,112,112,112	0
55	MG	2A	3129	1/1	0.46	0.62	75,75,75,75	0
55	MG	2A	3553	1/1	0.46	1.09	89,89,89,89	0
55	MG	1a	3149	1/1	0.48	0.23	104,104,104,104	0
55	MG	1A	3702	1/1	0.48	0.72	55,55,55,55	0
55	MG	2B	3011	1/1	0.48	0.21	90,90,90,90	0
55	MG	2A	3101	1/1	0.49	0.22	74,74,74,74	0
55	MG	1F	314	1/1	0.49	0.30	53,53,53,53	0
55	MG	2B	3012	1/1	0.49	0.09	87,87,87,87	0
55	MG	1a	3215	1/1	0.50	0.25	86,86,86,86	0
55	MG	2A	3752	1/1	0.51	0.36	77,77,77,77	0
55	MG	2A	3502	1/1	0.51	0.31	70,70,70,70	0
55	MG	2a	1686	1/1	0.51	0.25	108,108,108,108	0
55	MG	2A	3172	1/1	0.53	0.34	69,69,69,69	0
55	MG	1A	3516	1/1	0.54	0.51	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3511	1/1	0.55	0.14	90,90,90,90	0
55	MG	2A	3064	1/1	0.56	0.10	72,72,72,72	0
55	MG	2A	3142	1/1	0.56	0.97	60,60,60,60	0
55	MG	1Q	204	1/1	0.57	0.47	52,52,52,52	0
55	MG	2A	3162	1/1	0.57	0.36	82,82,82,82	0
55	MG	2d	504	1/1	0.57	0.14	90,90,90,90	0
55	MG	2n	502	1/1	0.57	0.42	82,82,82,82	0
55	MG	1A	3848	1/1	0.58	0.66	68,68,68,68	0
55	MG	1A	3181	1/1	0.59	0.24	51,51,51,51	0
55	MG	1A	3095	1/1	0.59	0.78	61,61,61,61	0
55	MG	1B	3006	1/1	0.60	0.21	59,59,59,59	0
55	MG	2A	3643	1/1	0.60	1.12	60,60,60,60	0
55	MG	2A	3706	1/1	0.60	0.13	90,90,90,90	0
55	MG	27	103	1/1	0.60	0.59	70,70,70,70	0
55	MG	2A	3080	1/1	0.60	0.41	69,69,69,69	0
55	MG	2A	3510	1/1	0.60	0.21	103,103,103,103	0
55	MG	2A	3563	1/1	0.60	0.65	77,77,77,77	0
55	MG	2a	1742	1/1	0.61	0.57	113,113,113,113	0
55	MG	2A	3672	1/1	0.61	0.28	59,59,59,59	0
55	MG	1A	3077	1/1	0.61	0.61	47,47,47,47	0
55	MG	1a	3058	1/1	0.62	0.69	82,82,82,82	0
55	MG	1A	3899	1/1	0.63	0.38	51,51,51,51	0
55	MG	1B	3002	1/1	0.63	0.28	69,69,69,69	0
55	MG	2e	3002	1/1	0.63	0.34	83,83,83,83	0
55	MG	2A	3019	1/1	0.63	0.22	45,45,45,45	0
55	MG	1A	3183	1/1	0.64	0.63	46,46,46,46	0
55	MG	2A	3574	1/1	0.64	0.23	98,98,98,98	0
55	MG	2A	3476	1/1	0.64	0.48	78,78,78,78	0
55	MG	2B	3013	1/1	0.64	0.12	84,84,84,84	0
55	MG	2D	302	1/1	0.64	0.45	58,58,58,58	0
55	MG	1A	3131	1/1	0.64	0.21	62,62,62,62	0
55	MG	2A	3507	1/1	0.64	0.56	69,69,69,69	0
55	MG	2A	3074	1/1	0.64	0.45	48,48,48,48	0
55	MG	2a	1770	1/1	0.64	0.18	75,75,75,75	0
55	MG	1A	3396	1/1	0.64	0.48	66,66,66,66	0
55	MG	1A	3456	1/1	0.64	0.23	59,59,59,59	0
55	MG	2A	3320	1/1	0.64	0.13	79,79,79,79	0
55	MG	2a	1731	1/1	0.65	0.10	90,90,90,90	0
55	MG	2A	3582	1/1	0.65	0.61	64,64,64,64	0
55	MG	2a	1747	1/1	0.65	0.23	94,94,94,94	0
55	MG	1A	3244	1/1	0.65	0.81	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	3022	1/1	0.65	0.69	66,66,66,66	0
55	MG	1A	3165	1/1	0.65	0.30	80,80,80,80	0
55	MG	1a	3004	1/1	0.65	0.19	69,69,69,69	0
55	MG	1A	3498	1/1	0.66	0.10	70,70,70,70	0
55	MG	1A	3684	1/1	0.66	0.26	49,49,49,49	0
55	MG	1A	3503	1/1	0.66	0.40	77,77,77,77	0
55	MG	2G	3003	1/1	0.66	0.12	81,81,81,81	0
55	MG	1n	502	1/1	0.66	0.29	63,63,63,63	0
55	MG	2a	1637	1/1	0.66	1.07	71,71,71,71	0
55	MG	2A	3441	1/1	0.66	0.21	90,90,90,90	0
55	MG	2A	3184	1/1	0.67	0.38	73,73,73,73	0
55	MG	2A	3246	1/1	0.67	0.09	92,92,92,92	0
55	MG	2a	1653	1/1	0.67	0.44	85,85,85,85	0
55	MG	2a	1674	1/1	0.67	0.19	89,89,89,89	0
55	MG	2A	3813	1/1	0.67	0.46	57,57,57,57	0
55	MG	1A	3084	1/1	0.67	0.69	47,47,47,47	0
55	MG	1A	3192	1/1	0.68	0.33	42,42,42,42	0
55	MG	2A	3637	1/1	0.68	0.07	61,61,61,61	0
55	MG	2a	1724	1/1	0.68	0.29	93,93,93,93	0
55	MG	2G	3001	1/1	0.68	0.29	90,90,90,90	0
55	MG	1A	3105	1/1	0.68	0.30	46,46,46,46	0
55	MG	2Q	8004	1/1	0.68	0.62	66,66,66,66	0
55	MG	2A	3342	1/1	0.68	0.21	76,76,76,76	0
55	MG	2a	1631	1/1	0.68	0.57	85,85,85,85	0
55	MG	1A	3592	1/1	0.68	0.38	70,70,70,70	0
55	MG	2A	3194	1/1	0.68	0.09	84,84,84,84	0
55	MG	2A	3742	1/1	0.69	0.38	70,70,70,70	0
55	MG	1A	3501	1/1	0.69	0.18	64,64,64,64	0
55	MG	1A	3889	1/1	0.69	0.40	46,46,46,46	0
55	MG	2G	3002	1/1	0.69	0.26	90,90,90,90	0
55	MG	2a	1734	1/1	0.69	0.40	57,57,57,57	0
55	MG	1A	3118	1/1	0.69	0.28	63,63,63,63	0
55	MG	2A	3425	1/1	0.69	0.22	71,71,71,71	0
55	MG	1a	3218	1/1	0.69	0.30	72,72,72,72	0
55	MG	2A	3816	1/1	0.69	0.32	51,51,51,51	0
55	MG	1a	3034	1/1	0.69	0.22	84,84,84,84	0
55	MG	1A	3611	1/1	0.69	0.46	65,65,65,65	0
55	MG	1a	3074	1/1	0.70	0.35	65,65,65,65	0
55	MG	1a	3114	1/1	0.70	0.11	74,74,74,74	0
55	MG	18	3301	1/1	0.70	0.63	70,70,70,70	0
55	MG	2D	304	1/1	0.70	0.27	55,55,55,55	0
55	MG	1A	3917	1/1	0.70	0.31	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	3168	1/1	0.70	0.10	79,79,79,79	0
55	MG	1A	3230	1/1	0.70	0.34	50,50,50,50	0
55	MG	2A	3480	1/1	0.70	0.23	81,81,81,81	0
55	MG	2A	3489	1/1	0.70	0.16	81,81,81,81	0
55	MG	2a	1609	1/1	0.70	1.46	77,77,77,77	0
55	MG	1a	3064	1/1	0.70	0.25	78,78,78,78	0
55	MG	2A	3099	1/1	0.70	0.31	52,52,52,52	0
55	MG	1A	3259	1/1	0.71	0.19	52,52,52,52	0
55	MG	1a	3132	1/1	0.71	0.24	91,91,91,91	0
55	MG	1A	3552	1/1	0.71	0.39	45,45,45,45	0
55	MG	2a	1717	1/1	0.71	0.17	73,73,73,73	0
55	MG	2a	1719	1/1	0.71	0.22	75,75,75,75	0
55	MG	1A	3236	1/1	0.71	0.23	79,79,79,79	0
55	MG	2A	3105	1/1	0.71	0.26	82,82,82,82	0
55	MG	1B	3015	1/1	0.71	0.16	66,66,66,66	0
55	MG	2A	3642	1/1	0.71	0.12	82,82,82,82	0
55	MG	1A	3734	1/1	0.71	0.41	45,45,45,45	0
55	MG	2A	3150	1/1	0.71	0.42	49,49,49,49	0
55	MG	2a	1772	1/1	0.71	0.38	92,92,92,92	0
55	MG	2a	1787	1/1	0.71	0.18	80,80,80,80	0
55	MG	2a	1636	1/1	0.71	0.62	83,83,83,83	0
55	MG	2A	3155	1/1	0.71	0.85	50,50,50,50	0
55	MG	2a	1651	1/1	0.71	0.12	69,69,69,69	0
55	MG	2a	1730	1/1	0.72	0.27	92,92,92,92	0
55	MG	1A	3895	1/1	0.72	0.48	65,65,65,65	0
55	MG	1a	3073	1/1	0.72	0.19	74,74,74,74	0
55	MG	2A	3004	1/1	0.72	0.28	56,56,56,56	0
55	MG	1A	3578	1/1	0.72	0.15	86,86,86,86	0
55	MG	2A	3719	1/1	0.72	0.17	70,70,70,70	0
55	MG	1a	3108	1/1	0.72	0.06	81,81,81,81	0
55	MG	1A	3623	1/1	0.72	0.30	56,56,56,56	0
55	MG	2a	1625	1/1	0.72	0.32	70,70,70,70	0
55	MG	2a	1722	1/1	0.72	0.17	82,82,82,82	0
55	MG	2A	3109	1/1	0.72	0.56	64,64,64,64	0
55	MG	2A	3104	1/1	0.73	0.16	56,56,56,56	0
55	MG	1A	3228	1/1	0.73	0.36	28,28,28,28	0
55	MG	2A	3445	1/1	0.73	0.32	48,48,48,48	0
55	MG	2A	3559	1/1	0.73	0.40	64,64,64,64	0
55	MG	1d	503	1/1	0.73	0.34	63,63,63,63	0
55	MG	1A	3659	1/1	0.73	0.12	57,57,57,57	0
55	MG	1A	3790	1/1	0.73	0.20	84,84,84,84	0
55	MG	2A	3586	1/1	0.73	0.17	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3809	1/1	0.73	0.29	75,75,75,75	0
55	MG	2A	3307	1/1	0.73	0.10	54,54,54,54	0
55	MG	2a	1768	1/1	0.73	0.10	80,80,80,80	0
55	MG	2A	3627	1/1	0.73	0.24	66,66,66,66	0
55	MG	2A	3819	1/1	0.73	0.17	90,90,90,90	0
55	MG	15	104	1/1	0.73	0.30	26,26,26,26	0
55	MG	1A	3186	1/1	0.73	0.23	72,72,72,72	0
55	MG	2a	1656	1/1	0.73	0.41	72,72,72,72	0
55	MG	2A	3386	1/1	0.73	0.28	102,102,102,102	0
55	MG	2A	3471	1/1	0.74	0.15	79,79,79,79	0
55	MG	1A	3361	1/1	0.74	0.10	75,75,75,75	0
55	MG	1A	3837	1/1	0.74	0.07	84,84,84,84	0
55	MG	2a	1710	1/1	0.74	0.43	86,86,86,86	0
55	MG	1a	3150	1/1	0.74	0.32	99,99,99,99	0
55	MG	1A	3058	1/1	0.74	0.16	65,65,65,65	0
55	MG	1a	3038	1/1	0.74	0.78	79,79,79,79	0
55	MG	2A	3717	1/1	0.74	0.18	92,92,92,92	0
55	MG	2A	3257	1/1	0.74	0.50	68,68,68,68	0
55	MG	1A	3654	1/1	0.74	0.11	41,41,41,41	0
55	MG	1a	3063	1/1	0.74	0.98	64,64,64,64	0
55	MG	2A	3329	1/1	0.74	0.11	88,88,88,88	0
55	MG	1A	3220	1/1	0.74	0.71	77,77,77,77	0
55	MG	1A	3563	1/1	0.74	0.23	59,59,59,59	0
55	MG	1A	3143	1/1	0.74	0.50	45,45,45,45	0
55	MG	1A	3913	1/1	0.74	0.42	63,63,63,63	0
55	MG	2a	1642	1/1	0.74	0.14	68,68,68,68	0
55	MG	2a	1643	1/1	0.74	0.32	73,73,73,73	0
55	MG	1A	3119	1/1	0.74	0.39	33,33,33,33	0
55	MG	2A	3047	1/1	0.74	0.89	63,63,63,63	0
55	MG	2A	3030	1/1	0.75	0.21	69,69,69,69	0
55	MG	1A	3808	1/1	0.75	0.25	38,38,38,38	0
55	MG	1A	3148	1/1	0.75	0.25	58,58,58,58	0
55	MG	2A	3673	1/1	0.75	0.35	65,65,65,65	0
55	MG	1A	3519	1/1	0.75	0.12	46,46,46,46	0
55	MG	2A	3138	1/1	0.75	0.71	48,48,48,48	0
55	MG	2a	1741	1/1	0.75	0.07	75,75,75,75	0
55	MG	2B	3015	1/1	0.75	0.15	85,85,85,85	0
55	MG	1A	3914	1/1	0.75	0.47	62,62,62,62	0
55	MG	2a	1652	1/1	0.75	0.35	90,90,90,90	0
55	MG	2A	3485	1/1	0.75	0.48	73,73,73,73	0
55	MG	1A	3509	1/1	0.75	0.34	38,38,38,38	0
55	MG	2A	3091	1/1	0.75	0.44	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3602	1/1	0.75	0.23	76,76,76,76	0
55	MG	1a	3184	1/1	0.75	0.11	73,73,73,73	0
55	MG	2A	3641	1/1	0.75	0.13	77,77,77,77	0
55	MG	1A	3554	1/1	0.76	0.23	69,69,69,69	0
55	MG	2A	3478	1/1	0.76	0.18	94,94,94,94	0
55	MG	2A	3024	1/1	0.76	0.26	58,58,58,58	0
55	MG	2P	202	1/1	0.76	0.54	73,73,73,73	0
55	MG	2A	3154	1/1	0.76	0.89	61,61,61,61	0
55	MG	2A	3650	1/1	0.76	0.34	55,55,55,55	0
55	MG	28	101	1/1	0.76	1.05	64,64,64,64	0
55	MG	1a	3179	1/1	0.76	0.07	78,78,78,78	0
55	MG	2a	1614	1/1	0.76	1.41	75,75,75,75	0
55	MG	2A	3773	1/1	0.76	0.12	85,85,85,85	0
55	MG	2A	3777	1/1	0.76	0.22	83,83,83,83	0
55	MG	1a	3123	1/1	0.76	0.17	86,86,86,86	0
55	MG	2m	201	1/1	0.76	0.11	79,79,79,79	0
55	MG	2A	3685	1/1	0.76	0.29	54,54,54,54	0
55	MG	1A	3144	1/1	0.77	0.38	64,64,64,64	0
55	MG	1A	3624	1/1	0.77	0.31	68,68,68,68	0
55	MG	2A	3522	1/1	0.77	0.16	82,82,82,82	0
55	MG	1A	3193	1/1	0.77	0.42	42,42,42,42	0
55	MG	2a	1694	1/1	0.77	0.23	78,78,78,78	0
55	MG	1A	3506	1/1	0.77	0.17	71,71,71,71	0
55	MG	2H	201	1/1	0.77	0.81	108,108,108,108	0
55	MG	2A	3008	1/1	0.77	0.35	69,69,69,69	0
55	MG	2A	3113	1/1	0.77	0.20	66,66,66,66	0
55	MG	1A	3204	1/1	0.77	0.63	39,39,39,39	0
55	MG	2a	1727	1/1	0.77	0.39	91,91,91,91	0
55	MG	1A	3900	1/1	0.77	0.23	58,58,58,58	0
55	MG	28	102	1/1	0.77	0.70	59,59,59,59	0
55	MG	1a	3144	1/1	0.77	0.28	75,75,75,75	0
55	MG	1A	3905	1/1	0.77	0.74	45,45,45,45	0
55	MG	1A	3589	1/1	0.77	0.27	36,36,36,36	0
55	MG	2A	3058	1/1	0.77	1.09	53,53,53,53	0
55	MG	1A	3733	1/1	0.77	0.39	27,27,27,27	0
55	MG	2A	3163	1/1	0.77	0.53	78,78,78,78	0
55	MG	1A	3210	1/1	0.77	0.25	45,45,45,45	0
55	MG	1A	3071	1/1	0.77	0.51	42,42,42,42	0
55	MG	2a	1644	1/1	0.77	0.18	67,67,67,67	0
55	MG	2a	1646	1/1	0.77	0.22	56,56,56,56	0
55	MG	1A	3604	1/1	0.77	0.13	52,52,52,52	0
55	MG	1A	3538	1/1	0.77	0.26	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3131	1/1	0.78	0.31	65,65,65,65	0
55	MG	2A	3393	1/1	0.78	0.14	52,52,52,52	0
55	MG	2A	3423	1/1	0.78	0.10	79,79,79,79	0
55	MG	1A	3124	1/1	0.78	0.24	63,63,63,63	0
55	MG	2A	3629	1/1	0.78	0.10	74,74,74,74	0
55	MG	1A	3648	1/1	0.78	0.12	90,90,90,90	0
55	MG	1A	3526	1/1	0.78	0.14	64,64,64,64	0
55	MG	1a	3048	1/1	0.78	0.14	66,66,66,66	0
55	MG	1A	3031	1/1	0.78	0.21	22,22,22,22	0
55	MG	1A	3878	1/1	0.78	0.28	46,46,46,46	0
55	MG	1E	306	1/1	0.78	0.18	52,52,52,52	0
55	MG	1A	3599	1/1	0.78	0.07	50,50,50,50	0
55	MG	1A	3890	1/1	0.78	0.21	73,73,73,73	0
55	MG	2A	3192	1/1	0.78	1.03	64,64,64,64	0
55	MG	2A	3193	1/1	0.78	0.10	76,76,76,76	0
55	MG	1a	3076	1/1	0.78	0.22	74,74,74,74	0
55	MG	2A	3736	1/1	0.78	0.12	95,95,95,95	0
55	MG	1A	3548	1/1	0.78	0.26	39,39,39,39	0
55	MG	2A	3248	1/1	0.78	0.05	81,81,81,81	0
55	MG	2A	3252	1/1	0.78	0.21	69,69,69,69	0
55	MG	2A	3771	1/1	0.78	0.13	68,68,68,68	0
55	MG	1A	3725	1/1	0.78	0.54	44,44,44,44	0
55	MG	2A	3543	1/1	0.78	0.39	82,82,82,82	0
55	MG	2A	3108	1/1	0.78	0.29	84,84,84,84	0
55	MG	1A	3196	1/1	0.78	0.24	36,36,36,36	0
55	MG	1A	3457	1/1	0.78	0.10	24,24,24,24	0
55	MG	1A	3173	1/1	0.78	1.04	63,63,63,63	0
55	MG	2B	3005	1/1	0.79	0.10	69,69,69,69	0
55	MG	1A	3630	1/1	0.79	0.21	55,55,55,55	0
55	MG	1V	201	1/1	0.79	0.66	25,25,25,25	0
55	MG	1a	3028	1/1	0.79	0.23	55,55,55,55	0
55	MG	2A	3762	1/1	0.79	0.61	60,60,60,60	0
55	MG	2A	3765	1/1	0.79	0.55	59,59,59,59	0
55	MG	2A	3375	1/1	0.79	0.48	49,49,49,49	0
55	MG	2A	3044	1/1	0.79	0.10	79,79,79,79	0
55	MG	1A	3634	1/1	0.79	0.23	38,38,38,38	0
55	MG	2A	3655	1/1	0.79	0.27	60,60,60,60	0
55	MG	1A	3853	1/1	0.79	0.10	25,25,25,25	0
55	MG	2A	3794	1/1	0.79	0.14	75,75,75,75	0
55	MG	2A	3136	1/1	0.79	0.48	55,55,55,55	0
55	MG	2X	102	1/1	0.79	0.47	82,82,82,82	0
55	MG	2A	3497	1/1	0.79	0.14	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	2A	3431	1/1	0.79	0.32	77,77,77,77	0
55	MG	2A	3438	1/1	0.79	0.09	81,81,81,81	0
55	MG	1A	3189	1/1	0.79	0.32	43,43,43,43	0
55	MG	1h	3001	1/1	0.80	0.67	63,63,63,63	0
55	MG	1A	3433	1/1	0.80	0.32	51,51,51,51	0
55	MG	1A	3098	1/1	0.80	0.37	38,38,38,38	0
55	MG	2A	3487	1/1	0.80	0.38	68,68,68,68	0
55	MG	1A	3134	1/1	0.80	0.23	65,65,65,65	0
55	MG	2A	3290	1/1	0.80	0.18	64,64,64,64	0
55	MG	1A	3533	1/1	0.80	0.15	60,60,60,60	0
55	MG	1A	3459	1/1	0.80	0.34	50,50,50,50	0
55	MG	2A	3677	1/1	0.80	0.19	56,56,56,56	0
55	MG	1A	3167	1/1	0.80	0.30	52,52,52,52	0
55	MG	1A	3896	1/1	0.80	0.60	37,37,37,37	0
55	MG	2A	3520	1/1	0.80	0.60	65,65,65,65	0
55	MG	1A	3253	1/1	0.80	0.24	53,53,53,53	0
55	MG	1A	3745	1/1	0.80	0.07	54,54,54,54	0
55	MG	1A	3758	1/1	0.80	0.63	53,53,53,53	0
55	MG	1A	3760	1/1	0.80	0.27	65,65,65,65	0
55	MG	2R	202	1/1	0.80	0.37	74,74,74,74	0
55	MG	2S	201	1/1	0.80	0.37	67,67,67,67	0
55	MG	2A	3555	1/1	0.80	0.53	52,52,52,52	0
55	MG	2A	3161	1/1	0.80	0.61	54,54,54,54	0
55	MG	1A	3190	1/1	0.80	0.12	72,72,72,72	0
55	MG	1A	3041	1/1	0.80	0.37	62,62,62,62	0
55	MG	1A	3835	1/1	0.80	0.07	48,48,48,48	0
55	MG	1a	3186	1/1	0.80	0.08	69,69,69,69	0
55	MG	2A	3779	1/1	0.80	0.08	72,72,72,72	0
55	MG	2a	1629	1/1	0.80	0.15	90,90,90,90	0
55	MG	1A	3574	1/1	0.80	0.29	64,64,64,64	0
55	MG	1A	3106	1/1	0.80	0.43	42,42,42,42	0
55	MG	2h	8001	1/1	0.80	0.29	77,77,77,77	0
55	MG	2l	201	1/1	0.80	0.15	79,79,79,79	0
55	MG	1B	3021	1/1	0.80	0.11	66,66,66,66	0
55	MG	2A	3632	1/1	0.80	0.24	97,97,97,97	0
55	MG	2A	3195	1/1	0.81	0.14	55,55,55,55	0
55	MG	1A	3854	1/1	0.81	0.12	72,72,72,72	0
55	MG	1A	3855	1/1	0.81	0.27	48,48,48,48	0
55	MG	2a	1623	1/1	0.81	0.25	78,78,78,78	0
55	MG	1B	3003	1/1	0.81	0.14	64,64,64,64	0
55	MG	1A	3400	1/1	0.81	0.23	63,63,63,63	0
55	MG	2A	3530	1/1	0.81	0.86	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3270	1/1	0.81	0.18	58,58,58,58	0
55	MG	1a	3040	1/1	0.81	0.25	75,75,75,75	0
55	MG	1A	3090	1/1	0.81	0.45	37,37,37,37	0
55	MG	1a	3057	1/1	0.81	0.34	81,81,81,81	0
55	MG	1b	3001	1/1	0.81	0.13	81,81,81,81	0
55	MG	2a	1645	1/1	0.81	0.32	63,63,63,63	0
55	MG	1A	3764	1/1	0.81	0.09	67,67,67,67	0
55	MG	1A	3175	1/1	0.81	0.55	56,56,56,56	0
55	MG	2A	3803	1/1	0.81	0.54	69,69,69,69	0
55	MG	2A	3804	1/1	0.81	0.20	35,35,35,35	0
55	MG	2A	3377	1/1	0.81	0.10	94,94,94,94	0
55	MG	2a	1670	1/1	0.81	0.12	84,84,84,84	0
55	MG	2A	3114	1/1	0.81	0.30	62,62,62,62	0
55	MG	2A	3117	1/1	0.81	0.25	58,58,58,58	0
55	MG	1F	303	1/1	0.81	0.63	43,43,43,43	0
55	MG	2a	1699	1/1	0.81	0.12	74,74,74,74	0
55	MG	1o	3001	1/1	0.81	0.26	52,52,52,52	0
55	MG	2A	3631	1/1	0.81	0.32	86,86,86,86	0
55	MG	1A	3794	1/1	0.81	0.22	59,59,59,59	0
55	MG	2A	3636	1/1	0.81	0.08	73,73,73,73	0
55	MG	1A	3164	1/1	0.81	0.31	59,59,59,59	0
55	MG	2B	3016	1/1	0.81	0.15	90,90,90,90	0
55	MG	2B	3018	1/1	0.81	0.39	92,92,92,92	0
55	MG	1A	3116	1/1	0.81	0.12	74,74,74,74	0
55	MG	1A	3315	1/1	0.81	0.28	45,45,45,45	0
55	MG	2a	1736	1/1	0.81	0.34	78,78,78,78	0
55	MG	2E	303	1/1	0.81	1.03	71,71,71,71	0
55	MG	2A	3022	1/1	0.81	0.14	68,68,68,68	0
55	MG	1W	3003	1/1	0.81	0.47	41,41,41,41	0
55	MG	2a	1766	1/1	0.81	0.10	91,91,91,91	0
55	MG	15	101	1/1	0.81	0.25	42,42,42,42	0
55	MG	1A	3901	1/1	0.81	0.16	42,42,42,42	0
55	MG	1a	3139	1/1	0.81	0.19	69,69,69,69	0
55	MG	1A	3840	1/1	0.81	0.29	61,61,61,61	0
55	MG	2A	3059	1/1	0.81	0.56	64,64,64,64	0
55	MG	1A	3032	1/1	0.81	0.29	45,45,45,45	0
55	MG	2g	3001	1/1	0.81	0.18	72,72,72,72	0
55	MG	2A	3707	1/1	0.81	0.46	75,75,75,75	0
55	MG	20	101	1/1	0.81	0.43	64,64,64,64	0
55	MG	2A	3072	1/1	0.81	0.33	57,57,57,57	0
55	MG	1A	3202	1/1	0.81	0.24	63,63,63,63	0
55	MG	1A	3838	1/1	0.82	0.47	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3839	1/1	0.82	0.15	59,59,59,59	0
55	MG	2A	3151	1/1	0.82	1.44	62,62,62,62	0
55	MG	1A	3660	1/1	0.82	0.36	56,56,56,56	0
55	MG	1D	308	1/1	0.82	0.09	58,58,58,58	0
55	MG	1A	3675	1/1	0.82	0.57	47,47,47,47	0
55	MG	1F	302	1/1	0.82	0.22	35,35,35,35	0
55	MG	2a	1641	1/1	0.82	0.23	77,77,77,77	0
55	MG	2A	3027	1/1	0.82	0.26	70,70,70,70	0
55	MG	1a	3077	1/1	0.82	0.44	81,81,81,81	0
55	MG	2A	3180	1/1	0.82	0.23	63,63,63,63	0
55	MG	2A	3034	1/1	0.82	0.20	54,54,54,54	0
55	MG	1A	3678	1/1	0.82	0.38	37,37,37,37	0
55	MG	1A	3248	1/1	0.82	0.41	51,51,51,51	0
55	MG	1A	3600	1/1	0.82	0.09	67,67,67,67	0
55	MG	1A	3703	1/1	0.82	0.50	30,30,30,30	0
55	MG	2A	3805	1/1	0.82	0.14	74,74,74,74	0
55	MG	2A	3201	1/1	0.82	0.23	48,48,48,48	0
55	MG	2A	3062	1/1	0.82	0.79	47,47,47,47	0
55	MG	2A	3815	1/1	0.82	0.46	67,67,67,67	0
55	MG	1A	3199	1/1	0.82	0.46	34,34,34,34	0
55	MG	2A	3068	1/1	0.82	0.33	56,56,56,56	0
55	MG	2A	3256	1/1	0.82	0.11	84,84,84,84	0
55	MG	1A	3404	1/1	0.82	0.09	60,60,60,60	0
55	MG	11	103	1/1	0.82	0.19	50,50,50,50	0
55	MG	1A	3610	1/1	0.82	0.20	70,70,70,70	0
55	MG	2A	3088	1/1	0.82	0.07	81,81,81,81	0
55	MG	1a	3160	1/1	0.82	0.25	84,84,84,84	0
55	MG	1A	3120	1/1	0.82	0.61	34,34,34,34	0
55	MG	1A	3753	1/1	0.82	0.17	67,67,67,67	0
55	MG	1A	3278	1/1	0.82	0.32	37,37,37,37	0
55	MG	1A	3569	1/1	0.82	0.16	43,43,43,43	0
55	MG	1a	3185	1/1	0.82	0.17	68,68,68,68	0
55	MG	1A	3573	1/1	0.82	0.68	37,37,37,37	0
55	MG	1a	3199	1/1	0.82	0.07	68,68,68,68	0
55	MG	2a	1754	1/1	0.82	0.17	85,85,85,85	0
55	MG	1A	3631	1/1	0.82	0.18	59,59,59,59	0
55	MG	1A	3517	1/1	0.82	0.20	68,68,68,68	0
55	MG	1A	3806	1/1	0.82	0.12	65,65,65,65	0
55	MG	1A	3221	1/1	0.82	0.15	56,56,56,56	0
55	MG	2a	1774	1/1	0.82	0.10	91,91,91,91	0
55	MG	2A	3675	1/1	0.82	0.16	70,70,70,70	0
55	MG	1a	3041	1/1	0.82	0.18	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	1A	3324	1/1	0.82	0.14	40,40,40,40	0
55	MG	2A	3456	1/1	0.82	0.36	70,70,70,70	0
55	MG	27	104	1/1	0.82	0.18	67,67,67,67	0
55	MG	2A	3462	1/1	0.82	0.19	62,62,62,62	0
55	MG	1A	3147	1/1	0.82	0.19	40,40,40,40	0
55	MG	2A	3140	1/1	0.82	0.33	61,61,61,61	0
55	MG	18	3302	1/1	0.83	0.54	40,40,40,40	0
55	MG	2A	3273	1/1	0.83	0.11	60,60,60,60	0
55	MG	1a	3001	1/1	0.83	0.05	76,76,76,76	0
55	MG	2A	3535	1/1	0.83	0.27	86,86,86,86	0
55	MG	2A	3304	1/1	0.83	0.09	48,48,48,48	0
55	MG	1B	3019	1/1	0.83	0.15	60,60,60,60	0
55	MG	2A	3784	1/1	0.83	0.14	94,94,94,94	0
55	MG	1a	3143	1/1	0.83	0.10	87,87,87,87	0
55	MG	1A	3111	1/1	0.83	0.41	42,42,42,42	0
55	MG	2A	3132	1/1	0.83	0.39	63,63,63,63	0
55	MG	1a	3012	1/1	0.83	0.15	68,68,68,68	0
55	MG	2A	3579	1/1	0.83	0.28	75,75,75,75	0
55	MG	1A	3464	1/1	0.83	0.64	35,35,35,35	0
55	MG	1D	315	1/1	0.83	0.35	68,68,68,68	0
55	MG	2A	3141	1/1	0.83	0.57	51,51,51,51	0
55	MG	2A	3610	1/1	0.83	0.11	81,81,81,81	0
55	MG	2A	3612	1/1	0.83	0.16	38,38,38,38	0
55	MG	1A	3490	1/1	0.83	0.18	62,62,62,62	0
55	MG	2B	3004	1/1	0.83	0.18	76,76,76,76	0
55	MG	2a	1697	1/1	0.83	0.08	80,80,80,80	0
55	MG	1A	3321	1/1	0.83	0.16	55,55,55,55	0
55	MG	1a	3169	1/1	0.83	0.37	95,95,95,95	0
55	MG	1a	3170	1/1	0.83	0.27	82,82,82,82	0
55	MG	1A	3676	1/1	0.83	0.22	70,70,70,70	0
55	MG	1a	3181	1/1	0.83	0.08	74,74,74,74	0
55	MG	1A	3089	1/1	0.83	0.37	37,37,37,37	0
55	MG	1A	3066	1/1	0.83	0.61	45,45,45,45	0
55	MG	2A	3457	1/1	0.83	0.34	90,90,90,90	0
55	MG	2A	3646	1/1	0.83	0.38	53,53,53,53	0
55	MG	1A	3695	1/1	0.83	0.30	60,60,60,60	0
55	MG	2A	3078	1/1	0.83	0.61	51,51,51,51	0
55	MG	1A	3004	1/1	0.83	0.27	41,41,41,41	0
55	MG	2A	3477	1/1	0.83	0.29	68,68,68,68	0
55	MG	1A	3608	1/1	0.83	0.23	74,74,74,74	0
55	MG	10	104	1/1	0.83	0.11	50,50,50,50	0
55	MG	11	101	1/1	0.83	1.57	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3094	1/1	0.83	0.82	59,59,59,59	0
55	MG	1A	3869	1/1	0.83	0.18	39,39,39,39	0
55	MG	2A	3224	1/1	0.83	0.17	69,69,69,69	0
55	MG	1d	504	1/1	0.83	0.27	75,75,75,75	0
55	MG	27	102	1/1	0.83	0.78	49,49,49,49	0
55	MG	1A	3875	1/1	0.83	0.26	44,44,44,44	0
55	MG	2d	505	1/1	0.83	0.38	101,101,101,101	0
55	MG	15	102	1/1	0.83	0.91	43,43,43,43	0
55	MG	2A	3747	1/1	0.83	0.08	75,75,75,75	0
55	MG	1A	3713	1/1	0.83	0.20	98,98,98,98	0
55	MG	2A	3754	1/1	0.83	0.24	101,101,101,101	0
55	MG	2A	3756	1/1	0.83	1.03	95,95,95,95	0
55	MG	1A	3722	1/1	0.83	0.14	62,62,62,62	0
55	MG	1a	3029	1/1	0.84	0.09	55,55,55,55	0
55	MG	1F	311	1/1	0.84	0.40	25,25,25,25	0
55	MG	1A	3135	1/1	0.84	0.20	37,37,37,37	0
55	MG	1a	3039	1/1	0.84	0.38	62,62,62,62	0
55	MG	1A	3570	1/1	0.84	0.28	48,48,48,48	0
55	MG	2A	3065	1/1	0.84	0.14	56,56,56,56	0
55	MG	2A	3469	1/1	0.84	0.13	68,68,68,68	0
55	MG	1A	3911	1/1	0.84	0.29	39,39,39,39	0
55	MG	2A	3175	1/1	0.84	0.99	69,69,69,69	0
55	MG	2a	1620	1/1	0.84	0.26	77,77,77,77	0
55	MG	1a	3047	1/1	0.84	0.20	68,68,68,68	0
55	MG	2A	3720	1/1	0.84	0.28	58,58,58,58	0
55	MG	1R	204	1/1	0.84	0.24	53,53,53,53	0
55	MG	1A	3150	1/1	0.84	0.15	39,39,39,39	0
55	MG	2A	3746	1/1	0.84	0.18	69,69,69,69	0
55	MG	2A	3482	1/1	0.84	0.39	54,54,54,54	0
55	MG	1a	3194	1/1	0.84	0.10	83,83,83,83	0
55	MG	2A	3486	1/1	0.84	1.38	57,57,57,57	0
55	MG	2A	3086	1/1	0.84	0.30	56,56,56,56	0
55	MG	1A	3227	1/1	0.84	0.41	34,34,34,34	0
55	MG	10	101	1/1	0.84	0.66	52,52,52,52	0
55	MG	2A	3211	1/1	0.84	0.14	45,45,45,45	0
55	MG	2A	3221	1/1	0.84	0.25	52,52,52,52	0
55	MG	1a	3216	1/1	0.84	0.07	100,100,100,100	0
55	MG	2A	3228	1/1	0.84	0.21	51,51,51,51	0
55	MG	2A	3244	1/1	0.84	0.54	53,53,53,53	0
55	MG	1A	3783	1/1	0.84	0.10	55,55,55,55	0
55	MG	2A	3523	1/1	0.84	0.25	61,61,61,61	0
55	MG	1a	3222	1/1	0.84	0.44	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3250	1/1	0.84	0.09	31,31,31,31	0
55	MG	1A	3180	1/1	0.84	0.37	48,48,48,48	0
55	MG	2A	3539	1/1	0.84	0.09	74,74,74,74	0
55	MG	2A	3542	1/1	0.84	0.16	88,88,88,88	0
55	MG	1A	3151	1/1	0.84	0.17	46,46,46,46	0
55	MG	2A	3812	1/1	0.84	0.23	60,60,60,60	0
55	MG	1A	3876	1/1	0.84	0.05	64,64,64,64	0
55	MG	1A	3011	1/1	0.84	0.36	41,41,41,41	0
55	MG	1A	3885	1/1	0.84	0.23	37,37,37,37	0
55	MG	1A	3184	1/1	0.84	0.48	37,37,37,37	0
55	MG	2A	3299	1/1	0.84	0.21	75,75,75,75	0
55	MG	1D	302	1/1	0.84	0.81	35,35,35,35	0
55	MG	2A	3305	1/1	0.84	0.07	84,84,84,84	0
55	MG	1A	3074	1/1	0.84	0.68	29,29,29,29	0
55	MG	2A	3590	1/1	0.84	0.47	65,65,65,65	0
55	MG	2B	3014	1/1	0.84	0.12	76,76,76,76	0
55	MG	1D	313	1/1	0.84	0.20	51,51,51,51	0
55	MG	1A	3205	1/1	0.84	0.51	44,44,44,44	0
55	MG	2A	3338	1/1	0.84	0.71	70,70,70,70	0
55	MG	1A	3658	1/1	0.84	0.50	38,38,38,38	0
55	MG	2A	3134	1/1	0.84	0.82	70,70,70,70	0
55	MG	1a	3148	1/1	0.84	0.13	82,82,82,82	0
55	MG	2a	1776	1/1	0.84	0.10	80,80,80,80	0
55	MG	1a	3017	1/1	0.84	0.31	65,65,65,65	0
55	MG	2A	3389	1/1	0.84	0.17	46,46,46,46	0
55	MG	1A	3092	1/1	0.84	0.28	37,37,37,37	0
55	MG	2A	3415	1/1	0.84	0.07	80,80,80,80	0
55	MG	1a	3152	1/1	0.84	0.16	91,91,91,91	0
55	MG	1A	3605	1/1	0.84	0.54	38,38,38,38	0
55	MG	2A	3146	1/1	0.84	0.62	53,53,53,53	0
55	MG	2A	3046	1/1	0.84	0.16	51,51,51,51	0
55	MG	2V	201	1/1	0.84	0.78	55,55,55,55	0
55	MG	2A	3054	1/1	0.85	0.63	51,51,51,51	0
55	MG	2A	3055	1/1	0.85	0.32	49,49,49,49	0
55	MG	1P	204	1/1	0.85	0.12	35,35,35,35	0
55	MG	2A	3152	1/1	0.85	0.44	59,59,59,59	0
55	MG	1A	3219	1/1	0.85	0.19	49,49,49,49	0
55	MG	1A	3668	1/1	0.85	0.08	85,85,85,85	0
55	MG	2A	3159	1/1	0.85	0.77	58,58,58,58	0
55	MG	1A	3856	1/1	0.85	0.32	46,46,46,46	0
55	MG	2A	3420	1/1	0.85	0.09	60,60,60,60	0
55	MG	1A	3859	1/1	0.85	0.34	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	1A	3072	1/1	0.85	0.17	43,43,43,43	0
55	MG	2A	3165	1/1	0.85	0.29	58,58,58,58	0
55	MG	1A	3398	1/1	0.85	0.24	37,37,37,37	0
55	MG	1A	3079	1/1	0.85	0.22	40,40,40,40	0
55	MG	1A	3681	1/1	0.85	0.07	38,38,38,38	0
55	MG	2a	1654	1/1	0.85	0.55	70,70,70,70	0
55	MG	1A	3101	1/1	0.85	0.68	63,63,63,63	0
55	MG	2A	3081	1/1	0.85	0.16	46,46,46,46	0
55	MG	1a	3075	1/1	0.85	0.18	48,48,48,48	0
55	MG	2a	1682	1/1	0.85	0.45	88,88,88,88	0
55	MG	2a	1683	1/1	0.85	0.16	67,67,67,67	0
55	MG	1B	3023	1/1	0.85	0.18	63,63,63,63	0
55	MG	2A	3463	1/1	0.85	0.33	76,76,76,76	0
55	MG	2A	3464	1/1	0.85	0.32	90,90,90,90	0
55	MG	1A	3262	1/1	0.85	0.20	84,84,84,84	0
55	MG	2a	1708	1/1	0.85	0.11	83,83,83,83	0
55	MG	17	105	1/1	0.85	0.25	52,52,52,52	0
55	MG	1D	307	1/1	0.85	0.74	44,44,44,44	0
55	MG	2A	3647	1/1	0.85	0.23	88,88,88,88	0
55	MG	1e	3002	1/1	0.85	0.50	58,58,58,58	0
55	MG	1A	3267	1/1	0.85	0.12	79,79,79,79	0
55	MG	2A	3661	1/1	0.85	0.07	85,85,85,85	0
55	MG	1a	3124	1/1	0.85	0.31	77,77,77,77	0
55	MG	1A	3815	1/1	0.85	0.58	51,51,51,51	0
55	MG	2F	309	1/1	0.85	0.21	60,60,60,60	0
55	MG	1A	3171	1/1	0.85	0.64	44,44,44,44	0
55	MG	1E	303	1/1	0.85	0.39	39,39,39,39	0
55	MG	2A	3681	1/1	0.85	0.10	71,71,71,71	0
55	MG	2A	3111	1/1	0.85	0.87	52,52,52,52	0
55	MG	1A	3053	1/1	0.85	0.30	58,58,58,58	0
55	MG	1A	3160	1/1	0.85	0.98	40,40,40,40	0
55	MG	1a	3018	1/1	0.85	0.16	64,64,64,64	0
55	MG	1A	3597	1/1	0.85	0.47	38,38,38,38	0
55	MG	1a	3151	1/1	0.85	0.15	76,76,76,76	0
55	MG	2A	3726	1/1	0.85	0.09	41,41,41,41	0
55	MG	2A	3285	1/1	0.85	0.11	47,47,47,47	0
55	MG	2A	3513	1/1	0.85	0.71	47,47,47,47	0
55	MG	2b	3001	1/1	0.85	0.18	85,85,85,85	0
55	MG	2d	503	1/1	0.85	0.43	79,79,79,79	0
55	MG	1F	310	1/1	0.85	0.47	27,27,27,27	0
55	MG	1A	3534	1/1	0.85	0.12	52,52,52,52	0
55	MG	2A	3040	1/1	0.85	0.35	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3465	1/1	0.85	0.24	54,54,54,54	0
55	MG	2a	1606	1/1	0.85	0.64	69,69,69,69	0
55	MG	1H	8001	1/1	0.85	0.11	76,76,76,76	0
55	MG	1A	3161	1/1	0.85	0.42	55,55,55,55	0
55	MG	2A	3050	1/1	0.85	0.42	64,64,64,64	0
55	MG	1A	3188	1/1	0.86	0.46	34,34,34,34	0
55	MG	2a	1602	1/1	0.86	0.51	55,55,55,55	0
55	MG	1a	3154	1/1	0.86	0.11	100,100,100,100	0
55	MG	1A	3377	1/1	0.86	0.06	70,70,70,70	0
55	MG	1A	3168	1/1	0.86	0.34	53,53,53,53	0
55	MG	1B	3009	1/1	0.86	0.26	60,60,60,60	0
55	MG	2a	1621	1/1	0.86	0.29	58,58,58,58	0
55	MG	2A	3525	1/1	0.86	0.07	50,50,50,50	0
55	MG	1A	3693	1/1	0.86	0.07	42,42,42,42	0
55	MG	2A	3328	1/1	0.86	0.27	72,72,72,72	0
55	MG	1B	3017	1/1	0.86	0.08	39,39,39,39	0
55	MG	2a	1633	1/1	0.86	0.28	79,79,79,79	0
55	MG	1a	3173	1/1	0.86	0.24	71,71,71,71	0
55	MG	2A	3148	1/1	0.86	0.32	57,57,57,57	0
55	MG	2A	3149	1/1	0.86	0.26	63,63,63,63	0
55	MG	1A	3485	1/1	0.86	0.21	47,47,47,47	0
55	MG	2A	3056	1/1	0.86	0.16	59,59,59,59	0
55	MG	1a	3180	1/1	0.86	0.21	102,102,102,102	0
55	MG	2A	3782	1/1	0.86	0.15	82,82,82,82	0
55	MG	1A	3883	1/1	0.86	0.08	58,58,58,58	0
55	MG	2a	1647	1/1	0.86	0.14	81,81,81,81	0
55	MG	2a	1648	1/1	0.86	0.13	63,63,63,63	0
55	MG	2A	3564	1/1	0.86	0.89	57,57,57,57	0
55	MG	2A	3394	1/1	0.86	0.18	65,65,65,65	0
55	MG	2A	3799	1/1	0.86	0.30	83,83,83,83	0
55	MG	2A	3060	1/1	0.86	0.80	52,52,52,52	0
55	MG	2A	3802	1/1	0.86	0.28	97,97,97,97	0
55	MG	1A	3169	1/1	0.86	0.20	62,62,62,62	0
55	MG	2A	3585	1/1	0.86	0.17	68,68,68,68	0
55	MG	1B	3024	1/1	0.86	0.12	62,62,62,62	0
55	MG	1A	3831	1/1	0.86	0.42	51,51,51,51	0
55	MG	2A	3596	1/1	0.86	0.13	65,65,65,65	0
55	MG	2a	1692	1/1	0.86	0.29	85,85,85,85	0
55	MG	1a	3065	1/1	0.86	0.31	65,65,65,65	0
55	MG	1a	3197	1/1	0.86	0.15	82,82,82,82	0
55	MG	1a	3069	1/1	0.86	0.20	62,62,62,62	0
55	MG	2A	3614	1/1	0.86	0.06	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2B	3002	1/1	0.86	0.11	78,78,78,78	0
55	MG	1a	3213	1/1	0.86	0.29	64,64,64,64	0
55	MG	2A	3449	1/1	0.86	0.21	84,84,84,84	0
55	MG	1A	3590	1/1	0.86	0.11	48,48,48,48	0
55	MG	1A	3893	1/1	0.86	0.06	103,103,103,103	0
55	MG	1A	3034	1/1	0.86	0.16	57,57,57,57	0
55	MG	1A	3593	1/1	0.86	0.17	34,34,34,34	0
55	MG	1D	318	1/1	0.86	0.18	50,50,50,50	0
55	MG	1A	3206	1/1	0.86	0.39	32,32,32,32	0
55	MG	2A	3465	1/1	0.86	0.20	71,71,71,71	0
55	MG	1a	3003	1/1	0.86	0.17	65,65,65,65	0
55	MG	2A	3095	1/1	0.86	0.17	64,64,64,64	0
55	MG	2A	3475	1/1	0.86	0.13	76,76,76,76	0
55	MG	2a	1752	1/1	0.86	0.09	86,86,86,86	0
55	MG	1E	304	1/1	0.86	0.11	46,46,46,46	0
55	MG	2a	1756	1/1	0.86	0.13	69,69,69,69	0
55	MG	2a	1764	1/1	0.86	0.08	59,59,59,59	0
55	MG	2A	3660	1/1	0.86	0.20	71,71,71,71	0
55	MG	1A	3551	1/1	0.86	0.35	60,60,60,60	0
55	MG	2A	3664	1/1	0.86	0.10	75,75,75,75	0
55	MG	1A	3046	1/1	0.86	0.28	38,38,38,38	0
55	MG	1a	3137	1/1	0.86	0.29	68,68,68,68	0
55	MG	1a	3016	1/1	0.86	0.41	80,80,80,80	0
55	MG	2a	1779	1/1	0.86	0.48	75,75,75,75	0
55	MG	2a	1785	1/1	0.86	0.07	68,68,68,68	0
55	MG	1A	3452	1/1	0.86	0.46	76,76,76,76	0
55	MG	2a	1792	1/1	0.86	0.33	52,52,52,52	0
55	MG	1A	3194	1/1	0.86	0.48	34,34,34,34	0
55	MG	1a	3020	1/1	0.86	0.19	58,58,58,58	0
55	MG	2A	3705	1/1	0.86	0.20	75,75,75,75	0
55	MG	1A	3672	1/1	0.86	0.17	49,49,49,49	0
55	MG	25	101	1/1	0.86	0.45	58,58,58,58	0
55	MG	25	103	1/1	0.86	0.64	62,62,62,62	0
55	MG	1A	3568	1/1	0.86	0.21	63,63,63,63	0
55	MG	2A	3025	1/1	0.86	0.20	38,38,38,38	0
55	MG	2A	3130	1/1	0.86	0.19	58,58,58,58	0
55	MG	1A	3146	1/1	0.86	0.12	54,54,54,54	0
55	MG	1A	3641	1/1	0.87	0.47	35,35,35,35	0
55	MG	2a	1635	1/1	0.87	0.49	77,77,77,77	0
55	MG	1a	3117	1/1	0.87	0.23	61,61,61,61	0
55	MG	2A	3589	1/1	0.87	0.25	82,82,82,82	0
55	MG	1d	502	1/1	0.87	0.10	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3593	1/1	0.87	0.20	68,68,68,68	0
55	MG	1A	3532	1/1	0.87	0.22	69,69,69,69	0
55	MG	2A	3605	1/1	0.87	0.26	63,63,63,63	0
55	MG	2A	3186	1/1	0.87	0.87	61,61,61,61	0
55	MG	2A	3454	1/1	0.87	0.13	81,81,81,81	0
55	MG	1A	3730	1/1	0.87	0.12	65,65,65,65	0
55	MG	1e	3001	1/1	0.87	0.20	55,55,55,55	0
55	MG	2a	1650	1/1	0.87	0.68	55,55,55,55	0
55	MG	1F	306	1/1	0.87	0.24	39,39,39,39	0
55	MG	1A	3057	1/1	0.87	0.07	54,54,54,54	0
55	MG	1A	3172	1/1	0.87	0.37	50,50,50,50	0
55	MG	1a	3140	1/1	0.87	0.20	84,84,84,84	0
55	MG	1F	312	1/1	0.87	0.30	44,44,44,44	0
55	MG	2a	1660	1/1	0.87	0.16	79,79,79,79	0
55	MG	1a	3019	1/1	0.87	0.22	54,54,54,54	0
55	MG	1A	3245	1/1	0.87	0.51	46,46,46,46	0
55	MG	2A	3015	1/1	0.87	0.69	50,50,50,50	0
55	MG	1A	3331	1/1	0.87	0.10	22,22,22,22	0
55	MG	2A	3021	1/1	0.87	0.43	43,43,43,43	0
55	MG	1a	3026	1/1	0.87	0.24	58,58,58,58	0
55	MG	1N	8003	1/1	0.87	0.18	69,69,69,69	0
55	MG	2B	3017	1/1	0.87	0.13	84,84,84,84	0
55	MG	1P	201	1/1	0.87	0.98	30,30,30,30	0
55	MG	1A	3549	1/1	0.87	0.33	31,31,31,31	0
55	MG	2D	303	1/1	0.87	0.57	50,50,50,50	0
55	MG	2a	1711	1/1	0.87	0.74	80,80,80,80	0
55	MG	2A	3268	1/1	0.87	0.15	69,69,69,69	0
55	MG	2a	1718	1/1	0.87	0.13	88,88,88,88	0
55	MG	2D	308	1/1	0.87	0.53	55,55,55,55	0
55	MG	1a	3159	1/1	0.87	0.12	65,65,65,65	0
55	MG	2F	306	1/1	0.87	0.54	43,43,43,43	0
55	MG	1A	3670	1/1	0.87	0.24	53,53,53,53	0
55	MG	2A	3039	1/1	0.87	0.80	60,60,60,60	0
55	MG	2A	3135	1/1	0.87	0.94	71,71,71,71	0
55	MG	1B	3013	1/1	0.87	0.12	58,58,58,58	0
55	MG	2A	3509	1/1	0.87	1.02	53,53,53,53	0
55	MG	1A	3761	1/1	0.87	0.13	64,64,64,64	0
55	MG	1A	3212	1/1	0.87	0.41	43,43,43,43	0
55	MG	1A	3767	1/1	0.87	0.06	51,51,51,51	0
55	MG	1A	3247	1/1	0.87	0.11	86,86,86,86	0
55	MG	1A	3087	1/1	0.87	0.77	33,33,33,33	0
55	MG	2X	101	1/1	0.87	0.20	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3174	1/1	0.87	0.16	44,44,44,44	0
55	MG	2A	3337	1/1	0.87	0.13	79,79,79,79	0
55	MG	20	104	1/1	0.87	0.24	81,81,81,81	0
55	MG	20	106	1/1	0.87	0.48	78,78,78,78	0
55	MG	1A	3255	1/1	0.87	0.17	34,34,34,34	0
55	MG	1A	3201	1/1	0.87	0.34	41,41,41,41	0
55	MG	2A	3534	1/1	0.87	0.67	80,80,80,80	0
55	MG	2A	3357	1/1	0.87	0.14	50,50,50,50	0
55	MG	2A	3538	1/1	0.87	0.59	62,62,62,62	0
55	MG	1A	3156	1/1	0.87	0.78	54,54,54,54	0
55	MG	1A	3443	1/1	0.87	0.14	22,22,22,22	0
55	MG	2A	3380	1/1	0.87	0.20	81,81,81,81	0
55	MG	2A	3547	1/1	0.87	0.16	41,41,41,41	0
55	MG	15	107	1/1	0.87	0.13	52,52,52,52	0
55	MG	1A	3834	1/1	0.87	0.11	61,61,61,61	0
55	MG	2e	3001	1/1	0.87	0.28	67,67,67,67	0
55	MG	2A	3158	1/1	0.87	0.30	72,72,72,72	0
55	MG	2f	8001	1/1	0.87	0.17	56,56,56,56	0
55	MG	1A	3009	1/1	0.87	0.24	28,28,28,28	0
55	MG	1A	3455	1/1	0.87	0.10	49,49,49,49	0
55	MG	19	101	1/1	0.87	0.31	41,41,41,41	0
55	MG	1a	3078	1/1	0.87	0.66	78,78,78,78	0
55	MG	1A	3149	1/1	0.87	0.68	43,43,43,43	0
55	MG	2o	3001	1/1	0.87	0.18	60,60,60,60	0
55	MG	2A	3032	1/1	0.88	0.63	66,66,66,66	0
55	MG	2A	3432	1/1	0.88	0.21	74,74,74,74	0
55	MG	1A	3759	1/1	0.88	0.24	61,61,61,61	0
55	MG	1A	3026	1/1	0.88	0.14	63,63,63,63	0
55	MG	1A	3577	1/1	0.88	0.74	40,40,40,40	0
55	MG	2A	3446	1/1	0.88	0.30	62,62,62,62	0
55	MG	2A	3652	1/1	0.88	0.63	53,53,53,53	0
55	MG	2A	3653	1/1	0.88	0.23	77,77,77,77	0
55	MG	1F	305	1/1	0.88	0.25	29,29,29,29	0
55	MG	1A	3021	1/1	0.88	0.16	42,42,42,42	0
55	MG	1a	3153	1/1	0.88	0.14	57,57,57,57	0
55	MG	1F	307	1/1	0.88	0.76	29,29,29,29	0
55	MG	1a	3024	1/1	0.88	0.21	57,57,57,57	0
55	MG	2a	1603	1/1	0.88	0.24	69,69,69,69	0
55	MG	2A	3459	1/1	0.88	0.31	71,71,71,71	0
55	MG	2a	1607	1/1	0.88	0.25	52,52,52,52	0
55	MG	1A	3579	1/1	0.88	0.14	64,64,64,64	0
55	MG	2A	3171	1/1	0.88	0.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2a	1615	1/1	0.88	0.16	47,47,47,47	0
55	MG	1A	3771	1/1	0.88	0.06	71,71,71,71	0
55	MG	1A	3781	1/1	0.88	0.63	28,28,28,28	0
55	MG	2A	3704	1/1	0.88	0.06	62,62,62,62	0
55	MG	2A	3468	1/1	0.88	0.11	80,80,80,80	0
55	MG	2A	3176	1/1	0.88	0.46	51,51,51,51	0
55	MG	1A	3581	1/1	0.88	0.53	35,35,35,35	0
55	MG	1A	3787	1/1	0.88	0.16	59,59,59,59	0
55	MG	1A	3136	1/1	0.88	0.10	68,68,68,68	0
55	MG	1a	3175	1/1	0.88	0.14	85,85,85,85	0
55	MG	2A	3721	1/1	0.88	0.26	42,42,42,42	0
55	MG	1A	3063	1/1	0.88	0.23	49,49,49,49	0
55	MG	2A	3727	1/1	0.88	0.51	65,65,65,65	0
55	MG	1A	3804	1/1	0.88	0.08	87,87,87,87	0
55	MG	2A	3071	1/1	0.88	0.57	62,62,62,62	0
55	MG	1A	3523	1/1	0.88	0.20	56,56,56,56	0
55	MG	1a	3183	1/1	0.88	0.18	84,84,84,84	0
55	MG	2A	3748	1/1	0.88	0.14	68,68,68,68	0
55	MG	2A	3215	1/1	0.88	0.24	80,80,80,80	0
55	MG	2a	1649	1/1	0.88	0.23	83,83,83,83	0
55	MG	1A	3524	1/1	0.88	0.17	52,52,52,52	0
55	MG	2A	3222	1/1	0.88	0.41	62,62,62,62	0
55	MG	1a	3052	1/1	0.88	0.22	51,51,51,51	0
55	MG	2A	3506	1/1	0.88	0.47	47,47,47,47	0
55	MG	2A	3225	1/1	0.88	0.09	51,51,51,51	0
55	MG	1a	3053	1/1	0.88	0.24	82,82,82,82	0
55	MG	2A	3240	1/1	0.88	0.16	34,34,34,34	0
55	MG	2A	3776	1/1	0.88	0.15	43,43,43,43	0
55	MG	1a	3056	1/1	0.88	0.10	69,69,69,69	0
55	MG	1A	3163	1/1	0.88	0.20	65,65,65,65	0
55	MG	1S	201	1/1	0.88	0.39	55,55,55,55	0
55	MG	1a	3208	1/1	0.88	0.23	75,75,75,75	0
55	MG	1U	207	1/1	0.88	0.23	47,47,47,47	0
55	MG	1A	3825	1/1	0.88	0.09	68,68,68,68	0
55	MG	2A	3796	1/1	0.88	0.68	67,67,67,67	0
55	MG	1A	3048	1/1	0.88	0.70	33,33,33,33	0
55	MG	2A	3258	1/1	0.88	0.08	59,59,59,59	0
55	MG	1a	3217	1/1	0.88	0.13	87,87,87,87	0
55	MG	2A	3102	1/1	0.88	0.40	56,56,56,56	0
55	MG	2a	1716	1/1	0.88	0.16	73,73,73,73	0
55	MG	1a	3067	1/1	0.88	0.14	65,65,65,65	0
55	MG	1A	3281	1/1	0.88	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3541	1/1	0.88	0.07	78,78,78,78	0
55	MG	2A	3810	1/1	0.88	0.32	51,51,51,51	0
55	MG	1A	3293	1/1	0.88	0.09	75,75,75,75	0
55	MG	1A	3313	1/1	0.88	0.20	55,55,55,55	0
55	MG	2A	3302	1/1	0.88	0.15	44,44,44,44	0
55	MG	1A	3200	1/1	0.88	0.91	37,37,37,37	0
55	MG	1A	3182	1/1	0.88	0.83	46,46,46,46	0
55	MG	2A	3822	1/1	0.88	0.31	53,53,53,53	0
55	MG	1A	3709	1/1	0.88	0.18	49,49,49,49	0
55	MG	2A	3319	1/1	0.88	0.06	78,78,78,78	0
55	MG	2a	1745	1/1	0.88	0.28	67,67,67,67	0
55	MG	1A	3478	1/1	0.88	0.16	44,44,44,44	0
55	MG	2B	3007	1/1	0.88	0.12	81,81,81,81	0
55	MG	1a	3092	1/1	0.88	0.07	85,85,85,85	0
55	MG	1A	3239	1/1	0.88	0.24	35,35,35,35	0
55	MG	2a	1758	1/1	0.88	0.24	70,70,70,70	0
55	MG	2a	1759	1/1	0.88	0.15	72,72,72,72	0
55	MG	1A	3097	1/1	0.88	0.52	48,48,48,48	0
55	MG	2A	3583	1/1	0.88	0.23	72,72,72,72	0
55	MG	2A	3001	1/1	0.88	0.18	55,55,55,55	0
55	MG	1A	3555	1/1	0.88	0.10	61,61,61,61	0
55	MG	2A	3587	1/1	0.88	0.08	68,68,68,68	0
55	MG	2a	1773	1/1	0.88	0.25	89,89,89,89	0
55	MG	2A	3348	1/1	0.88	0.10	76,76,76,76	0
55	MG	1A	3731	1/1	0.88	0.12	72,72,72,72	0
55	MG	2a	1777	1/1	0.88	0.11	77,77,77,77	0
55	MG	1A	3070	1/1	0.88	0.49	32,32,32,32	0
55	MG	1A	3038	1/1	0.88	0.50	66,66,66,66	0
55	MG	1a	3134	1/1	0.88	0.26	78,78,78,78	0
55	MG	2A	3381	1/1	0.88	0.08	77,77,77,77	0
55	MG	2F	304	1/1	0.88	0.58	49,49,49,49	0
55	MG	1A	3128	1/1	0.88	0.16	31,31,31,31	0
55	MG	1A	3088	1/1	0.88	0.64	30,30,30,30	0
55	MG	2A	3144	1/1	0.88	0.14	73,73,73,73	0
55	MG	2A	3625	1/1	0.88	0.09	74,74,74,74	0
55	MG	1A	3757	1/1	0.88	0.20	37,37,37,37	0
55	MG	2A	3147	1/1	0.88	0.11	78,78,78,78	0
55	MG	1a	3006	1/1	0.88	0.48	74,74,74,74	0
55	MG	2A	3421	1/1	0.88	0.30	58,58,58,58	0
55	MG	2A	3634	1/1	0.88	0.18	83,83,83,83	0
55	MG	1A	3507	1/1	0.88	0.28	48,48,48,48	0
55	MG	2U	201	1/1	0.88	0.46	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	1a	3146	1/1	0.88	0.07	80,80,80,80	0
55	MG	1A	3287	1/1	0.89	0.23	45,45,45,45	0
55	MG	2A	3686	1/1	0.89	0.08	95,95,95,95	0
55	MG	2A	3692	1/1	0.89	0.07	54,54,54,54	0
55	MG	1A	3625	1/1	0.89	0.46	35,35,35,35	0
55	MG	1A	3877	1/1	0.89	0.20	63,63,63,63	0
55	MG	2A	3218	1/1	0.89	0.07	52,52,52,52	0
55	MG	2A	3479	1/1	0.89	0.22	40,40,40,40	0
55	MG	2A	3716	1/1	0.89	0.15	92,92,92,92	0
55	MG	1A	3747	1/1	0.89	0.07	45,45,45,45	0
55	MG	1a	3055	1/1	0.89	0.58	47,47,47,47	0
55	MG	1a	3191	1/1	0.89	0.13	47,47,47,47	0
55	MG	1A	3093	1/1	0.89	0.33	43,43,43,43	0
55	MG	1A	3756	1/1	0.89	0.19	40,40,40,40	0
55	MG	2A	3089	1/1	0.89	0.10	56,56,56,56	0
55	MG	2A	3731	1/1	0.89	0.16	70,70,70,70	0
55	MG	2A	3732	1/1	0.89	0.74	61,61,61,61	0
55	MG	2A	3241	1/1	0.89	0.16	49,49,49,49	0
55	MG	2a	1632	1/1	0.89	0.23	75,75,75,75	0
55	MG	1A	3887	1/1	0.89	0.28	44,44,44,44	0
55	MG	2A	3504	1/1	0.89	0.21	55,55,55,55	0
55	MG	1A	3301	1/1	0.89	0.21	41,41,41,41	0
55	MG	1A	3302	1/1	0.89	0.10	42,42,42,42	0
55	MG	2A	3751	1/1	0.89	0.18	67,67,67,67	0
55	MG	1A	3640	1/1	0.89	0.40	34,34,34,34	0
55	MG	2A	3753	1/1	0.89	0.15	71,71,71,71	0
55	MG	1A	3484	1/1	0.89	0.12	47,47,47,47	0
55	MG	1A	3642	1/1	0.89	0.54	36,36,36,36	0
55	MG	2A	3761	1/1	0.89	0.12	38,38,38,38	0
55	MG	1a	3071	1/1	0.89	0.17	53,53,53,53	0
55	MG	1A	3646	1/1	0.89	0.20	31,31,31,31	0
55	MG	2A	3259	1/1	0.89	0.12	34,34,34,34	0
55	MG	1A	3126	1/1	0.89	0.16	34,34,34,34	0
55	MG	2A	3106	1/1	0.89	0.53	60,60,60,60	0
55	MG	1A	3060	1/1	0.89	0.12	36,36,36,36	0
55	MG	1A	3317	1/1	0.89	0.12	73,73,73,73	0
55	MG	1A	3178	1/1	0.89	0.29	39,39,39,39	0
55	MG	1A	3179	1/1	0.89	0.60	38,38,38,38	0
55	MG	2a	1658	1/1	0.89	0.08	74,74,74,74	0
55	MG	1A	3788	1/1	0.89	0.07	48,48,48,48	0
55	MG	2a	1666	1/1	0.89	0.20	79,79,79,79	0
55	MG	2A	3790	1/1	0.89	0.05	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3115	1/1	0.89	0.17	66,66,66,66	0
55	MG	2a	1677	1/1	0.89	0.22	71,71,71,71	0
55	MG	1a	3107	1/1	0.89	0.18	67,67,67,67	0
55	MG	2A	3128	1/1	0.89	0.11	61,61,61,61	0
55	MG	2A	3798	1/1	0.89	0.19	93,93,93,93	0
55	MG	1A	3662	1/1	0.89	0.09	52,52,52,52	0
55	MG	1A	3130	1/1	0.89	0.25	33,33,33,33	0
55	MG	2a	1696	1/1	0.89	0.09	77,77,77,77	0
55	MG	1A	3359	1/1	0.89	0.10	64,64,64,64	0
55	MG	1A	3145	1/1	0.89	0.39	29,29,29,29	0
55	MG	2A	3331	1/1	0.89	0.10	61,61,61,61	0
55	MG	1B	3007	1/1	0.89	0.13	51,51,51,51	0
55	MG	1a	3129	1/1	0.89	0.08	66,66,66,66	0
55	MG	1A	3807	1/1	0.89	0.26	48,48,48,48	0
55	MG	2A	3345	1/1	0.89	0.20	81,81,81,81	0
55	MG	1B	3012	1/1	0.89	0.07	44,44,44,44	0
55	MG	2A	3020	1/1	0.89	0.10	42,42,42,42	0
55	MG	1A	3580	1/1	0.89	0.14	61,61,61,61	0
55	MG	1A	3812	1/1	0.89	0.11	28,28,28,28	0
55	MG	1A	3514	1/1	0.89	0.12	35,35,35,35	0
55	MG	1A	3214	1/1	0.89	0.21	40,40,40,40	0
55	MG	1A	3216	1/1	0.89	0.24	52,52,52,52	0
55	MG	1a	3145	1/1	0.89	0.24	77,77,77,77	0
55	MG	1A	3254	1/1	0.89	0.33	50,50,50,50	0
55	MG	2A	3602	1/1	0.89	0.06	73,73,73,73	0
55	MG	1A	3690	1/1	0.89	0.11	67,67,67,67	0
55	MG	2A	3403	1/1	0.89	0.26	79,79,79,79	0
55	MG	2A	3035	1/1	0.89	0.42	32,32,32,32	0
55	MG	2A	3038	1/1	0.89	0.11	49,49,49,49	0
55	MG	1A	3195	1/1	0.89	0.34	46,46,46,46	0
55	MG	2A	3621	1/1	0.89	0.51	54,54,54,54	0
55	MG	2A	3622	1/1	0.89	0.35	49,49,49,49	0
55	MG	1D	304	1/1	0.89	0.37	37,37,37,37	0
55	MG	1A	3157	1/1	0.89	0.16	57,57,57,57	0
55	MG	2A	3045	1/1	0.89	0.25	46,46,46,46	0
55	MG	1A	3408	1/1	0.89	0.20	43,43,43,43	0
55	MG	2A	3435	1/1	0.89	0.28	76,76,76,76	0
55	MG	1A	3530	1/1	0.89	0.13	44,44,44,44	0
55	MG	1A	3847	1/1	0.89	0.12	58,58,58,58	0
55	MG	2A	3442	1/1	0.89	0.23	81,81,81,81	0
55	MG	2A	3053	1/1	0.89	0.18	57,57,57,57	0
55	MG	2A	3167	1/1	0.89	0.26	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3708	1/1	0.89	0.50	53,53,53,53	0
55	MG	2A	3451	1/1	0.89	0.30	67,67,67,67	0
55	MG	1A	3260	1/1	0.89	0.51	36,36,36,36	0
55	MG	2a	1788	1/1	0.89	0.04	86,86,86,86	0
55	MG	2A	3174	1/1	0.89	0.17	58,58,58,58	0
55	MG	2a	1793	1/1	0.89	0.15	61,61,61,61	0
55	MG	1A	3198	1/1	0.89	0.59	28,28,28,28	0
55	MG	1A	3264	1/1	0.89	0.14	37,37,37,37	0
55	MG	1A	3222	1/1	0.89	0.56	36,36,36,36	0
55	MG	1a	3035	1/1	0.89	1.15	64,64,64,64	0
55	MG	2W	3001	1/1	0.89	0.22	60,60,60,60	0
55	MG	2A	3185	1/1	0.89	0.80	62,62,62,62	0
55	MG	2A	3061	1/1	0.89	0.21	62,62,62,62	0
55	MG	1A	3857	1/1	0.89	0.28	71,71,71,71	0
55	MG	1A	3019	1/1	0.89	0.66	39,39,39,39	0
55	MG	1A	3054	1/1	0.89	0.31	49,49,49,49	0
55	MG	1A	3550	1/1	0.89	0.27	44,44,44,44	0
55	MG	2A	3678	1/1	0.89	0.09	92,92,92,92	0
55	MG	2A	3472	1/1	0.89	0.35	88,88,88,88	0
56	A	1B	3025	1/23	0.89	0.61	57,57,57,57	0
55	MG	1A	3866	1/1	0.90	0.21	61,61,61,61	0
55	MG	28	103	1/1	0.90	0.10	77,77,77,77	0
55	MG	1A	3348	1/1	0.90	0.09	71,71,71,71	0
55	MG	1A	3001	1/1	0.90	0.10	32,32,32,32	0
55	MG	1a	3066	1/1	0.90	0.11	68,68,68,68	0
55	MG	1A	3094	1/1	0.90	0.72	30,30,30,30	0
55	MG	2A	3537	1/1	0.90	0.16	61,61,61,61	0
55	MG	2A	3346	1/1	0.90	0.06	77,77,77,77	0
55	MG	2A	3347	1/1	0.90	0.09	80,80,80,80	0
55	MG	2A	3057	1/1	0.90	1.07	49,49,49,49	0
55	MG	15	105	1/1	0.90	0.32	43,43,43,43	0
55	MG	2A	3366	1/1	0.90	0.05	92,92,92,92	0
55	MG	1A	3133	1/1	0.90	0.56	35,35,35,35	0
55	MG	17	103	1/1	0.90	0.84	43,43,43,43	0
55	MG	1A	3467	1/1	0.90	0.23	32,32,32,32	0
55	MG	1A	3792	1/1	0.90	0.21	55,55,55,55	0
55	MG	2A	3766	1/1	0.90	0.18	81,81,81,81	0
55	MG	1a	3203	1/1	0.90	0.12	67,67,67,67	0
55	MG	1A	3002	1/1	0.90	0.21	48,48,48,48	0
55	MG	2A	3571	1/1	0.90	0.12	41,41,41,41	0
55	MG	1A	3802	1/1	0.90	0.17	39,39,39,39	0
55	MG	2A	3069	1/1	0.90	0.83	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	1A	3231	1/1	0.90	0.72	31,31,31,31	0
55	MG	2A	3412	1/1	0.90	0.54	70,70,70,70	0
55	MG	2A	3413	1/1	0.90	0.13	70,70,70,70	0
55	MG	2A	3786	1/1	0.90	0.11	49,49,49,49	0
55	MG	2A	3788	1/1	0.90	0.17	88,88,88,88	0
55	MG	2A	3789	1/1	0.90	0.21	62,62,62,62	0
55	MG	1A	3715	1/1	0.90	0.04	85,85,85,85	0
55	MG	1a	3095	1/1	0.90	0.14	62,62,62,62	0
55	MG	2A	3075	1/1	0.90	0.26	53,53,53,53	0
55	MG	1A	3721	1/1	0.90	0.18	50,50,50,50	0
55	MG	1A	3258	1/1	0.90	0.67	44,44,44,44	0
55	MG	2A	3429	1/1	0.90	0.10	64,64,64,64	0
55	MG	2A	3598	1/1	0.90	0.12	62,62,62,62	0
55	MG	1A	3487	1/1	0.90	0.33	57,57,57,57	0
55	MG	2a	1659	1/1	0.90	0.12	71,71,71,71	0
55	MG	1a	3007	1/1	0.90	0.17	74,74,74,74	0
55	MG	1A	3729	1/1	0.90	0.20	47,47,47,47	0
55	MG	1A	3817	1/1	0.90	0.37	72,72,72,72	0
55	MG	1A	3073	1/1	0.90	0.73	43,43,43,43	0
55	MG	1A	3539	1/1	0.90	0.17	62,62,62,62	0
55	MG	2A	3615	1/1	0.90	0.20	56,56,56,56	0
55	MG	1a	3133	1/1	0.90	0.32	74,74,74,74	0
55	MG	2A	3814	1/1	0.90	0.91	68,68,68,68	0
55	MG	2A	3207	1/1	0.90	0.12	70,70,70,70	0
55	MG	2A	3624	1/1	0.90	0.82	62,62,62,62	0
55	MG	2A	3208	1/1	0.90	0.15	60,60,60,60	0
55	MG	1A	3907	1/1	0.90	0.29	46,46,46,46	0
55	MG	1a	3136	1/1	0.90	0.36	79,79,79,79	0
55	MG	2B	3003	1/1	0.90	0.35	73,73,73,73	0
55	MG	1t	3001	1/1	0.90	0.36	76,76,76,76	0
55	MG	1A	3656	1/1	0.90	0.25	79,79,79,79	0
55	MG	2B	3006	1/1	0.90	0.41	80,80,80,80	0
55	MG	1a	3021	1/1	0.90	0.22	63,63,63,63	0
55	MG	2B	3008	1/1	0.90	0.11	83,83,83,83	0
55	MG	2B	3010	1/1	0.90	0.07	72,72,72,72	0
55	MG	1A	3491	1/1	0.90	0.29	55,55,55,55	0
55	MG	1A	3742	1/1	0.90	0.89	71,71,71,71	0
55	MG	2a	1726	1/1	0.90	0.09	78,78,78,78	0
55	MG	2A	3639	1/1	0.90	0.19	76,76,76,76	0
55	MG	2a	1729	1/1	0.90	0.14	60,60,60,60	0
55	MG	2A	3107	1/1	0.90	0.17	57,57,57,57	0
55	MG	2A	3232	1/1	0.90	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3011	1/1	0.90	0.43	58,58,58,58	0
55	MG	1A	3113	1/1	0.90	0.33	41,41,41,41	0
55	MG	2A	3110	1/1	0.90	0.54	53,53,53,53	0
55	MG	2A	3649	1/1	0.90	0.41	49,49,49,49	0
55	MG	2a	1744	1/1	0.90	0.15	76,76,76,76	0
55	MG	2A	3470	1/1	0.90	0.12	63,63,63,63	0
55	MG	2A	3245	1/1	0.90	0.32	78,78,78,78	0
55	MG	2D	307	1/1	0.90	1.69	64,64,64,64	0
55	MG	1a	3027	1/1	0.90	0.46	70,70,70,70	0
55	MG	1A	3432	1/1	0.90	0.07	49,49,49,49	0
55	MG	2a	1757	1/1	0.90	0.11	71,71,71,71	0
55	MG	2E	307	1/1	0.90	0.08	73,73,73,73	0
55	MG	1A	3138	1/1	0.90	0.13	52,52,52,52	0
55	MG	2a	1760	1/1	0.90	0.06	90,90,90,90	0
55	MG	2a	1761	1/1	0.90	0.21	67,67,67,67	0
55	MG	1A	3139	1/1	0.90	0.22	59,59,59,59	0
55	MG	2F	307	1/1	0.90	0.87	60,60,60,60	0
55	MG	1Q	201	1/1	0.90	0.50	44,44,44,44	0
55	MG	2A	3121	1/1	0.90	0.15	81,81,81,81	0
55	MG	1A	3027	1/1	0.90	0.31	31,31,31,31	0
55	MG	2A	3026	1/1	0.90	0.32	73,73,73,73	0
55	MG	1A	3454	1/1	0.90	0.08	56,56,56,56	0
55	MG	1A	3607	1/1	0.90	0.07	60,60,60,60	0
55	MG	1U	204	1/1	0.90	0.70	29,29,29,29	0
55	MG	2A	3684	1/1	0.90	0.12	57,57,57,57	0
55	MG	2A	3277	1/1	0.90	0.25	36,36,36,36	0
55	MG	1a	3043	1/1	0.90	0.43	68,68,68,68	0
55	MG	2U	203	1/1	0.90	0.10	71,71,71,71	0
55	MG	2A	3690	1/1	0.90	0.20	84,84,84,84	0
55	MG	2V	202	1/1	0.90	1.02	55,55,55,55	0
55	MG	1A	3556	1/1	0.90	0.15	14,14,14,14	0
55	MG	2A	3295	1/1	0.90	0.27	71,71,71,71	0
55	MG	2A	3036	1/1	0.90	0.52	48,48,48,48	0
55	MG	2X	103	1/1	0.90	0.11	58,58,58,58	0
55	MG	1A	3510	1/1	0.90	0.10	70,70,70,70	0
55	MG	20	103	1/1	0.90	0.30	59,59,59,59	0
55	MG	1W	3001	1/1	0.90	0.23	38,38,38,38	0
55	MG	1B	3016	1/1	0.90	0.07	51,51,51,51	0
55	MG	1A	3272	1/1	0.90	0.26	56,56,56,56	0
55	MG	2A	3143	1/1	0.90	0.28	53,53,53,53	0
55	MG	10	103	1/1	0.90	0.22	65,65,65,65	0
55	MG	2A	3521	1/1	0.90	0.19	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3612	1/1	0.90	0.07	78,78,78,78	0
55	MG	1A	3338	1/1	0.90	0.16	20,20,20,20	0
55	MG	1A	3728	1/1	0.91	0.10	54,54,54,54	0
55	MG	1D	309	1/1	0.91	0.51	41,41,41,41	0
55	MG	2A	3448	1/1	0.91	0.25	51,51,51,51	0
55	MG	1D	311	1/1	0.91	0.22	38,38,38,38	0
55	MG	1A	3017	1/1	0.91	0.40	31,31,31,31	0
55	MG	2A	3654	1/1	0.91	0.08	34,34,34,34	0
55	MG	1D	314	1/1	0.91	0.27	34,34,34,34	0
55	MG	2A	3659	1/1	0.91	0.17	73,73,73,73	0
55	MG	1A	3633	1/1	0.91	0.24	79,79,79,79	0
55	MG	2A	3196	1/1	0.91	0.18	77,77,77,77	0
55	MG	2A	3197	1/1	0.91	0.20	48,48,48,48	0
55	MG	2A	3666	1/1	0.91	0.05	70,70,70,70	0
55	MG	2A	3458	1/1	0.91	0.10	78,78,78,78	0
55	MG	2A	3200	1/1	0.91	0.99	65,65,65,65	0
55	MG	1D	316	1/1	0.91	0.10	73,73,73,73	0
55	MG	1A	3052	1/1	0.91	0.81	36,36,36,36	0
55	MG	1A	3635	1/1	0.91	0.26	39,39,39,39	0
55	MG	1A	3636	1/1	0.91	0.11	38,38,38,38	0
55	MG	2A	3212	1/1	0.91	0.16	60,60,60,60	0
55	MG	1A	3008	1/1	0.91	0.26	46,46,46,46	0
55	MG	1A	3033	1/1	0.91	0.59	45,45,45,45	0
55	MG	2A	3689	1/1	0.91	0.19	67,67,67,67	0
55	MG	1A	3005	1/1	0.91	0.21	22,22,22,22	0
55	MG	1a	3178	1/1	0.91	0.15	75,75,75,75	0
55	MG	2A	3697	1/1	0.91	0.07	57,57,57,57	0
55	MG	2A	3703	1/1	0.91	0.25	93,93,93,93	0
55	MG	1F	304	1/1	0.91	0.96	39,39,39,39	0
55	MG	1a	3036	1/1	0.91	0.12	49,49,49,49	0
55	MG	2a	1611	1/1	0.91	0.10	58,58,58,58	0
55	MG	1A	3870	1/1	0.91	0.26	54,54,54,54	0
55	MG	1a	3182	1/1	0.91	0.50	71,71,71,71	0
55	MG	2a	1617	1/1	0.91	0.38	65,65,65,65	0
55	MG	1A	3645	1/1	0.91	0.31	54,54,54,54	0
55	MG	1A	3122	1/1	0.91	0.53	30,30,30,30	0
55	MG	2A	3481	1/1	0.91	0.23	67,67,67,67	0
55	MG	1F	309	1/1	0.91	0.11	28,28,28,28	0
55	MG	2A	3483	1/1	0.91	0.65	55,55,55,55	0
55	MG	2A	3722	1/1	0.91	0.08	67,67,67,67	0
55	MG	2A	3724	1/1	0.91	0.11	45,45,45,45	0
55	MG	2A	3725	1/1	0.91	0.05	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3440	1/1	0.91	0.15	47,47,47,47	0
55	MG	1A	3511	1/1	0.91	0.15	26,26,26,26	0
55	MG	1A	3882	1/1	0.91	0.13	62,62,62,62	0
55	MG	2a	1640	1/1	0.91	0.72	61,61,61,61	0
55	MG	1a	3049	1/1	0.91	0.45	69,69,69,69	0
55	MG	2A	3096	1/1	0.91	0.14	46,46,46,46	0
55	MG	1A	3513	1/1	0.91	0.09	27,27,27,27	0
55	MG	1A	3314	1/1	0.91	0.12	52,52,52,52	0
55	MG	1a	3207	1/1	0.91	0.12	76,76,76,76	0
55	MG	1N	8002	1/1	0.91	0.15	64,64,64,64	0
55	MG	2A	3750	1/1	0.91	0.33	63,63,63,63	0
55	MG	2A	3260	1/1	0.91	0.12	66,66,66,66	0
55	MG	1A	3445	1/1	0.91	0.17	65,65,65,65	0
55	MG	1A	3449	1/1	0.91	0.17	21,21,21,21	0
55	MG	1A	3076	1/1	0.91	0.23	63,63,63,63	0
55	MG	1a	3062	1/1	0.91	0.38	79,79,79,79	0
55	MG	2A	3758	1/1	0.91	0.15	77,77,77,77	0
55	MG	2A	3759	1/1	0.91	0.30	88,88,88,88	0
55	MG	2A	3278	1/1	0.91	0.11	56,56,56,56	0
55	MG	1A	3891	1/1	0.91	0.18	64,64,64,64	0
55	MG	1A	3666	1/1	0.91	0.23	45,45,45,45	0
55	MG	1A	3778	1/1	0.91	0.07	83,83,83,83	0
55	MG	1A	3218	1/1	0.91	0.43	35,35,35,35	0
55	MG	2A	3769	1/1	0.91	0.17	75,75,75,75	0
55	MG	2a	1673	1/1	0.91	0.15	63,63,63,63	0
55	MG	2A	3301	1/1	0.91	0.14	49,49,49,49	0
55	MG	1R	205	1/1	0.91	0.28	34,34,34,34	0
55	MG	1A	3023	1/1	0.91	0.14	21,21,21,21	0
55	MG	1A	3595	1/1	0.91	0.10	67,67,67,67	0
55	MG	2a	1684	1/1	0.91	0.07	76,76,76,76	0
55	MG	1A	3078	1/1	0.91	0.56	39,39,39,39	0
55	MG	1f	8001	1/1	0.91	0.21	60,60,60,60	0
55	MG	1A	3598	1/1	0.91	0.13	83,83,83,83	0
55	MG	1A	3099	1/1	0.91	0.30	62,62,62,62	0
55	MG	1A	3007	1/1	0.91	0.12	38,38,38,38	0
55	MG	1A	3154	1/1	0.91	0.64	28,28,28,28	0
55	MG	2a	1701	1/1	0.91	0.23	90,90,90,90	0
55	MG	1A	3349	1/1	0.91	0.17	25,25,25,25	0
55	MG	1A	3350	1/1	0.91	0.16	46,46,46,46	0
55	MG	2A	3556	1/1	0.91	0.71	57,57,57,57	0
55	MG	2A	3557	1/1	0.91	0.14	67,67,67,67	0
55	MG	2A	3340	1/1	0.91	0.27	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3560	1/1	0.91	0.19	53,53,53,53	0
55	MG	1a	3094	1/1	0.91	0.10	46,46,46,46	0
55	MG	2a	1720	1/1	0.91	0.10	73,73,73,73	0
55	MG	2a	1721	1/1	0.91	0.17	84,84,84,84	0
55	MG	1A	3694	1/1	0.91	0.10	35,35,35,35	0
55	MG	2A	3569	1/1	0.91	0.65	48,48,48,48	0
55	MG	2A	3570	1/1	0.91	0.14	57,57,57,57	0
55	MG	1a	3103	1/1	0.91	0.17	72,72,72,72	0
55	MG	2A	3808	1/1	0.91	0.22	44,44,44,44	0
55	MG	1A	3474	1/1	0.91	0.20	69,69,69,69	0
55	MG	2A	3575	1/1	0.91	0.20	48,48,48,48	0
55	MG	2A	3811	1/1	0.91	0.17	67,67,67,67	0
55	MG	1A	3696	1/1	0.91	0.10	29,29,29,29	0
55	MG	2a	1739	1/1	0.91	0.08	86,86,86,86	0
55	MG	1A	3102	1/1	0.91	0.33	42,42,42,42	0
55	MG	2A	3363	1/1	0.91	0.14	50,50,50,50	0
55	MG	2A	3584	1/1	0.91	0.23	62,62,62,62	0
55	MG	1a	3116	1/1	0.91	0.44	76,76,76,76	0
55	MG	1A	3479	1/1	0.91	0.13	39,39,39,39	0
55	MG	2a	1750	1/1	0.91	0.11	83,83,83,83	0
55	MG	1a	3118	1/1	0.91	0.08	70,70,70,70	0
55	MG	1a	3120	1/1	0.91	0.10	65,65,65,65	0
55	MG	1A	3824	1/1	0.91	0.15	47,47,47,47	0
55	MG	1A	3707	1/1	0.91	0.22	72,72,72,72	0
55	MG	2A	3595	1/1	0.91	0.11	52,52,52,52	0
55	MG	2A	3387	1/1	0.91	0.15	68,68,68,68	0
55	MG	17	101	1/1	0.91	0.42	35,35,35,35	0
55	MG	2A	3600	1/1	0.91	0.50	54,54,54,54	0
55	MG	2A	3031	1/1	0.91	0.35	59,59,59,59	0
55	MG	1a	3130	1/1	0.91	0.30	62,62,62,62	0
55	MG	2a	1767	1/1	0.91	0.17	79,79,79,79	0
55	MG	2A	3401	1/1	0.91	0.19	66,66,66,66	0
55	MG	1A	3042	1/1	0.91	0.14	25,25,25,25	0
55	MG	2A	3404	1/1	0.91	0.05	63,63,63,63	0
55	MG	2A	3406	1/1	0.91	0.56	62,62,62,62	0
55	MG	1A	3833	1/1	0.91	0.21	69,69,69,69	0
55	MG	2A	3618	1/1	0.91	0.21	55,55,55,55	0
55	MG	1A	3371	1/1	0.91	0.19	63,63,63,63	0
55	MG	2D	301	1/1	0.91	0.78	47,47,47,47	0
55	MG	1a	3135	1/1	0.91	0.13	77,77,77,77	0
55	MG	1A	3711	1/1	0.91	0.26	39,39,39,39	0
55	MG	1A	3618	1/1	0.91	0.24	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	2a	1791	1/1	0.91	0.21	71,71,71,71	0
55	MG	2D	305	1/1	0.91	0.95	59,59,59,59	0
55	MG	1A	3376	1/1	0.91	0.06	72,72,72,72	0
55	MG	2a	1795	1/1	0.91	0.17	57,57,57,57	0
55	MG	1A	3488	1/1	0.91	0.46	43,43,43,43	0
55	MG	2A	3426	1/1	0.91	0.20	70,70,70,70	0
55	MG	2A	3427	1/1	0.91	0.13	61,61,61,61	0
55	MG	2A	3633	1/1	0.91	0.11	82,82,82,82	0
55	MG	2F	305	1/1	0.91	0.13	46,46,46,46	0
55	MG	2A	3428	1/1	0.91	0.28	71,71,71,71	0
55	MG	1A	3064	1/1	0.91	0.33	29,29,29,29	0
55	MG	1D	303	1/1	0.91	0.30	52,52,52,52	0
55	MG	2A	3048	1/1	0.91	0.24	56,56,56,56	0
55	MG	1A	3014	1/1	0.91	0.64	41,41,41,41	0
55	MG	1D	306	1/1	0.91	0.28	35,35,35,35	0
55	MG	1a	3009	1/1	0.91	0.31	69,69,69,69	0
55	MG	2N	201	1/1	0.91	0.63	82,82,82,82	0
55	MG	1A	3726	1/1	0.91	0.24	29,29,29,29	0
55	MG	2A	3359	1/1	0.92	0.07	51,51,51,51	0
55	MG	2A	3360	1/1	0.92	0.11	64,64,64,64	0
55	MG	2A	3164	1/1	0.92	0.40	56,56,56,56	0
55	MG	2A	3740	1/1	0.92	0.26	68,68,68,68	0
55	MG	1A	3727	1/1	0.92	0.23	40,40,40,40	0
55	MG	2a	1605	1/1	0.92	0.30	56,56,56,56	0
55	MG	2A	3743	1/1	0.92	0.26	59,59,59,59	0
55	MG	2A	3549	1/1	0.92	0.05	74,74,74,74	0
55	MG	2a	1608	1/1	0.92	0.08	51,51,51,51	0
55	MG	1A	3836	1/1	0.92	0.12	54,54,54,54	0
55	MG	2A	3168	1/1	0.92	0.28	53,53,53,53	0
55	MG	1A	3446	1/1	0.92	0.21	49,49,49,49	0
55	MG	1a	3189	1/1	0.92	0.25	84,84,84,84	0
55	MG	2a	1616	1/1	0.92	0.14	68,68,68,68	0
55	MG	2A	3383	1/1	0.92	0.17	57,57,57,57	0
55	MG	2a	1619	1/1	0.92	0.33	72,72,72,72	0
55	MG	10	105	1/1	0.92	0.10	57,57,57,57	0
55	MG	1A	3237	1/1	0.92	0.15	53,53,53,53	0
55	MG	2A	3755	1/1	0.92	0.12	63,63,63,63	0
55	MG	1a	3196	1/1	0.92	0.09	77,77,77,77	0
55	MG	2a	1626	1/1	0.92	0.12	60,60,60,60	0
55	MG	2A	3757	1/1	0.92	0.35	53,53,53,53	0
55	MG	2A	3568	1/1	0.92	0.24	68,68,68,68	0
55	MG	1A	3451	1/1	0.92	0.06	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3181	1/1	0.92	0.23	79,79,79,79	0
55	MG	2A	3398	1/1	0.92	0.17	81,81,81,81	0
55	MG	2A	3573	1/1	0.92	0.13	71,71,71,71	0
55	MG	1A	3341	1/1	0.92	0.12	20,20,20,20	0
55	MG	1A	3582	1/1	0.92	0.30	69,69,69,69	0
55	MG	1A	3586	1/1	0.92	0.07	59,59,59,59	0
55	MG	1A	3849	1/1	0.92	0.26	89,89,89,89	0
55	MG	1A	3741	1/1	0.92	0.11	56,56,56,56	0
55	MG	2A	3774	1/1	0.92	0.21	79,79,79,79	0
55	MG	1A	3036	1/1	0.92	0.15	28,28,28,28	0
55	MG	1A	3243	1/1	0.92	1.04	44,44,44,44	0
55	MG	2A	3416	1/1	0.92	0.17	56,56,56,56	0
55	MG	2A	3418	1/1	0.92	0.11	55,55,55,55	0
55	MG	2A	3588	1/1	0.92	0.22	67,67,67,67	0
55	MG	1A	3037	1/1	0.92	0.08	56,56,56,56	0
55	MG	1A	3750	1/1	0.92	0.09	52,52,52,52	0
55	MG	2A	3198	1/1	0.92	0.17	27,27,27,27	0
55	MG	1A	3123	1/1	0.92	0.57	27,27,27,27	0
55	MG	1a	3223	1/1	0.92	0.19	54,54,54,54	0
55	MG	2A	3793	1/1	0.92	0.27	67,67,67,67	0
55	MG	2A	3597	1/1	0.92	0.10	51,51,51,51	0
55	MG	1A	3285	1/1	0.92	0.28	47,47,47,47	0
55	MG	2A	3797	1/1	0.92	0.15	75,75,75,75	0
55	MG	2A	3599	1/1	0.92	0.12	75,75,75,75	0
55	MG	2a	1668	1/1	0.92	0.08	51,51,51,51	0
55	MG	1A	3863	1/1	0.92	0.24	58,58,58,58	0
55	MG	1A	3596	1/1	0.92	0.22	58,58,58,58	0
55	MG	2A	3430	1/1	0.92	0.20	74,74,74,74	0
55	MG	1A	3525	1/1	0.92	0.19	57,57,57,57	0
55	MG	2A	3608	1/1	0.92	0.16	62,62,62,62	0
55	MG	1A	3671	1/1	0.92	0.20	46,46,46,46	0
55	MG	1A	3363	1/1	0.92	0.08	26,26,26,26	0
55	MG	2A	3436	1/1	0.92	0.12	72,72,72,72	0
55	MG	2a	1688	1/1	0.92	0.09	56,56,56,56	0
55	MG	2A	3100	1/1	0.92	0.20	58,58,58,58	0
55	MG	1A	3012	1/1	0.92	0.18	22,22,22,22	0
55	MG	1E	302	1/1	0.92	0.93	39,39,39,39	0
55	MG	1l	201	1/1	0.92	0.22	74,74,74,74	0
55	MG	1A	3051	1/1	0.92	0.57	30,30,30,30	0
55	MG	2A	3447	1/1	0.92	0.17	73,73,73,73	0
55	MG	2a	1707	1/1	0.92	0.19	92,92,92,92	0
55	MG	2A	3229	1/1	0.92	0.16	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3230	1/1	0.92	0.36	51,51,51,51	0
55	MG	1A	3470	1/1	0.92	0.10	28,28,28,28	0
55	MG	2A	3237	1/1	0.92	0.17	67,67,67,67	0
55	MG	1A	3294	1/1	0.92	0.06	33,33,33,33	0
55	MG	1A	3772	1/1	0.92	0.17	37,37,37,37	0
55	MG	2A	3635	1/1	0.92	0.05	92,92,92,92	0
55	MG	1A	3775	1/1	0.92	0.16	72,72,72,72	0
55	MG	2A	3005	1/1	0.92	0.13	44,44,44,44	0
55	MG	1A	3477	1/1	0.92	0.12	20,20,20,20	0
55	MG	2A	3640	1/1	0.92	0.22	78,78,78,78	0
55	MG	1A	3381	1/1	0.92	0.11	62,62,62,62	0
55	MG	1A	3691	1/1	0.92	0.13	26,26,26,26	0
55	MG	1a	3023	1/1	0.92	0.27	53,53,53,53	0
55	MG	1A	3547	1/1	0.92	0.44	35,35,35,35	0
55	MG	1A	3892	1/1	0.92	0.22	62,62,62,62	0
55	MG	2a	1733	1/1	0.92	0.17	67,67,67,67	0
55	MG	2A	3125	1/1	0.92	1.07	58,58,58,58	0
55	MG	1A	3384	1/1	0.92	0.47	58,58,58,58	0
55	MG	1A	3385	1/1	0.92	0.12	57,57,57,57	0
55	MG	1A	3115	1/1	0.92	0.07	54,54,54,54	0
55	MG	1a	3032	1/1	0.92	0.14	45,45,45,45	0
55	MG	1A	3701	1/1	0.92	0.49	40,40,40,40	0
55	MG	2A	3276	1/1	0.92	0.14	48,48,48,48	0
55	MG	2A	3133	1/1	0.92	0.37	60,60,60,60	0
55	MG	1G	3002	1/1	0.92	0.07	62,62,62,62	0
55	MG	2a	1751	1/1	0.92	0.17	107,107,107,107	0
55	MG	2A	3028	1/1	0.92	0.30	64,64,64,64	0
55	MG	1A	3039	1/1	0.92	0.32	55,55,55,55	0
55	MG	2E	304	1/1	0.92	0.83	46,46,46,46	0
55	MG	2A	3670	1/1	0.92	0.08	84,84,84,84	0
55	MG	2F	301	1/1	0.92	1.03	47,47,47,47	0
55	MG	2F	303	1/1	0.92	0.48	62,62,62,62	0
55	MG	2A	3294	1/1	0.92	0.16	55,55,55,55	0
55	MG	1A	3226	1/1	0.92	0.46	31,31,31,31	0
55	MG	2A	3297	1/1	0.92	0.14	78,78,78,78	0
55	MG	2A	3676	1/1	0.92	0.38	73,73,73,73	0
55	MG	1A	3903	1/1	0.92	0.23	59,59,59,59	0
55	MG	1A	3904	1/1	0.92	0.31	17,17,17,17	0
55	MG	1A	3402	1/1	0.92	0.29	43,43,43,43	0
55	MG	1A	3117	1/1	0.92	0.11	44,44,44,44	0
55	MG	1A	3494	1/1	0.92	0.19	59,59,59,59	0
55	MG	1a	3165	1/1	0.92	0.61	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3310	1/1	0.92	0.10	57,57,57,57	0
55	MG	2Q	8002	1/1	0.92	0.08	62,62,62,62	0
55	MG	2A	3317	1/1	0.92	0.15	55,55,55,55	0
55	MG	2R	201	1/1	0.92	0.79	56,56,56,56	0
55	MG	2a	1786	1/1	0.92	0.07	90,90,90,90	0
55	MG	1a	3166	1/1	0.92	0.09	80,80,80,80	0
55	MG	2A	3041	1/1	0.92	0.09	73,73,73,73	0
55	MG	2A	3321	1/1	0.92	0.18	34,34,34,34	0
55	MG	1A	3710	1/1	0.92	0.10	42,42,42,42	0
55	MG	1A	3257	1/1	0.92	0.23	40,40,40,40	0
55	MG	1A	3916	1/1	0.92	0.41	29,29,29,29	0
55	MG	2V	203	1/1	0.92	0.15	59,59,59,59	0
55	MG	1A	3499	1/1	0.92	0.12	59,59,59,59	0
55	MG	2A	3712	1/1	0.92	0.16	63,63,63,63	0
55	MG	1U	201	1/1	0.92	0.27	34,34,34,34	0
55	MG	1A	3316	1/1	0.92	0.11	58,58,58,58	0
55	MG	2A	3528	1/1	0.92	0.17	34,34,34,34	0
55	MG	2A	3157	1/1	0.92	0.29	62,62,62,62	0
55	MG	1A	3132	1/1	0.92	0.17	35,35,35,35	0
55	MG	1A	3208	1/1	0.92	0.23	37,37,37,37	0
55	MG	1A	3020	1/1	0.92	0.59	39,39,39,39	0
55	MG	1W	3002	1/1	0.92	0.20	49,49,49,49	0
55	MG	2A	3350	1/1	0.92	0.09	49,49,49,49	0
55	MG	1A	3104	1/1	0.92	0.67	37,37,37,37	0
55	MG	2A	3729	1/1	0.92	0.14	70,70,70,70	0
55	MG	2A	3339	1/1	0.93	0.05	71,71,71,71	0
55	MG	2A	3531	1/1	0.93	0.09	83,83,83,83	0
55	MG	1a	3163	1/1	0.93	0.10	74,74,74,74	0
55	MG	2A	3728	1/1	0.93	0.11	34,34,34,34	0
55	MG	1a	3044	1/1	0.93	0.10	66,66,66,66	0
55	MG	2A	3343	1/1	0.93	0.04	73,73,73,73	0
55	MG	1A	3481	1/1	0.93	0.10	23,23,23,23	0
55	MG	2A	3733	1/1	0.93	0.07	60,60,60,60	0
55	MG	1a	3167	1/1	0.93	0.11	86,86,86,86	0
55	MG	1U	206	1/1	0.93	0.26	28,28,28,28	0
55	MG	1A	3679	1/1	0.93	0.22	44,44,44,44	0
55	MG	2a	1610	1/1	0.93	0.55	74,74,74,74	0
55	MG	2A	3049	1/1	0.93	0.21	38,38,38,38	0
55	MG	1a	3050	1/1	0.93	0.15	45,45,45,45	0
55	MG	2A	3544	1/1	0.93	0.06	90,90,90,90	0
55	MG	1a	3172	1/1	0.93	0.17	77,77,77,77	0
55	MG	2A	3169	1/1	0.93	0.81	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	1A	3406	1/1	0.93	0.19	46,46,46,46	0
55	MG	1A	3407	1/1	0.93	0.05	48,48,48,48	0
55	MG	2A	3369	1/1	0.93	0.12	58,58,58,58	0
55	MG	1A	3069	1/1	0.93	0.17	38,38,38,38	0
55	MG	1A	3411	1/1	0.93	0.17	52,52,52,52	0
55	MG	1A	3346	1/1	0.93	0.10	52,52,52,52	0
55	MG	2A	3177	1/1	0.93	0.15	62,62,62,62	0
55	MG	2a	1630	1/1	0.93	0.50	50,50,50,50	0
55	MG	2A	3382	1/1	0.93	0.19	65,65,65,65	0
55	MG	2A	3565	1/1	0.93	0.07	56,56,56,56	0
55	MG	10	102	1/1	0.93	0.45	52,52,52,52	0
55	MG	2A	3385	1/1	0.93	0.18	32,32,32,32	0
55	MG	1A	3865	1/1	0.93	0.14	75,75,75,75	0
55	MG	2A	3182	1/1	0.93	0.27	72,72,72,72	0
55	MG	1A	3080	1/1	0.93	0.59	36,36,36,36	0
55	MG	2A	3392	1/1	0.93	0.19	31,31,31,31	0
55	MG	1A	3620	1/1	0.93	0.05	50,50,50,50	0
55	MG	2A	3772	1/1	0.93	0.08	63,63,63,63	0
55	MG	2A	3577	1/1	0.93	0.10	56,56,56,56	0
55	MG	10	108	1/1	0.93	0.68	43,43,43,43	0
55	MG	2A	3187	1/1	0.93	0.61	73,73,73,73	0
55	MG	2A	3399	1/1	0.93	0.16	45,45,45,45	0
55	MG	2A	3190	1/1	0.93	0.47	68,68,68,68	0
55	MG	2A	3191	1/1	0.93	0.17	61,61,61,61	0
55	MG	2A	3783	1/1	0.93	0.12	78,78,78,78	0
55	MG	1D	305	1/1	0.93	0.63	42,42,42,42	0
55	MG	2A	3785	1/1	0.93	0.09	60,60,60,60	0
55	MG	1A	3436	1/1	0.93	0.17	49,49,49,49	0
55	MG	2A	3410	1/1	0.93	0.10	83,83,83,83	0
55	MG	13	102	1/1	0.93	0.35	44,44,44,44	0
55	MG	1a	3193	1/1	0.93	0.21	74,74,74,74	0
55	MG	2A	3592	1/1	0.93	0.17	89,89,89,89	0
55	MG	2A	3414	1/1	0.93	0.24	72,72,72,72	0
55	MG	2a	1662	1/1	0.93	0.09	74,74,74,74	0
55	MG	2A	3594	1/1	0.93	0.11	56,56,56,56	0
55	MG	1A	3215	1/1	0.93	0.42	38,38,38,38	0
55	MG	1A	3233	1/1	0.93	0.36	63,63,63,63	0
55	MG	2A	3417	1/1	0.93	0.76	58,58,58,58	0
55	MG	1A	3444	1/1	0.93	0.10	75,75,75,75	0
55	MG	1A	3706	1/1	0.93	0.16	54,54,54,54	0
55	MG	2a	1681	1/1	0.93	0.12	84,84,84,84	0
55	MG	1A	3358	1/1	0.93	0.13	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3204	1/1	0.93	0.30	54,54,54,54	0
55	MG	1A	3256	1/1	0.93	0.20	41,41,41,41	0
55	MG	2A	3082	1/1	0.93	0.14	56,56,56,56	0
55	MG	1A	3235	1/1	0.93	0.37	38,38,38,38	0
55	MG	2a	1689	1/1	0.93	0.10	58,58,58,58	0
55	MG	2a	1690	1/1	0.93	0.24	83,83,83,83	0
55	MG	1a	3210	1/1	0.93	0.15	78,78,78,78	0
55	MG	1a	3087	1/1	0.93	0.06	57,57,57,57	0
55	MG	1A	3886	1/1	0.93	0.16	61,61,61,61	0
55	MG	1D	317	1/1	0.93	0.24	57,57,57,57	0
55	MG	1A	3155	1/1	0.93	0.59	27,27,27,27	0
55	MG	2A	3619	1/1	0.93	0.12	50,50,50,50	0
55	MG	2a	1706	1/1	0.93	0.28	63,63,63,63	0
55	MG	1A	3575	1/1	0.93	0.31	23,23,23,23	0
55	MG	1a	3220	1/1	0.93	0.09	65,65,65,65	0
55	MG	1a	3106	1/1	0.93	0.06	60,60,60,60	0
55	MG	1A	3137	1/1	0.93	0.96	46,46,46,46	0
55	MG	2a	1712	1/1	0.93	0.33	69,69,69,69	0
55	MG	2a	1713	1/1	0.93	0.06	69,69,69,69	0
55	MG	1A	3022	1/1	0.93	0.42	31,31,31,31	0
55	MG	1a	3109	1/1	0.93	0.24	53,53,53,53	0
55	MG	2A	3103	1/1	0.93	0.51	65,65,65,65	0
55	MG	1a	3112	1/1	0.93	0.17	86,86,86,86	0
55	MG	1A	3805	1/1	0.93	0.07	65,65,65,65	0
55	MG	1F	301	1/1	0.93	0.31	28,28,28,28	0
55	MG	1A	3718	1/1	0.93	0.21	67,67,67,67	0
55	MG	2a	1723	1/1	0.93	0.23	110,110,110,110	0
55	MG	1A	3719	1/1	0.93	0.10	45,45,45,45	0
55	MG	1a	3008	1/1	0.93	0.43	60,60,60,60	0
55	MG	2A	3638	1/1	0.93	0.16	86,86,86,86	0
55	MG	2a	1728	1/1	0.93	0.13	86,86,86,86	0
55	MG	1A	3512	1/1	0.93	0.28	46,46,46,46	0
55	MG	1a	3010	1/1	0.93	0.14	78,78,78,78	0
55	MG	1a	3128	1/1	0.93	0.18	71,71,71,71	0
55	MG	2a	1732	1/1	0.93	0.10	74,74,74,74	0
55	MG	1A	3898	1/1	0.93	0.38	63,63,63,63	0
55	MG	1A	3159	1/1	0.93	0.27	30,30,30,30	0
55	MG	2a	1735	1/1	0.93	0.08	81,81,81,81	0
55	MG	2A	3002	1/1	0.93	0.12	63,63,63,63	0
55	MG	2a	1737	1/1	0.93	0.24	69,69,69,69	0
55	MG	1A	3724	1/1	0.93	0.06	71,71,71,71	0
55	MG	2A	3265	1/1	0.93	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3378	1/1	0.93	0.12	20,20,20,20	0
55	MG	2A	3126	1/1	0.93	0.14	55,55,55,55	0
55	MG	1A	3515	1/1	0.93	0.20	54,54,54,54	0
55	MG	2A	3009	1/1	0.93	0.49	59,59,59,59	0
55	MG	2a	1748	1/1	0.93	0.05	79,79,79,79	0
55	MG	1A	3044	1/1	0.93	0.31	33,33,33,33	0
55	MG	2A	3657	1/1	0.93	0.08	66,66,66,66	0
55	MG	2A	3474	1/1	0.93	0.10	70,70,70,70	0
55	MG	2a	1753	1/1	0.93	0.50	69,69,69,69	0
55	MG	1A	3207	1/1	0.93	0.35	45,45,45,45	0
55	MG	2A	3281	1/1	0.93	0.10	61,61,61,61	0
55	MG	2A	3013	1/1	0.93	0.11	60,60,60,60	0
55	MG	2A	3287	1/1	0.93	0.09	39,39,39,39	0
55	MG	2A	3668	1/1	0.93	0.12	66,66,66,66	0
55	MG	1A	3270	1/1	0.93	0.17	18,18,18,18	0
55	MG	2A	3018	1/1	0.93	1.18	52,52,52,52	0
55	MG	2F	308	1/1	0.93	0.41	59,59,59,59	0
55	MG	1a	3138	1/1	0.93	0.12	58,58,58,58	0
55	MG	1A	3386	1/1	0.93	0.08	61,61,61,61	0
55	MG	1A	3387	1/1	0.93	0.13	70,70,70,70	0
55	MG	2A	3484	1/1	0.93	0.48	46,46,46,46	0
55	MG	1H	8002	1/1	0.93	0.10	46,46,46,46	0
55	MG	1A	3323	1/1	0.93	0.20	46,46,46,46	0
55	MG	2A	3303	1/1	0.93	0.12	88,88,88,88	0
55	MG	1A	3471	1/1	0.93	0.13	65,65,65,65	0
55	MG	2A	3494	1/1	0.93	0.10	77,77,77,77	0
55	MG	2a	1778	1/1	0.93	0.06	79,79,79,79	0
55	MG	2A	3688	1/1	0.93	0.13	66,66,66,66	0
55	MG	2a	1781	1/1	0.93	0.26	76,76,76,76	0
55	MG	2a	1784	1/1	0.93	0.09	80,80,80,80	0
55	MG	1A	3140	1/1	0.93	0.17	37,37,37,37	0
55	MG	2A	3499	1/1	0.93	0.09	65,65,65,65	0
55	MG	2A	3691	1/1	0.93	0.12	70,70,70,70	0
55	MG	2U	202	1/1	0.93	0.62	46,46,46,46	0
55	MG	2a	1789	1/1	0.93	0.11	86,86,86,86	0
55	MG	2a	1790	1/1	0.93	0.46	80,80,80,80	0
55	MG	2A	3500	1/1	0.93	0.31	41,41,41,41	0
55	MG	1a	3031	1/1	0.93	0.09	61,61,61,61	0
55	MG	1A	3476	1/1	0.93	0.21	45,45,45,45	0
55	MG	1A	3327	1/1	0.93	0.14	18,18,18,18	0
55	MG	2A	3318	1/1	0.93	0.21	67,67,67,67	0
55	MG	1B	3005	1/1	0.93	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1Q	203	1/1	0.93	0.21	38,38,38,38	0
55	MG	2A	3708	1/1	0.93	0.16	66,66,66,66	0
55	MG	1A	3842	1/1	0.93	0.08	84,84,84,84	0
55	MG	20	102	1/1	0.93	0.17	75,75,75,75	0
55	MG	2A	3324	1/1	0.93	0.17	61,61,61,61	0
55	MG	1A	3129	1/1	0.93	0.27	36,36,36,36	0
55	MG	1a	3158	1/1	0.93	0.07	88,88,88,88	0
55	MG	2I	101	1/1	0.93	0.76	61,61,61,61	0
55	MG	1A	3748	1/1	0.93	0.09	50,50,50,50	0
55	MG	2A	3334	1/1	0.93	0.17	45,45,45,45	0
55	MG	1A	3279	1/1	0.93	0.11	56,56,56,56	0
55	MG	1A	3480	1/1	0.93	0.27	34,34,34,34	0
56	A	2A	3821	1/23	0.93	0.16	79,79,79,79	0
55	MG	1A	3289	1/1	0.94	0.13	53,53,53,53	0
55	MG	1A	3698	1/1	0.94	0.13	48,48,48,48	0
55	MG	2D	311	1/1	0.94	0.16	53,53,53,53	0
55	MG	1A	3820	1/1	0.94	0.60	41,41,41,41	0
55	MG	2A	3335	1/1	0.94	0.07	71,71,71,71	0
55	MG	1A	3822	1/1	0.94	0.09	58,58,58,58	0
55	MG	1A	3823	1/1	0.94	0.12	28,28,28,28	0
55	MG	1A	3520	1/1	0.94	0.18	56,56,56,56	0
55	MG	2A	3112	1/1	0.94	0.62	77,77,77,77	0
55	MG	1A	3521	1/1	0.94	0.20	45,45,45,45	0
55	MG	1a	3187	1/1	0.94	0.07	89,89,89,89	0
55	MG	1a	3188	1/1	0.94	0.18	64,64,64,64	0
55	MG	1A	3829	1/1	0.94	0.20	60,60,60,60	0
55	MG	2A	3118	1/1	0.94	0.32	52,52,52,52	0
55	MG	2A	3120	1/1	0.94	0.81	56,56,56,56	0
55	MG	1A	3177	1/1	0.94	0.57	52,52,52,52	0
55	MG	2A	3356	1/1	0.94	0.19	43,43,43,43	0
55	MG	2A	3123	1/1	0.94	0.24	43,43,43,43	0
55	MG	1D	312	1/1	0.94	0.24	15,15,15,15	0
55	MG	2P	201	1/1	0.94	0.56	51,51,51,51	0
55	MG	2A	3609	1/1	0.94	0.12	38,38,38,38	0
55	MG	1A	3704	1/1	0.94	0.06	42,42,42,42	0
55	MG	2A	3361	1/1	0.94	0.07	64,64,64,64	0
55	MG	2A	3362	1/1	0.94	0.18	61,61,61,61	0
55	MG	1A	3368	1/1	0.94	0.19	29,29,29,29	0
55	MG	2A	3617	1/1	0.94	0.09	33,33,33,33	0
55	MG	1A	3370	1/1	0.94	0.16	41,41,41,41	0
55	MG	1A	3209	1/1	0.94	0.17	72,72,72,72	0
55	MG	2A	3371	1/1	0.94	0.17	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3374	1/1	0.94	0.16	62,62,62,62	0
55	MG	1a	3200	1/1	0.94	0.08	93,93,93,93	0
55	MG	1A	3528	1/1	0.94	0.15	57,57,57,57	0
55	MG	2A	3626	1/1	0.94	0.17	60,60,60,60	0
55	MG	2A	3379	1/1	0.94	0.09	61,61,61,61	0
55	MG	2A	3628	1/1	0.94	0.32	63,63,63,63	0
55	MG	1a	3204	1/1	0.94	0.06	72,72,72,72	0
55	MG	2A	3630	1/1	0.94	0.32	58,58,58,58	0
55	MG	1A	3373	1/1	0.94	0.12	58,58,58,58	0
55	MG	1A	3375	1/1	0.94	0.14	51,51,51,51	0
55	MG	1a	3209	1/1	0.94	0.12	52,52,52,52	0
55	MG	1A	3298	1/1	0.94	0.19	27,27,27,27	0
55	MG	2A	3139	1/1	0.94	0.51	53,53,53,53	0
55	MG	1a	3211	1/1	0.94	0.23	59,59,59,59	0
55	MG	25	102	1/1	0.94	0.35	62,62,62,62	0
55	MG	1a	3212	1/1	0.94	0.05	51,51,51,51	0
55	MG	1A	3714	1/1	0.94	0.10	68,68,68,68	0
55	MG	1a	3046	1/1	0.94	0.26	54,54,54,54	0
55	MG	1E	305	1/1	0.94	0.16	26,26,26,26	0
55	MG	2A	3396	1/1	0.94	0.19	71,71,71,71	0
55	MG	2A	3397	1/1	0.94	0.09	76,76,76,76	0
55	MG	2A	3145	1/1	0.94	0.16	79,79,79,79	0
55	MG	1A	3845	1/1	0.94	0.18	43,43,43,43	0
55	MG	1A	3049	1/1	0.94	0.53	45,45,45,45	0
55	MG	1A	3469	1/1	0.94	0.18	39,39,39,39	0
55	MG	1A	3030	1/1	0.94	0.12	30,30,30,30	0
55	MG	2A	3651	1/1	0.94	0.22	56,56,56,56	0
55	MG	1A	3545	1/1	0.94	0.49	36,36,36,36	0
55	MG	2A	3408	1/1	0.94	0.14	67,67,67,67	0
55	MG	2A	3409	1/1	0.94	0.13	48,48,48,48	0
55	MG	1A	3308	1/1	0.94	0.08	42,42,42,42	0
55	MG	2a	1613	1/1	0.94	0.41	61,61,61,61	0
55	MG	2A	3656	1/1	0.94	0.11	42,42,42,42	0
55	MG	1A	3628	1/1	0.94	0.07	50,50,50,50	0
55	MG	2A	3658	1/1	0.94	0.18	76,76,76,76	0
55	MG	1A	3383	1/1	0.94	0.12	20,20,20,20	0
55	MG	1F	308	1/1	0.94	0.53	32,32,32,32	0
55	MG	1d	505	1/1	0.94	0.06	74,74,74,74	0
55	MG	1d	506	1/1	0.94	0.09	91,91,91,91	0
55	MG	2a	1622	1/1	0.94	0.44	50,50,50,50	0
55	MG	2A	3665	1/1	0.94	0.09	59,59,59,59	0
55	MG	1a	3060	1/1	0.94	0.21	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3309	1/1	0.94	0.17	32,32,32,32	0
55	MG	1A	3858	1/1	0.94	0.11	56,56,56,56	0
55	MG	1g	3001	1/1	0.94	0.20	66,66,66,66	0
55	MG	1A	3311	1/1	0.94	0.06	34,34,34,34	0
55	MG	1A	3860	1/1	0.94	0.14	53,53,53,53	0
55	MG	1A	3312	1/1	0.94	0.07	64,64,64,64	0
55	MG	1F	315	1/1	0.94	0.45	43,43,43,43	0
55	MG	1F	316	1/1	0.94	0.10	69,69,69,69	0
55	MG	1a	3070	1/1	0.94	0.18	62,62,62,62	0
55	MG	1A	3062	1/1	0.94	0.22	37,37,37,37	0
55	MG	1A	3392	1/1	0.94	0.14	35,35,35,35	0
55	MG	1A	3395	1/1	0.94	0.11	44,44,44,44	0
55	MG	2A	3434	1/1	0.94	0.11	65,65,65,65	0
55	MG	1N	8001	1/1	0.94	0.44	51,51,51,51	0
55	MG	1A	3121	1/1	0.94	0.15	43,43,43,43	0
55	MG	2A	3179	1/1	0.94	0.99	48,48,48,48	0
55	MG	2A	3439	1/1	0.94	0.39	64,64,64,64	0
55	MG	2A	3694	1/1	0.94	0.04	65,65,65,65	0
55	MG	2A	3696	1/1	0.94	0.09	62,62,62,62	0
55	MG	1A	3560	1/1	0.94	0.06	72,72,72,72	0
55	MG	1A	3873	1/1	0.94	0.10	49,49,49,49	0
55	MG	1a	3082	1/1	0.94	0.20	62,62,62,62	0
55	MG	1a	3084	1/1	0.94	0.29	64,64,64,64	0
55	MG	2A	3017	1/1	0.94	0.53	54,54,54,54	0
55	MG	1A	3735	1/1	0.94	0.35	27,27,27,27	0
55	MG	1a	3090	1/1	0.94	0.06	40,40,40,40	0
55	MG	2A	3188	1/1	0.94	0.17	45,45,45,45	0
55	MG	1A	3737	1/1	0.94	0.11	14,14,14,14	0
55	MG	1A	3643	1/1	0.94	0.11	34,34,34,34	0
55	MG	2A	3718	1/1	0.94	0.08	83,83,83,83	0
55	MG	1A	3561	1/1	0.94	0.09	47,47,47,47	0
55	MG	1a	3097	1/1	0.94	0.10	61,61,61,61	0
55	MG	1A	3880	1/1	0.94	0.10	66,66,66,66	0
55	MG	1a	3104	1/1	0.94	0.30	82,82,82,82	0
55	MG	2a	1676	1/1	0.94	0.17	55,55,55,55	0
55	MG	1a	3105	1/1	0.94	0.14	58,58,58,58	0
55	MG	1A	3018	1/1	0.94	0.41	23,23,23,23	0
55	MG	1A	3567	1/1	0.94	0.23	30,30,30,30	0
55	MG	1A	3884	1/1	0.94	0.07	18,18,18,18	0
55	MG	1A	3650	1/1	0.94	0.37	49,49,49,49	0
55	MG	1A	3653	1/1	0.94	0.13	62,62,62,62	0
55	MG	1A	3238	1/1	0.94	0.39	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	1a	3115	1/1	0.94	0.40	66,66,66,66	0
55	MG	2A	3210	1/1	0.94	0.09	95,95,95,95	0
55	MG	1A	3217	1/1	0.94	0.42	45,45,45,45	0
55	MG	2A	3737	1/1	0.94	0.07	80,80,80,80	0
55	MG	2A	3738	1/1	0.94	0.10	86,86,86,86	0
55	MG	1A	3265	1/1	0.94	0.18	44,44,44,44	0
55	MG	2A	3213	1/1	0.94	0.16	33,33,33,33	0
55	MG	1A	3266	1/1	0.94	0.17	70,70,70,70	0
55	MG	2a	1703	1/1	0.94	0.08	61,61,61,61	0
55	MG	2a	1704	1/1	0.94	0.14	68,68,68,68	0
55	MG	1a	3119	1/1	0.94	0.10	81,81,81,81	0
55	MG	2A	3042	1/1	0.94	0.17	27,27,27,27	0
55	MG	1A	3242	1/1	0.94	0.42	29,29,29,29	0
55	MG	2A	3749	1/1	0.94	0.05	85,85,85,85	0
55	MG	1A	3268	1/1	0.94	0.18	35,35,35,35	0
55	MG	1A	3894	1/1	0.94	0.82	38,38,38,38	0
55	MG	1A	3664	1/1	0.94	0.13	59,59,59,59	0
55	MG	2a	1715	1/1	0.94	0.14	82,82,82,82	0
55	MG	1A	3762	1/1	0.94	0.65	48,48,48,48	0
55	MG	1A	3075	1/1	0.94	0.76	41,41,41,41	0
55	MG	1A	3765	1/1	0.94	0.10	39,39,39,39	0
55	MG	2A	3236	1/1	0.94	0.08	80,80,80,80	0
55	MG	2A	3051	1/1	0.94	0.84	61,61,61,61	0
55	MG	2A	3493	1/1	0.94	0.27	51,51,51,51	0
55	MG	10	106	1/1	0.94	0.07	58,58,58,58	0
55	MG	10	107	1/1	0.94	0.18	57,57,57,57	0
55	MG	2A	3242	1/1	0.94	0.24	40,40,40,40	0
55	MG	2a	1725	1/1	0.94	0.12	86,86,86,86	0
55	MG	2A	3764	1/1	0.94	0.12	72,72,72,72	0
55	MG	1A	3420	1/1	0.94	0.14	27,27,27,27	0
55	MG	1A	3045	1/1	0.94	0.18	12,12,12,12	0
55	MG	1A	3339	1/1	0.94	0.15	18,18,18,18	0
55	MG	13	101	1/1	0.94	0.36	32,32,32,32	0
55	MG	1A	3435	1/1	0.94	0.08	69,69,69,69	0
55	MG	2A	3508	1/1	0.94	0.56	57,57,57,57	0
55	MG	1A	3674	1/1	0.94	0.15	26,26,26,26	0
55	MG	2A	3253	1/1	0.94	0.16	56,56,56,56	0
55	MG	2A	3775	1/1	0.94	0.16	57,57,57,57	0
55	MG	1a	3141	1/1	0.94	0.10	75,75,75,75	0
55	MG	2A	3512	1/1	0.94	0.19	61,61,61,61	0
55	MG	1A	3780	1/1	0.94	0.04	58,58,58,58	0
55	MG	2A	3780	1/1	0.94	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3515	1/1	0.94	0.23	52,52,52,52	0
55	MG	2A	3517	1/1	0.94	0.12	64,64,64,64	0
55	MG	1A	3908	1/1	0.94	0.36	33,33,33,33	0
55	MG	1A	3276	1/1	0.94	0.24	3,3,3,3	0
55	MG	2A	3066	1/1	0.94	0.40	58,58,58,58	0
55	MG	2A	3261	1/1	0.94	0.11	88,88,88,88	0
55	MG	2A	3524	1/1	0.94	0.09	67,67,67,67	0
55	MG	1A	3912	1/1	0.94	0.14	43,43,43,43	0
55	MG	2A	3526	1/1	0.94	0.13	73,73,73,73	0
55	MG	2A	3527	1/1	0.94	0.31	73,73,73,73	0
55	MG	1A	3035	1/1	0.94	0.15	37,37,37,37	0
55	MG	2A	3529	1/1	0.94	0.13	75,75,75,75	0
55	MG	17	102	1/1	0.94	0.49	36,36,36,36	0
55	MG	2A	3271	1/1	0.94	0.15	36,36,36,36	0
55	MG	2A	3272	1/1	0.94	0.10	41,41,41,41	0
55	MG	1A	3784	1/1	0.94	0.07	42,42,42,42	0
55	MG	2A	3073	1/1	0.94	0.56	48,48,48,48	0
55	MG	1A	3786	1/1	0.94	0.14	23,23,23,23	0
55	MG	1A	3588	1/1	0.94	0.14	62,62,62,62	0
55	MG	2A	3279	1/1	0.94	0.15	45,45,45,45	0
55	MG	2A	3806	1/1	0.94	0.20	73,73,73,73	0
55	MG	2A	3540	1/1	0.94	0.18	64,64,64,64	0
55	MG	2A	3076	1/1	0.94	0.28	55,55,55,55	0
55	MG	2A	3282	1/1	0.94	0.12	34,34,34,34	0
55	MG	1A	3067	1/1	0.94	1.04	37,37,37,37	0
55	MG	2A	3286	1/1	0.94	0.11	42,42,42,42	0
55	MG	1A	3055	1/1	0.94	0.24	53,53,53,53	0
55	MG	2A	3548	1/1	0.94	0.07	65,65,65,65	0
55	MG	1A	3682	1/1	0.94	0.27	61,61,61,61	0
55	MG	2A	3291	1/1	0.94	0.15	34,34,34,34	0
55	MG	2A	3818	1/1	0.94	0.24	57,57,57,57	0
55	MG	2A	3554	1/1	0.94	0.22	58,58,58,58	0
55	MG	1A	3591	1/1	0.94	0.08	30,30,30,30	0
55	MG	1A	3800	1/1	0.94	0.16	64,64,64,64	0
55	MG	1B	3008	1/1	0.94	0.18	57,57,57,57	0
55	MG	2A	3558	1/1	0.94	0.08	59,59,59,59	0
55	MG	1A	3801	1/1	0.94	0.04	56,56,56,56	0
55	MG	1A	3686	1/1	0.94	0.08	35,35,35,35	0
55	MG	1A	3803	1/1	0.94	0.07	39,39,39,39	0
55	MG	2A	3093	1/1	0.94	0.39	46,46,46,46	0
55	MG	2a	1796	1/1	0.94	0.14	60,60,60,60	0
55	MG	1A	3689	1/1	0.94	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3283	1/1	0.94	0.12	25,25,25,25	0
55	MG	1a	3011	1/1	0.94	0.15	32,32,32,32	0
55	MG	2A	3098	1/1	0.94	0.19	53,53,53,53	0
55	MG	2A	3311	1/1	0.94	0.15	42,42,42,42	0
55	MG	2A	3313	1/1	0.94	0.09	40,40,40,40	0
55	MG	1A	3352	1/1	0.94	0.10	22,22,22,22	0
55	MG	1A	3029	1/1	0.94	0.19	38,38,38,38	0
55	MG	1B	3020	1/1	0.94	0.27	73,73,73,73	0
55	MG	1A	3450	1/1	0.94	0.13	19,19,19,19	0
55	MG	1a	3176	1/1	0.94	0.14	92,92,92,92	0
55	MG	1A	3809	1/1	0.94	0.16	13,13,13,13	0
55	MG	2A	3327	1/1	0.94	0.35	67,67,67,67	0
55	MG	1A	3082	1/1	0.94	0.73	37,37,37,37	0
55	MG	2D	306	1/1	0.94	0.21	57,57,57,57	0
55	MG	2R	203	1/1	0.95	0.20	39,39,39,39	0
55	MG	1A	3687	1/1	0.95	0.17	56,56,56,56	0
55	MG	1A	3688	1/1	0.95	0.09	26,26,26,26	0
55	MG	2A	3063	1/1	0.95	1.28	49,49,49,49	0
55	MG	1a	3155	1/1	0.95	0.11	78,78,78,78	0
55	MG	2U	204	1/1	0.95	0.19	55,55,55,55	0
55	MG	2A	3450	1/1	0.95	0.16	40,40,40,40	0
55	MG	2A	3233	1/1	0.95	0.16	73,73,73,73	0
55	MG	1a	3156	1/1	0.95	0.18	69,69,69,69	0
55	MG	2V	205	1/1	0.95	0.31	73,73,73,73	0
55	MG	1a	3157	1/1	0.95	0.07	82,82,82,82	0
55	MG	1A	3431	1/1	0.95	0.12	40,40,40,40	0
55	MG	1A	3213	1/1	0.95	0.85	32,32,32,32	0
55	MG	1B	3018	1/1	0.95	0.10	37,37,37,37	0
55	MG	1A	3162	1/1	0.95	0.64	37,37,37,37	0
55	MG	2A	3461	1/1	0.95	0.11	34,34,34,34	0
55	MG	1a	3162	1/1	0.95	0.07	77,77,77,77	0
55	MG	1A	3297	1/1	0.95	0.16	15,15,15,15	0
55	MG	1A	3813	1/1	0.95	0.08	25,25,25,25	0
55	MG	2A	3674	1/1	0.95	0.17	66,66,66,66	0
55	MG	23	101	1/1	0.95	0.88	64,64,64,64	0
55	MG	1A	3261	1/1	0.95	0.36	28,28,28,28	0
55	MG	2A	3077	1/1	0.95	0.19	56,56,56,56	0
55	MG	1A	3025	1/1	0.95	0.61	33,33,33,33	0
55	MG	27	101	1/1	0.95	0.22	55,55,55,55	0
55	MG	2A	3255	1/1	0.95	0.19	62,62,62,62	0
55	MG	1A	3819	1/1	0.95	0.12	58,58,58,58	0
55	MG	1A	3442	1/1	0.95	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3821	1/1	0.95	0.10	54,54,54,54	0
55	MG	1A	3114	1/1	0.95	0.27	37,37,37,37	0
55	MG	2A	3687	1/1	0.95	0.17	49,49,49,49	0
55	MG	2a	1601	1/1	0.95	0.32	79,79,79,79	0
55	MG	1A	3700	1/1	0.95	0.12	24,24,24,24	0
55	MG	1A	3303	1/1	0.95	0.15	13,13,13,13	0
55	MG	2A	3262	1/1	0.95	0.23	74,74,74,74	0
55	MG	1A	3367	1/1	0.95	0.19	30,30,30,30	0
55	MG	1a	3177	1/1	0.95	0.08	74,74,74,74	0
55	MG	2A	3092	1/1	0.95	0.66	49,49,49,49	0
55	MG	1A	3827	1/1	0.95	0.12	64,64,64,64	0
55	MG	1D	310	1/1	0.95	0.52	42,42,42,42	0
55	MG	2A	3702	1/1	0.95	0.16	34,34,34,34	0
55	MG	1A	3241	1/1	0.95	0.23	30,30,30,30	0
55	MG	1a	3030	1/1	0.95	0.93	61,61,61,61	0
55	MG	1A	3050	1/1	0.95	0.36	29,29,29,29	0
55	MG	1A	3310	1/1	0.95	0.26	41,41,41,41	0
55	MG	1A	3166	1/1	0.95	0.44	46,46,46,46	0
55	MG	2a	1618	1/1	0.95	0.42	81,81,81,81	0
55	MG	1A	3609	1/1	0.95	0.10	62,62,62,62	0
55	MG	1A	3127	1/1	0.95	0.21	14,14,14,14	0
55	MG	2A	3715	1/1	0.95	0.08	66,66,66,66	0
55	MG	2A	3496	1/1	0.95	0.16	43,43,43,43	0
55	MG	1A	3269	1/1	0.95	0.07	62,62,62,62	0
55	MG	1A	3100	1/1	0.95	0.25	25,25,25,25	0
55	MG	1A	3615	1/1	0.95	0.14	19,19,19,19	0
55	MG	1A	3616	1/1	0.95	0.05	48,48,48,48	0
55	MG	1a	3192	1/1	0.95	0.11	49,49,49,49	0
55	MG	1a	3042	1/1	0.95	0.20	53,53,53,53	0
55	MG	1A	3841	1/1	0.95	0.08	64,64,64,64	0
55	MG	1a	3195	1/1	0.95	0.10	62,62,62,62	0
55	MG	2a	1634	1/1	0.95	0.56	81,81,81,81	0
55	MG	2A	3298	1/1	0.95	0.12	56,56,56,56	0
55	MG	1A	3056	1/1	0.95	0.20	28,28,28,28	0
55	MG	1A	3716	1/1	0.95	0.07	46,46,46,46	0
55	MG	2a	1639	1/1	0.95	0.55	50,50,50,50	0
55	MG	1A	3187	1/1	0.95	0.09	52,52,52,52	0
55	MG	1A	3621	1/1	0.95	0.12	40,40,40,40	0
55	MG	1a	3201	1/1	0.95	0.13	92,92,92,92	0
55	MG	1A	3720	1/1	0.95	0.06	65,65,65,65	0
55	MG	2A	3519	1/1	0.95	0.10	73,73,73,73	0
55	MG	1A	3852	1/1	0.95	0.22	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3622	1/1	0.95	0.09	76,76,76,76	0
55	MG	1A	3531	1/1	0.95	0.05	46,46,46,46	0
55	MG	2A	3741	1/1	0.95	0.05	70,70,70,70	0
55	MG	1A	3458	1/1	0.95	0.10	46,46,46,46	0
55	MG	1A	3277	1/1	0.95	0.16	30,30,30,30	0
55	MG	1A	3462	1/1	0.95	0.04	40,40,40,40	0
55	MG	1A	3463	1/1	0.95	0.10	28,28,28,28	0
55	MG	1a	3059	1/1	0.95	0.16	80,80,80,80	0
55	MG	1A	3318	1/1	0.95	0.26	61,61,61,61	0
55	MG	2A	3322	1/1	0.95	0.07	62,62,62,62	0
55	MG	1a	3061	1/1	0.95	0.17	74,74,74,74	0
55	MG	1A	3543	1/1	0.95	0.17	63,63,63,63	0
55	MG	2A	3532	1/1	0.95	0.06	84,84,84,84	0
55	MG	1F	313	1/1	0.95	0.16	32,32,32,32	0
55	MG	2a	1664	1/1	0.95	0.34	69,69,69,69	0
55	MG	1A	3320	1/1	0.95	0.15	62,62,62,62	0
55	MG	2A	3330	1/1	0.95	0.14	57,57,57,57	0
55	MG	2A	3536	1/1	0.95	0.06	64,64,64,64	0
55	MG	2a	1672	1/1	0.95	0.13	57,57,57,57	0
55	MG	1A	3862	1/1	0.95	0.12	59,59,59,59	0
55	MG	2A	3332	1/1	0.95	0.08	46,46,46,46	0
55	MG	1A	3006	1/1	0.95	0.11	21,21,21,21	0
55	MG	1A	3016	1/1	0.95	0.50	19,19,19,19	0
55	MG	2a	1679	1/1	0.95	0.10	63,63,63,63	0
55	MG	2A	3763	1/1	0.95	0.12	41,41,41,41	0
55	MG	1A	3637	1/1	0.95	0.17	38,38,38,38	0
55	MG	1A	3868	1/1	0.95	0.09	29,29,29,29	0
55	MG	1A	3638	1/1	0.95	0.43	31,31,31,31	0
55	MG	1A	3158	1/1	0.95	0.15	37,37,37,37	0
55	MG	2A	3545	1/1	0.95	0.17	97,97,97,97	0
55	MG	2A	3770	1/1	0.95	0.04	79,79,79,79	0
55	MG	2A	3341	1/1	0.95	0.17	34,34,34,34	0
55	MG	1A	3871	1/1	0.95	0.09	21,21,21,21	0
55	MG	1A	3738	1/1	0.95	0.13	14,14,14,14	0
55	MG	2A	3344	1/1	0.95	0.11	55,55,55,55	0
55	MG	1A	3393	1/1	0.95	0.11	53,53,53,53	0
55	MG	1A	3472	1/1	0.95	0.17	58,58,58,58	0
55	MG	1A	3743	1/1	0.95	0.11	45,45,45,45	0
55	MG	1a	3079	1/1	0.95	0.17	55,55,55,55	0
55	MG	1A	3473	1/1	0.95	0.05	63,63,63,63	0
55	MG	2a	1705	1/1	0.95	0.21	69,69,69,69	0
55	MG	2A	3352	1/1	0.95	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3353	1/1	0.95	0.07	72,72,72,72	0
55	MG	2A	3561	1/1	0.95	0.08	59,59,59,59	0
55	MG	1m	201	1/1	0.95	0.16	72,72,72,72	0
55	MG	1A	3746	1/1	0.95	0.14	31,31,31,31	0
55	MG	1Q	205	1/1	0.95	0.12	43,43,43,43	0
55	MG	2A	3566	1/1	0.95	0.33	64,64,64,64	0
55	MG	1R	201	1/1	0.95	0.97	46,46,46,46	0
55	MG	1R	203	1/1	0.95	0.23	19,19,19,19	0
55	MG	1A	3881	1/1	0.95	0.25	43,43,43,43	0
55	MG	1A	3644	1/1	0.95	0.12	18,18,18,18	0
55	MG	2A	3795	1/1	0.95	0.13	72,72,72,72	0
55	MG	2A	3365	1/1	0.95	0.22	39,39,39,39	0
55	MG	1a	3096	1/1	0.95	0.16	78,78,78,78	0
55	MG	2A	3006	1/1	0.95	0.12	36,36,36,36	0
55	MG	2A	3007	1/1	0.95	0.19	61,61,61,61	0
55	MG	1A	3553	1/1	0.95	0.24	37,37,37,37	0
55	MG	1a	3102	1/1	0.95	0.09	48,48,48,48	0
55	MG	1A	3394	1/1	0.95	0.20	50,50,50,50	0
55	MG	2A	3166	1/1	0.95	0.41	44,44,44,44	0
55	MG	1U	202	1/1	0.95	0.19	43,43,43,43	0
55	MG	1U	203	1/1	0.95	0.52	42,42,42,42	0
55	MG	1A	3751	1/1	0.95	0.20	39,39,39,39	0
55	MG	1A	3475	1/1	0.95	0.99	32,32,32,32	0
55	MG	1A	3649	1/1	0.95	0.12	33,33,33,33	0
55	MG	1A	3282	1/1	0.95	0.10	26,26,26,26	0
55	MG	1A	3651	1/1	0.95	0.15	40,40,40,40	0
55	MG	1a	3113	1/1	0.95	0.29	66,66,66,66	0
55	MG	2A	3391	1/1	0.95	0.07	43,43,43,43	0
55	MG	1A	3083	1/1	0.95	0.06	57,57,57,57	0
55	MG	2a	1738	1/1	0.95	0.80	85,85,85,85	0
55	MG	2A	3178	1/1	0.95	0.68	38,38,38,38	0
55	MG	1A	3335	1/1	0.95	0.18	19,19,19,19	0
55	MG	2A	3395	1/1	0.95	0.14	35,35,35,35	0
55	MG	2A	3820	1/1	0.95	0.11	69,69,69,69	0
55	MG	1A	3336	1/1	0.95	0.11	21,21,21,21	0
55	MG	1A	3566	1/1	0.95	0.11	23,23,23,23	0
55	MG	2A	3601	1/1	0.95	0.11	58,58,58,58	0
55	MG	2a	1749	1/1	0.95	0.05	80,80,80,80	0
55	MG	1A	3401	1/1	0.95	0.06	62,62,62,62	0
55	MG	2A	3604	1/1	0.95	0.33	65,65,65,65	0
55	MG	2A	3183	1/1	0.95	0.20	75,75,75,75	0
55	MG	1A	3068	1/1	0.95	0.29	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	2A	3607	1/1	0.95	0.12	80,80,80,80	0
55	MG	2B	3009	1/1	0.95	0.09	71,71,71,71	0
55	MG	1A	3766	1/1	0.95	0.07	39,39,39,39	0
55	MG	1A	3403	1/1	0.95	0.09	53,53,53,53	0
55	MG	1A	3768	1/1	0.95	0.10	46,46,46,46	0
55	MG	2A	3611	1/1	0.95	0.42	83,83,83,83	0
55	MG	1a	3127	1/1	0.95	0.10	53,53,53,53	0
55	MG	1A	3663	1/1	0.95	0.09	26,26,26,26	0
55	MG	1A	3211	1/1	0.95	0.77	31,31,31,31	0
55	MG	2A	3616	1/1	0.95	0.12	53,53,53,53	0
55	MG	2A	3037	1/1	0.95	0.18	24,24,24,24	0
55	MG	1A	3572	1/1	0.95	0.12	41,41,41,41	0
55	MG	1a	3131	1/1	0.95	0.15	76,76,76,76	0
55	MG	1A	3010	1/1	0.95	0.41	37,37,37,37	0
55	MG	1A	3669	1/1	0.95	0.26	56,56,56,56	0
55	MG	2A	3623	1/1	0.95	0.31	66,66,66,66	0
55	MG	1A	3344	1/1	0.95	0.08	25,25,25,25	0
55	MG	1A	3910	1/1	0.95	0.51	35,35,35,35	0
55	MG	1A	3291	1/1	0.95	0.16	30,30,30,30	0
55	MG	2D	309	1/1	0.95	0.20	30,30,30,30	0
55	MG	2D	310	1/1	0.95	0.10	55,55,55,55	0
55	MG	1A	3347	1/1	0.95	0.12	18,18,18,18	0
55	MG	2A	3422	1/1	0.95	0.09	52,52,52,52	0
55	MG	2A	3203	1/1	0.95	1.10	63,63,63,63	0
55	MG	2A	3424	1/1	0.95	0.20	50,50,50,50	0
55	MG	1A	3414	1/1	0.95	0.15	19,19,19,19	0
55	MG	2F	302	1/1	0.95	0.62	55,55,55,55	0
55	MG	1A	3495	1/1	0.95	0.14	49,49,49,49	0
55	MG	1A	3497	1/1	0.95	0.14	66,66,66,66	0
55	MG	1A	3789	1/1	0.95	0.10	31,31,31,31	0
55	MG	17	104	1/1	0.95	0.32	61,61,61,61	0
55	MG	1A	3677	1/1	0.95	0.09	56,56,56,56	0
55	MG	1A	3292	1/1	0.95	0.18	52,52,52,52	0
55	MG	2A	3214	1/1	0.95	0.14	37,37,37,37	0
55	MG	2F	310	1/1	0.95	0.15	75,75,75,75	0
55	MG	1A	3424	1/1	0.95	0.04	62,62,62,62	0
55	MG	2A	3217	1/1	0.95	0.15	32,32,32,32	0
55	MG	1A	3680	1/1	0.95	0.10	59,59,59,59	0
55	MG	1A	3425	1/1	0.95	0.14	20,20,20,20	0
55	MG	1A	3427	1/1	0.95	0.08	42,42,42,42	0
55	MG	2A	3440	1/1	0.95	0.17	74,74,74,74	0
55	MG	1A	3505	1/1	0.95	0.18	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	1A	3428	1/1	0.95	0.10	68,68,68,68	0
55	MG	2Q	8003	1/1	0.95	0.18	57,57,57,57	0
55	MG	2n	503	1/1	0.95	0.32	85,85,85,85	0
55	MG	2A	3443	1/1	0.95	0.17	63,63,63,63	0
55	MG	2A	3444	1/1	0.95	0.15	31,31,31,31	0
55	MG	2A	3227	1/1	0.95	0.15	65,65,65,65	0
57	ZN	1n	501	1/1	0.95	0.15	88,88,88,88	0
57	ZN	2n	501	1/1	0.95	0.08	108,108,108,108	0
55	MG	1A	3110	1/1	0.96	0.25	38,38,38,38	0
55	MG	2A	3223	1/1	0.96	0.13	68,68,68,68	0
55	MG	2A	3744	1/1	0.96	0.21	64,64,64,64	0
55	MG	2A	3745	1/1	0.96	0.18	70,70,70,70	0
55	MG	1A	3657	1/1	0.96	0.06	50,50,50,50	0
55	MG	1A	3736	1/1	0.96	0.18	55,55,55,55	0
55	MG	2A	3226	1/1	0.96	0.12	44,44,44,44	0
55	MG	2A	3562	1/1	0.96	0.16	74,74,74,74	0
55	MG	1A	3362	1/1	0.96	0.15	20,20,20,20	0
55	MG	2A	3097	1/1	0.96	0.16	35,35,35,35	0
55	MG	1a	3098	1/1	0.96	0.18	61,61,61,61	0
55	MG	2A	3400	1/1	0.96	0.12	43,43,43,43	0
55	MG	2A	3567	1/1	0.96	0.43	51,51,51,51	0
55	MG	1a	3101	1/1	0.96	0.14	39,39,39,39	0
55	MG	1A	3583	1/1	0.96	0.23	37,37,37,37	0
55	MG	1a	3221	1/1	0.96	0.26	71,71,71,71	0
55	MG	2A	3234	1/1	0.96	0.19	45,45,45,45	0
55	MG	2a	1628	1/1	0.96	0.15	54,54,54,54	0
55	MG	2A	3235	1/1	0.96	0.08	69,69,69,69	0
55	MG	2A	3760	1/1	0.96	0.08	40,40,40,40	0
55	MG	15	103	1/1	0.96	0.33	34,34,34,34	0
55	MG	1A	3584	1/1	0.96	0.07	37,37,37,37	0
55	MG	1B	3022	1/1	0.96	0.40	63,63,63,63	0
55	MG	1A	3518	1/1	0.96	0.12	77,77,77,77	0
55	MG	2A	3580	1/1	0.96	0.24	73,73,73,73	0
55	MG	2A	3581	1/1	0.96	0.08	72,72,72,72	0
55	MG	1A	3153	1/1	0.96	0.19	49,49,49,49	0
55	MG	2A	3243	1/1	0.96	0.07	72,72,72,72	0
55	MG	1A	3249	1/1	0.96	0.14	21,21,21,21	0
55	MG	1A	3846	1/1	0.96	0.12	53,53,53,53	0
55	MG	1A	3251	1/1	0.96	0.54	34,34,34,34	0
55	MG	2A	3419	1/1	0.96	0.08	33,33,33,33	0
55	MG	1A	3522	1/1	0.96	0.13	26,26,26,26	0
55	MG	1A	3326	1/1	0.96	0.12	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3850	1/1	0.96	0.08	21,21,21,21	0
55	MG	18	3303	1/1	0.96	0.07	52,52,52,52	0
55	MG	2A	3254	1/1	0.96	0.27	54,54,54,54	0
55	MG	1A	3413	1/1	0.96	0.09	43,43,43,43	0
55	MG	1h	3002	1/1	0.96	0.08	76,76,76,76	0
55	MG	2A	3116	1/1	0.96	0.13	43,43,43,43	0
55	MG	1k	3001	1/1	0.96	0.16	48,48,48,48	0
55	MG	19	103	1/1	0.96	0.08	61,61,61,61	0
55	MG	1A	3594	1/1	0.96	0.16	24,24,24,24	0
55	MG	2A	3787	1/1	0.96	0.13	61,61,61,61	0
55	MG	2a	1657	1/1	0.96	0.12	65,65,65,65	0
55	MG	1A	3234	1/1	0.96	0.12	48,48,48,48	0
55	MG	2A	3122	1/1	0.96	0.38	46,46,46,46	0
55	MG	2A	3263	1/1	0.96	0.18	46,46,46,46	0
55	MG	2A	3791	1/1	0.96	0.09	45,45,45,45	0
55	MG	2a	1663	1/1	0.96	0.29	63,63,63,63	0
55	MG	2A	3603	1/1	0.96	0.11	61,61,61,61	0
55	MG	2A	3264	1/1	0.96	0.11	65,65,65,65	0
55	MG	1a	3122	1/1	0.96	0.32	71,71,71,71	0
55	MG	2a	1669	1/1	0.96	0.10	46,46,46,46	0
55	MG	2A	3437	1/1	0.96	0.20	78,78,78,78	0
55	MG	1A	3755	1/1	0.96	0.07	69,69,69,69	0
55	MG	2A	3269	1/1	0.96	0.08	45,45,45,45	0
55	MG	1A	3418	1/1	0.96	0.14	26,26,26,26	0
55	MG	2a	1675	1/1	0.96	0.09	51,51,51,51	0
55	MG	2A	3127	1/1	0.96	0.37	60,60,60,60	0
55	MG	1A	3527	1/1	0.96	0.08	35,35,35,35	0
55	MG	1A	3419	1/1	0.96	0.14	37,37,37,37	0
55	MG	2A	3274	1/1	0.96	0.05	61,61,61,61	0
55	MG	1A	3372	1/1	0.96	0.18	29,29,29,29	0
55	MG	1A	3271	1/1	0.96	0.10	22,22,22,22	0
55	MG	1A	3601	1/1	0.96	0.34	37,37,37,37	0
55	MG	2A	3807	1/1	0.96	0.38	48,48,48,48	0
55	MG	1A	3332	1/1	0.96	0.14	28,28,28,28	0
55	MG	1E	301	1/1	0.96	0.12	15,15,15,15	0
55	MG	1a	3013	1/1	0.96	0.05	72,72,72,72	0
55	MG	2a	1691	1/1	0.96	0.15	56,56,56,56	0
55	MG	2A	3283	1/1	0.96	0.09	37,37,37,37	0
55	MG	2A	3284	1/1	0.96	0.10	37,37,37,37	0
55	MG	1A	3763	1/1	0.96	0.16	22,22,22,22	0
55	MG	2A	3012	1/1	0.96	0.17	38,38,38,38	0
55	MG	2a	1698	1/1	0.96	0.66	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3203	1/1	0.96	0.30	35,35,35,35	0
55	MG	1A	3275	1/1	0.96	0.16	27,27,27,27	0
55	MG	2a	1702	1/1	0.96	0.06	67,67,67,67	0
55	MG	2A	3016	1/1	0.96	0.75	46,46,46,46	0
55	MG	2A	3460	1/1	0.96	0.10	55,55,55,55	0
55	MG	2A	3293	1/1	0.96	0.12	40,40,40,40	0
55	MG	1A	3535	1/1	0.96	0.13	38,38,38,38	0
55	MG	1A	3536	1/1	0.96	0.08	44,44,44,44	0
55	MG	1A	3537	1/1	0.96	0.28	38,38,38,38	0
55	MG	2a	1709	1/1	0.96	0.15	82,82,82,82	0
55	MG	1A	3305	1/1	0.96	0.15	16,16,16,16	0
55	MG	2A	3467	1/1	0.96	0.08	57,57,57,57	0
55	MG	1A	3380	1/1	0.96	0.18	52,52,52,52	0
55	MG	1A	3541	1/1	0.96	0.61	34,34,34,34	0
55	MG	1a	3025	1/1	0.96	0.11	55,55,55,55	0
55	MG	1A	3777	1/1	0.96	0.05	41,41,41,41	0
55	MG	1A	3482	1/1	0.96	0.20	43,43,43,43	0
55	MG	1A	3692	1/1	0.96	0.08	43,43,43,43	0
55	MG	2A	3306	1/1	0.96	0.21	39,39,39,39	0
55	MG	1A	3879	1/1	0.96	0.10	41,41,41,41	0
55	MG	2A	3644	1/1	0.96	0.14	63,63,63,63	0
55	MG	2A	3309	1/1	0.96	0.09	65,65,65,65	0
55	MG	1A	3483	1/1	0.96	0.19	38,38,38,38	0
55	MG	1A	3047	1/1	0.96	0.15	24,24,24,24	0
55	MG	1A	3382	1/1	0.96	0.16	52,52,52,52	0
55	MG	1A	3486	1/1	0.96	0.14	63,63,63,63	0
55	MG	1A	3340	1/1	0.96	0.12	22,22,22,22	0
55	MG	1A	3438	1/1	0.96	0.09	57,57,57,57	0
55	MG	1A	3489	1/1	0.96	0.09	33,33,33,33	0
55	MG	1A	3191	1/1	0.96	0.18	66,66,66,66	0
55	MG	1A	3112	1/1	0.96	0.18	42,42,42,42	0
55	MG	1A	3629	1/1	0.96	0.22	42,42,42,42	0
55	MG	1A	3796	1/1	0.96	0.11	43,43,43,43	0
55	MG	2A	3490	1/1	0.96	0.22	33,33,33,33	0
55	MG	1A	3705	1/1	0.96	0.27	48,48,48,48	0
55	MG	1A	3345	1/1	0.96	0.17	45,45,45,45	0
55	MG	2E	301	1/1	0.96	0.27	43,43,43,43	0
55	MG	2A	3495	1/1	0.96	0.09	59,59,59,59	0
55	MG	1a	3045	1/1	0.96	0.26	57,57,57,57	0
55	MG	2E	306	1/1	0.96	0.14	49,49,49,49	0
55	MG	1A	3061	1/1	0.96	0.28	47,47,47,47	0
55	MG	2A	3498	1/1	0.96	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3557	1/1	0.96	0.10	24,24,24,24	0
55	MG	2A	3333	1/1	0.96	0.13	42,42,42,42	0
55	MG	2A	3173	1/1	0.96	0.56	42,42,42,42	0
55	MG	1P	202	1/1	0.96	0.39	28,28,28,28	0
55	MG	2A	3505	1/1	0.96	0.18	44,44,44,44	0
55	MG	1A	3559	1/1	0.96	0.19	26,26,26,26	0
55	MG	1A	3388	1/1	0.96	0.20	48,48,48,48	0
55	MG	1A	3389	1/1	0.96	0.17	48,48,48,48	0
55	MG	2A	3680	1/1	0.96	0.10	66,66,66,66	0
55	MG	1A	3712	1/1	0.96	0.16	52,52,52,52	0
55	MG	2A	3682	1/1	0.96	0.18	67,67,67,67	0
55	MG	1a	3054	1/1	0.96	0.14	82,82,82,82	0
55	MG	1A	3448	1/1	0.96	0.16	23,23,23,23	0
55	MG	1A	3902	1/1	0.96	0.13	56,56,56,56	0
55	MG	1A	3564	1/1	0.96	0.16	43,43,43,43	0
55	MG	2a	1763	1/1	0.96	0.09	55,55,55,55	0
55	MG	1A	3810	1/1	0.96	0.11	27,27,27,27	0
55	MG	1A	3639	1/1	0.96	0.11	47,47,47,47	0
55	MG	1A	3906	1/1	0.96	0.10	59,59,59,59	0
55	MG	1A	3390	1/1	0.96	0.14	23,23,23,23	0
55	MG	2a	1769	1/1	0.96	0.27	76,76,76,76	0
55	MG	1T	201	1/1	0.96	0.19	54,54,54,54	0
55	MG	2A	3693	1/1	0.96	0.06	95,95,95,95	0
55	MG	2A	3351	1/1	0.96	0.11	68,68,68,68	0
55	MG	2A	3695	1/1	0.96	0.10	97,97,97,97	0
55	MG	1A	3103	1/1	0.96	0.55	35,35,35,35	0
55	MG	1A	3504	1/1	0.96	0.19	19,19,19,19	0
55	MG	2A	3700	1/1	0.96	0.16	87,87,87,87	0
55	MG	1A	3818	1/1	0.96	0.06	24,24,24,24	0
55	MG	1A	3040	1/1	0.96	0.17	37,37,37,37	0
55	MG	2a	1782	1/1	0.96	0.21	70,70,70,70	0
55	MG	2a	1783	1/1	0.96	0.17	53,53,53,53	0
55	MG	1A	3125	1/1	0.96	0.17	45,45,45,45	0
55	MG	1a	3068	1/1	0.96	0.29	73,73,73,73	0
55	MG	1A	3028	1/1	0.96	0.53	37,37,37,37	0
55	MG	1A	3263	1/1	0.96	0.18	17,17,17,17	0
55	MG	1A	3647	1/1	0.96	0.12	39,39,39,39	0
55	MG	2A	3364	1/1	0.96	0.07	60,60,60,60	0
55	MG	2A	3713	1/1	0.96	0.03	79,79,79,79	0
55	MG	1a	3072	1/1	0.96	0.06	65,65,65,65	0
55	MG	1A	3355	1/1	0.96	0.13	53,53,53,53	0
55	MG	2A	3367	1/1	0.96	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3399	1/1	0.96	0.20	15,15,15,15	0
55	MG	2A	3370	1/1	0.96	0.11	76,76,76,76	0
55	MG	2A	3202	1/1	0.96	0.15	56,56,56,56	0
55	MG	1X	8001	1/1	0.96	0.10	31,31,31,31	0
55	MG	1A	3826	1/1	0.96	0.12	59,59,59,59	0
55	MG	2A	3723	1/1	0.96	0.05	73,73,73,73	0
55	MG	1A	3357	1/1	0.96	0.18	20,20,20,20	0
55	MG	2A	3378	1/1	0.96	0.15	51,51,51,51	0
55	MG	1A	3828	1/1	0.96	0.17	61,61,61,61	0
55	MG	1A	3013	1/1	0.96	0.07	51,51,51,51	0
55	MG	2A	3083	1/1	0.96	0.31	57,57,57,57	0
55	MG	2A	3546	1/1	0.96	0.06	87,87,87,87	0
55	MG	1A	3652	1/1	0.96	0.11	34,34,34,34	0
55	MG	2A	3087	1/1	0.96	0.18	62,62,62,62	0
55	MG	1B	3010	1/1	0.96	0.04	59,59,59,59	0
55	MG	2A	3550	1/1	0.96	0.10	48,48,48,48	0
55	MG	1a	3085	1/1	0.96	0.27	64,64,64,64	0
55	MG	1A	3832	1/1	0.96	0.11	55,55,55,55	0
55	MG	1A	3461	1/1	0.96	0.09	63,63,63,63	0
57	ZN	24	501	1/1	0.96	0.03	129,129,129,129	0
57	ZN	26	101	1/1	0.96	0.12	64,64,64,64	0
55	MG	1A	3108	1/1	0.96	0.20	24,24,24,24	0
55	MG	1A	3299	1/1	0.97	0.18	28,28,28,28	0
55	MG	1A	3558	1/1	0.97	0.12	27,27,27,27	0
55	MG	1A	3613	1/1	0.97	0.04	82,82,82,82	0
55	MG	2A	3572	1/1	0.97	0.13	55,55,55,55	0
55	MG	1A	3415	1/1	0.97	0.07	20,20,20,20	0
55	MG	1A	3416	1/1	0.97	0.14	26,26,26,26	0
55	MG	1G	3003	1/1	0.97	0.08	47,47,47,47	0
55	MG	2A	3576	1/1	0.97	0.41	52,52,52,52	0
55	MG	1A	3417	1/1	0.97	0.10	22,22,22,22	0
55	MG	1A	3085	1/1	0.97	0.35	34,34,34,34	0
55	MG	1A	3322	1/1	0.97	0.24	48,48,48,48	0
55	MG	1A	3565	1/1	0.97	0.14	20,20,20,20	0
55	MG	1A	3091	1/1	0.97	0.29	16,16,16,16	0
55	MG	1a	3033	1/1	0.97	0.10	50,50,50,50	0
55	MG	2A	3266	1/1	0.97	0.15	65,65,65,65	0
55	MG	2A	3267	1/1	0.97	0.26	61,61,61,61	0
55	MG	2A	3014	1/1	0.97	0.26	66,66,66,66	0
55	MG	1A	3421	1/1	0.97	0.12	28,28,28,28	0
55	MG	1A	3683	1/1	0.97	0.30	51,51,51,51	0
55	MG	1A	3422	1/1	0.97	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3137	1/1	0.97	0.84	60,60,60,60	0
55	MG	2A	3591	1/1	0.97	0.19	53,53,53,53	0
55	MG	2a	1638	1/1	0.97	0.16	73,73,73,73	0
55	MG	1A	3830	1/1	0.97	0.04	47,47,47,47	0
55	MG	1a	3147	1/1	0.97	0.13	85,85,85,85	0
55	MG	2A	3433	1/1	0.97	0.11	66,66,66,66	0
55	MG	2A	3275	1/1	0.97	0.10	47,47,47,47	0
55	MG	1A	3685	1/1	0.97	0.13	52,52,52,52	0
55	MG	1Q	202	1/1	0.97	0.07	39,39,39,39	0
55	MG	1A	3626	1/1	0.97	0.13	44,44,44,44	0
55	MG	1A	3754	1/1	0.97	0.05	39,39,39,39	0
55	MG	2A	3280	1/1	0.97	0.07	51,51,51,51	0
55	MG	2A	3778	1/1	0.97	0.22	50,50,50,50	0
55	MG	1A	3627	1/1	0.97	0.49	44,44,44,44	0
55	MG	1A	3423	1/1	0.97	0.13	20,20,20,20	0
55	MG	2A	3781	1/1	0.97	0.07	51,51,51,51	0
55	MG	1R	202	1/1	0.97	0.18	46,46,46,46	0
55	MG	1A	3915	1/1	0.97	0.20	60,60,60,60	0
55	MG	2A	3029	1/1	0.97	0.25	61,61,61,61	0
55	MG	2a	1655	1/1	0.97	0.06	84,84,84,84	0
55	MG	1A	3351	1/1	0.97	0.30	54,54,54,54	0
55	MG	1A	3185	1/1	0.97	0.66	32,32,32,32	0
55	MG	1A	3354	1/1	0.97	0.09	36,36,36,36	0
55	MG	2A	3033	1/1	0.97	0.09	59,59,59,59	0
55	MG	2A	3292	1/1	0.97	0.28	77,77,77,77	0
55	MG	2a	1661	1/1	0.97	0.26	63,63,63,63	0
55	MG	1A	3632	1/1	0.97	0.11	49,49,49,49	0
55	MG	1B	3004	1/1	0.97	0.11	44,44,44,44	0
55	MG	2A	3453	1/1	0.97	0.18	81,81,81,81	0
55	MG	2A	3156	1/1	0.97	0.52	39,39,39,39	0
55	MG	2a	1667	1/1	0.97	0.11	64,64,64,64	0
55	MG	2A	3296	1/1	0.97	0.15	42,42,42,42	0
55	MG	1A	3250	1/1	0.97	0.17	11,11,11,11	0
55	MG	1A	3356	1/1	0.97	0.15	25,25,25,25	0
55	MG	2a	1671	1/1	0.97	0.08	80,80,80,80	0
55	MG	1A	3576	1/1	0.97	0.51	47,47,47,47	0
55	MG	2A	3620	1/1	0.97	0.10	45,45,45,45	0
55	MG	1a	3164	1/1	0.97	0.14	61,61,61,61	0
55	MG	1A	3843	1/1	0.97	0.21	49,49,49,49	0
55	MG	1A	3844	1/1	0.97	0.07	27,27,27,27	0
55	MG	1A	3307	1/1	0.97	0.06	63,63,63,63	0
55	MG	2A	3043	1/1	0.97	0.12	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2a	1680	1/1	0.97	0.09	55,55,55,55	0
55	MG	1V	202	1/1	0.97	0.25	25,25,25,25	0
55	MG	1V	203	1/1	0.97	0.12	60,60,60,60	0
55	MG	2A	3308	1/1	0.97	0.23	52,52,52,52	0
55	MG	1A	3330	1/1	0.97	0.11	37,37,37,37	0
55	MG	1A	3699	1/1	0.97	0.08	38,38,38,38	0
55	MG	2a	1687	1/1	0.97	0.23	55,55,55,55	0
55	MG	2A	3170	1/1	0.97	0.23	73,73,73,73	0
55	MG	2A	3312	1/1	0.97	0.16	53,53,53,53	0
55	MG	1A	3434	1/1	0.97	0.21	16,16,16,16	0
55	MG	2A	3473	1/1	0.97	0.09	61,61,61,61	0
55	MG	2A	3315	1/1	0.97	0.16	67,67,67,67	0
55	MG	2a	1693	1/1	0.97	0.21	54,54,54,54	0
55	MG	1a	3174	1/1	0.97	0.11	70,70,70,70	0
55	MG	1A	3391	1/1	0.97	0.16	18,18,18,18	0
55	MG	1Y	502	1/1	0.97	0.10	74,74,74,74	0
55	MG	2A	3052	1/1	0.97	0.42	42,42,42,42	0
55	MG	1A	3770	1/1	0.97	0.14	34,34,34,34	0
55	MG	1A	3851	1/1	0.97	0.07	21,21,21,21	0
55	MG	2B	3001	1/1	0.97	0.12	64,64,64,64	0
55	MG	1A	3086	1/1	0.97	0.06	50,50,50,50	0
55	MG	2A	3326	1/1	0.97	0.10	35,35,35,35	0
55	MG	1A	3529	1/1	0.97	0.15	58,58,58,58	0
55	MG	1A	3773	1/1	0.97	0.17	44,44,44,44	0
55	MG	1A	3774	1/1	0.97	0.25	45,45,45,45	0
55	MG	2A	3648	1/1	0.97	0.06	34,34,34,34	0
55	MG	1A	3176	1/1	0.97	0.27	52,52,52,52	0
55	MG	1A	3776	1/1	0.97	0.10	43,43,43,43	0
55	MG	2A	3488	1/1	0.97	0.13	58,58,58,58	0
55	MG	1D	301	1/1	0.97	0.22	32,32,32,32	0
55	MG	1A	3333	1/1	0.97	0.18	17,17,17,17	0
55	MG	2a	1714	1/1	0.97	0.14	71,71,71,71	0
55	MG	2A	3491	1/1	0.97	0.11	51,51,51,51	0
55	MG	1A	3286	1/1	0.97	0.11	64,64,64,64	0
55	MG	1A	3366	1/1	0.97	0.12	26,26,26,26	0
55	MG	2A	3336	1/1	0.97	0.22	56,56,56,56	0
55	MG	1A	3024	1/1	0.97	0.36	30,30,30,30	0
55	MG	2A	3189	1/1	0.97	0.16	43,43,43,43	0
55	MG	1A	3109	1/1	0.97	0.12	30,30,30,30	0
55	MG	1a	3080	1/1	0.97	0.12	69,69,69,69	0
55	MG	2A	3662	1/1	0.97	0.07	68,68,68,68	0
55	MG	2A	3663	1/1	0.97	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	3081	1/1	0.97	0.23	69,69,69,69	0
55	MG	2A	3501	1/1	0.97	0.11	76,76,76,76	0
55	MG	2A	3070	1/1	0.97	0.18	35,35,35,35	0
55	MG	2A	3667	1/1	0.97	0.12	57,57,57,57	0
55	MG	2A	3503	1/1	0.97	0.23	53,53,53,53	0
55	MG	2A	3669	1/1	0.97	0.13	40,40,40,40	0
55	MG	1A	3369	1/1	0.97	0.07	14,14,14,14	0
55	MG	1a	3083	1/1	0.97	0.26	67,67,67,67	0
55	MG	2E	302	1/1	0.97	0.06	35,35,35,35	0
55	MG	1A	3864	1/1	0.97	0.10	49,49,49,49	0
55	MG	1A	3015	1/1	0.97	0.42	23,23,23,23	0
55	MG	2E	305	1/1	0.97	0.12	34,34,34,34	0
55	MG	1a	3198	1/1	0.97	0.05	47,47,47,47	0
55	MG	2A	3199	1/1	0.97	0.27	65,65,65,65	0
55	MG	2A	3349	1/1	0.97	0.06	77,77,77,77	0
55	MG	1a	3086	1/1	0.97	0.34	68,68,68,68	0
55	MG	1A	3493	1/1	0.97	0.12	30,30,30,30	0
55	MG	2a	1743	1/1	0.97	0.04	55,55,55,55	0
55	MG	1a	3088	1/1	0.97	0.37	63,63,63,63	0
55	MG	2A	3514	1/1	0.97	0.48	53,53,53,53	0
55	MG	2a	1746	1/1	0.97	0.06	69,69,69,69	0
55	MG	1A	3867	1/1	0.97	0.67	37,37,37,37	0
55	MG	2A	3354	1/1	0.97	0.17	26,26,26,26	0
55	MG	1A	3170	1/1	0.97	0.54	34,34,34,34	0
55	MG	2A	3205	1/1	0.97	0.68	52,52,52,52	0
55	MG	1a	3205	1/1	0.97	0.07	77,77,77,77	0
55	MG	1a	3206	1/1	0.97	0.04	68,68,68,68	0
55	MG	2A	3209	1/1	0.97	0.09	81,81,81,81	0
55	MG	2A	3085	1/1	0.97	0.26	62,62,62,62	0
55	MG	2a	1755	1/1	0.97	0.73	81,81,81,81	0
55	MG	1a	3093	1/1	0.97	0.06	73,73,73,73	0
55	MG	1A	3229	1/1	0.97	0.23	62,62,62,62	0
55	MG	1A	3496	1/1	0.97	0.07	51,51,51,51	0
55	MG	1A	3342	1/1	0.97	0.09	21,21,21,21	0
55	MG	2Q	8001	1/1	0.97	0.03	79,79,79,79	0
55	MG	1A	3872	1/1	0.97	0.08	29,29,29,29	0
55	MG	2a	1762	1/1	0.97	0.10	74,74,74,74	0
55	MG	1A	3793	1/1	0.97	0.06	52,52,52,52	0
55	MG	2A	3698	1/1	0.97	0.14	42,42,42,42	0
55	MG	2a	1765	1/1	0.97	0.10	71,71,71,71	0
55	MG	2Q	8005	1/1	0.97	0.09	62,62,62,62	0
55	MG	2A	3699	1/1	0.97	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	3100	1/1	0.97	0.31	60,60,60,60	0
55	MG	2A	3219	1/1	0.97	0.37	22,22,22,22	0
55	MG	2A	3373	1/1	0.97	0.11	48,48,48,48	0
55	MG	1A	3874	1/1	0.97	0.17	59,59,59,59	0
55	MG	1A	3717	1/1	0.97	0.10	35,35,35,35	0
55	MG	2A	3376	1/1	0.97	0.11	31,31,31,31	0
55	MG	1A	3795	1/1	0.97	0.35	46,46,46,46	0
55	MG	1A	3655	1/1	0.97	0.32	41,41,41,41	0
55	MG	2A	3710	1/1	0.97	0.10	60,60,60,60	0
55	MG	2A	3711	1/1	0.97	0.08	70,70,70,70	0
55	MG	2a	1780	1/1	0.97	0.06	68,68,68,68	0
55	MG	2V	204	1/1	0.97	0.39	77,77,77,77	0
55	MG	1a	3002	1/1	0.97	0.15	82,82,82,82	0
55	MG	1A	3546	1/1	0.97	0.33	25,25,25,25	0
55	MG	2A	3714	1/1	0.97	0.10	49,49,49,49	0
55	MG	1A	3343	1/1	0.97	0.09	26,26,26,26	0
55	MG	1A	3081	1/1	0.97	0.51	33,33,33,33	0
55	MG	1E	307	1/1	0.97	0.19	33,33,33,33	0
55	MG	1E	308	1/1	0.97	0.15	49,49,49,49	0
55	MG	2A	3231	1/1	0.97	0.19	48,48,48,48	0
55	MG	1A	3500	1/1	0.97	0.37	65,65,65,65	0
55	MG	1A	3723	1/1	0.97	0.10	47,47,47,47	0
55	MG	1A	3096	1/1	0.97	0.54	34,34,34,34	0
55	MG	1A	3603	1/1	0.97	0.08	49,49,49,49	0
55	MG	1A	3409	1/1	0.97	0.08	49,49,49,49	0
55	MG	2A	3551	1/1	0.97	0.06	71,71,71,71	0
55	MG	1A	3410	1/1	0.97	0.20	42,42,42,42	0
55	MG	1a	3014	1/1	0.97	0.32	81,81,81,81	0
55	MG	1a	3015	1/1	0.97	0.21	74,74,74,74	0
55	MG	1a	3121	1/1	0.97	0.51	62,62,62,62	0
55	MG	2A	3730	1/1	0.97	0.12	56,56,56,56	0
55	MG	1A	3665	1/1	0.97	0.26	51,51,51,51	0
55	MG	1A	3232	1/1	0.97	0.99	35,35,35,35	0
55	MG	1A	3412	1/1	0.97	0.16	12,12,12,12	0
55	MG	2A	3735	1/1	0.97	0.18	49,49,49,49	0
55	MG	1a	3126	1/1	0.97	0.15	74,74,74,74	0
55	MG	2A	3247	1/1	0.97	0.17	35,35,35,35	0
55	MG	1A	3379	1/1	0.97	0.15	43,43,43,43	0
55	MG	2A	3739	1/1	0.97	0.07	69,69,69,69	0
55	MG	2A	3249	1/1	0.97	0.25	43,43,43,43	0
55	MG	2A	3407	1/1	0.97	0.32	74,74,74,74	0
55	MG	1A	3508	1/1	0.97	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	ZN	14	501	1/1	0.97	0.04	109,109,109,109	0
55	MG	1A	3816	1/1	0.97	0.11	19,19,19,19	0
57	ZN	2Y	501	1/1	0.97	0.06	95,95,95,95	0
55	MG	2A	3119	1/1	0.97	0.54	49,49,49,49	0
55	MG	2a	1612	1/1	0.97	0.12	51,51,51,51	0
55	MG	2A	3411	1/1	0.97	0.11	63,63,63,63	0
55	MG	2a	1695	1/1	0.98	0.26	58,58,58,58	0
55	MG	1A	3430	1/1	0.98	0.12	16,16,16,16	0
55	MG	2A	3153	1/1	0.98	0.10	52,52,52,52	0
55	MG	2A	3552	1/1	0.98	0.32	52,52,52,52	0
55	MG	1a	3142	1/1	0.98	0.09	85,85,85,85	0
55	MG	2a	1700	1/1	0.98	0.13	76,76,76,76	0
55	MG	1A	3397	1/1	0.98	0.03	64,64,64,64	0
55	MG	1A	3003	1/1	0.98	0.09	20,20,20,20	0
55	MG	1A	3296	1/1	0.98	0.15	20,20,20,20	0
55	MG	1A	3141	1/1	0.98	0.31	37,37,37,37	0
55	MG	1A	3280	1/1	0.98	0.09	29,29,29,29	0
55	MG	2A	3452	1/1	0.98	0.07	51,51,51,51	0
55	MG	2A	3160	1/1	0.98	0.39	46,46,46,46	0
55	MG	2A	3251	1/1	0.98	0.04	79,79,79,79	0
55	MG	1A	3319	1/1	0.98	0.20	34,34,34,34	0
55	MG	20	105	1/1	0.98	0.12	81,81,81,81	0
55	MG	2A	3671	1/1	0.98	0.25	73,73,73,73	0
55	MG	1A	3437	1/1	0.98	0.07	34,34,34,34	0
55	MG	21	102	1/1	0.98	0.07	60,60,60,60	0
55	MG	1A	3142	1/1	0.98	0.92	32,32,32,32	0
55	MG	1A	3439	1/1	0.98	0.07	54,54,54,54	0
55	MG	1A	3606	1/1	0.98	0.17	56,56,56,56	0
55	MG	2A	3355	1/1	0.98	0.03	76,76,76,76	0
55	MG	1A	3374	1/1	0.98	0.09	62,62,62,62	0
55	MG	1A	3562	1/1	0.98	0.23	20,20,20,20	0
55	MG	2A	3679	1/1	0.98	0.08	52,52,52,52	0
55	MG	1A	3441	1/1	0.98	0.14	40,40,40,40	0
55	MG	1A	3405	1/1	0.98	0.09	42,42,42,42	0
55	MG	2A	3084	1/1	0.98	0.27	45,45,45,45	0
55	MG	1A	3300	1/1	0.98	0.07	44,44,44,44	0
55	MG	1A	3661	1/1	0.98	0.08	33,33,33,33	0
55	MG	1A	3909	1/1	0.98	0.16	32,32,32,32	0
55	MG	1A	3240	1/1	0.98	0.18	58,58,58,58	0
55	MG	2a	1604	1/1	0.98	0.15	53,53,53,53	0
55	MG	1A	3223	1/1	0.98	0.08	42,42,42,42	0
55	MG	2A	3578	1/1	0.98	0.06	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3614	1/1	0.98	0.15	70,70,70,70	0
55	MG	2A	3368	1/1	0.98	0.05	42,42,42,42	0
55	MG	1G	3001	1/1	0.98	0.10	67,67,67,67	0
55	MG	1A	3284	1/1	0.98	0.12	43,43,43,43	0
55	MG	1A	3779	1/1	0.98	0.10	24,24,24,24	0
55	MG	1A	3325	1/1	0.98	0.06	28,28,28,28	0
55	MG	1A	3667	1/1	0.98	0.19	46,46,46,46	0
55	MG	1A	3782	1/1	0.98	0.06	33,33,33,33	0
55	MG	1B	3001	1/1	0.98	0.23	55,55,55,55	0
55	MG	2a	1740	1/1	0.98	0.05	70,70,70,70	0
55	MG	1a	3089	1/1	0.98	0.06	52,52,52,52	0
55	MG	1a	3171	1/1	0.98	0.10	50,50,50,50	0
55	MG	2A	3701	1/1	0.98	0.06	60,60,60,60	0
55	MG	2A	3817	1/1	0.98	0.12	65,65,65,65	0
55	MG	1A	3617	1/1	0.98	0.05	38,38,38,38	0
55	MG	1A	3304	1/1	0.98	0.08	45,45,45,45	0
55	MG	1A	3785	1/1	0.98	0.09	25,25,25,25	0
55	MG	1A	3619	1/1	0.98	0.16	44,44,44,44	0
55	MG	1A	3571	1/1	0.98	0.31	54,54,54,54	0
55	MG	2A	3384	1/1	0.98	0.09	68,68,68,68	0
55	MG	1A	3225	1/1	0.98	0.10	34,34,34,34	0
55	MG	1A	3673	1/1	0.98	0.13	35,35,35,35	0
55	MG	1A	3353	1/1	0.98	0.12	67,67,67,67	0
55	MG	2A	3492	1/1	0.98	0.08	52,52,52,52	0
55	MG	2A	3388	1/1	0.98	0.14	60,60,60,60	0
55	MG	2A	3023	1/1	0.98	0.32	47,47,47,47	0
55	MG	2A	3390	1/1	0.98	0.14	49,49,49,49	0
55	MG	1A	3791	1/1	0.98	0.06	33,33,33,33	0
55	MG	1B	3011	1/1	0.98	0.15	48,48,48,48	0
55	MG	2A	3289	1/1	0.98	0.13	46,46,46,46	0
55	MG	1A	3328	1/1	0.98	0.12	22,22,22,22	0
55	MG	1A	3492	1/1	0.98	0.16	50,50,50,50	0
55	MG	1B	3014	1/1	0.98	0.07	41,41,41,41	0
55	MG	1A	3329	1/1	0.98	0.11	40,40,40,40	0
55	MG	1A	3252	1/1	0.98	0.50	36,36,36,36	0
55	MG	1A	3273	1/1	0.98	0.25	19,19,19,19	0
55	MG	1A	3797	1/1	0.98	0.06	28,28,28,28	0
55	MG	2A	3613	1/1	0.98	0.08	55,55,55,55	0
55	MG	1A	3798	1/1	0.98	0.09	48,48,48,48	0
55	MG	1a	3110	1/1	0.98	0.08	52,52,52,52	0
55	MG	2a	1771	1/1	0.98	0.07	55,55,55,55	0
55	MG	2A	3206	1/1	0.98	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3405	1/1	0.98	0.08	43,43,43,43	0
55	MG	2A	3300	1/1	0.98	0.12	36,36,36,36	0
55	MG	2a	1775	1/1	0.98	0.08	63,63,63,63	0
55	MG	1A	3799	1/1	0.98	0.11	49,49,49,49	0
55	MG	1A	3288	1/1	0.98	0.14	26,26,26,26	0
55	MG	2A	3734	1/1	0.98	0.04	67,67,67,67	0
55	MG	1A	3274	1/1	0.98	0.18	27,27,27,27	0
55	MG	1U	205	1/1	0.98	0.36	29,29,29,29	0
55	MG	1A	3360	1/1	0.98	0.12	21,21,21,21	0
55	MG	2A	3516	1/1	0.98	0.09	45,45,45,45	0
55	MG	1A	3290	1/1	0.98	0.04	49,49,49,49	0
55	MG	1A	3059	1/1	0.98	0.19	35,35,35,35	0
55	MG	1A	3739	1/1	0.98	0.17	22,22,22,22	0
55	MG	1A	3740	1/1	0.98	0.04	26,26,26,26	0
55	MG	2A	3216	1/1	0.98	0.24	41,41,41,41	0
55	MG	1A	3337	1/1	0.98	0.10	39,39,39,39	0
55	MG	1A	3585	1/1	0.98	0.25	59,59,59,59	0
55	MG	1A	3542	1/1	0.98	0.11	77,77,77,77	0
55	MG	2A	3220	1/1	0.98	0.10	66,66,66,66	0
55	MG	2A	3316	1/1	0.98	0.17	43,43,43,43	0
55	MG	1A	3744	1/1	0.98	0.06	55,55,55,55	0
55	MG	2a	1794	1/1	0.98	0.07	70,70,70,70	0
55	MG	1a	3125	1/1	0.98	0.30	74,74,74,74	0
55	MG	1A	3811	1/1	0.98	0.05	56,56,56,56	0
55	MG	1A	3587	1/1	0.98	0.06	50,50,50,50	0
55	MG	1A	3502	1/1	0.98	0.11	62,62,62,62	0
55	MG	1A	3814	1/1	0.98	0.10	18,18,18,18	0
55	MG	1A	3544	1/1	0.98	0.30	34,34,34,34	0
55	MG	2A	3325	1/1	0.98	0.07	51,51,51,51	0
55	MG	1a	3051	1/1	0.98	0.42	57,57,57,57	0
55	MG	2a	1678	1/1	0.98	0.47	65,65,65,65	0
55	MG	1A	3364	1/1	0.98	0.25	36,36,36,36	0
55	MG	2A	3645	1/1	0.98	0.08	62,62,62,62	0
55	MG	1a	3214	1/1	0.98	0.04	71,71,71,71	0
55	MG	1A	3365	1/1	0.98	0.11	40,40,40,40	0
55	MG	1A	3466	1/1	0.98	0.08	46,46,46,46	0
55	MG	1A	3752	1/1	0.98	0.07	22,22,22,22	0
55	MG	1A	3043	1/1	0.98	0.30	10,10,10,10	0
55	MG	1a	3219	1/1	0.98	0.16	63,63,63,63	0
55	MG	1A	3468	1/1	0.98	0.06	49,49,49,49	0
55	MG	2A	3767	1/1	0.98	0.06	65,65,65,65	0
55	MG	1A	3888	1/1	0.98	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3238	1/1	0.98	0.10	38,38,38,38	0
55	MG	2A	3239	1/1	0.98	0.10	38,38,38,38	0
55	MG	1A	3107	1/1	0.98	0.47	36,36,36,36	0
57	ZN	29	501	1/1	0.98	0.10	75,75,75,75	0
55	MG	1A	3697	1/1	0.98	0.13	19,19,19,19	0
55	MG	1A	3453	1/1	0.99	0.13	19,19,19,19	0
55	MG	2A	3801	1/1	0.99	0.26	21,21,21,21	0
55	MG	2A	3402	1/1	0.99	0.11	37,37,37,37	0
55	MG	1A	3334	1/1	0.99	0.14	20,20,20,20	0
55	MG	1A	3749	1/1	0.99	0.06	36,36,36,36	0
55	MG	1A	3426	1/1	0.99	0.06	18,18,18,18	0
55	MG	2T	201	1/1	0.99	0.12	47,47,47,47	0
55	MG	2A	3372	1/1	0.99	0.13	38,38,38,38	0
55	MG	1a	3111	1/1	0.99	0.14	56,56,56,56	0
55	MG	1A	3540	1/1	0.99	0.17	19,19,19,19	0
55	MG	1a	3202	1/1	0.99	0.07	47,47,47,47	0
55	MG	1a	3091	1/1	0.99	0.08	37,37,37,37	0
55	MG	1A	3065	1/1	0.99	0.19	32,32,32,32	0
55	MG	2A	3314	1/1	0.99	0.14	60,60,60,60	0
55	MG	11	102	1/1	0.99	0.05	56,56,56,56	0
55	MG	2A	3518	1/1	0.99	0.14	71,71,71,71	0
55	MG	1A	3295	1/1	0.99	0.13	13,13,13,13	0
55	MG	1a	3037	1/1	0.99	0.18	68,68,68,68	0
55	MG	2A	3288	1/1	0.99	0.07	30,30,30,30	0
55	MG	1A	3897	1/1	0.99	0.20	11,11,11,11	0
55	MG	2A	3067	1/1	0.99	0.09	62,62,62,62	0
55	MG	2a	1665	1/1	0.99	0.09	74,74,74,74	0
55	MG	2d	502	1/1	0.99	0.13	74,74,74,74	0
55	MG	1A	3769	1/1	0.99	0.07	61,61,61,61	0
55	MG	2a	1624	1/1	0.99	0.20	53,53,53,53	0
55	MG	1A	3447	1/1	0.99	0.15	17,17,17,17	0
55	MG	2A	3323	1/1	0.99	0.22	66,66,66,66	0
55	MG	2a	1627	1/1	0.99	0.26	84,84,84,84	0
55	MG	2A	3124	1/1	0.99	0.23	47,47,47,47	0
55	MG	2A	3709	1/1	0.99	0.09	45,45,45,45	0
55	MG	1a	3099	1/1	0.99	0.14	61,61,61,61	0
55	MG	1A	3429	1/1	0.99	0.10	26,26,26,26	0
55	MG	2A	3358	1/1	0.99	0.16	45,45,45,45	0
55	MG	1A	3460	1/1	0.99	0.13	20,20,20,20	0
55	MG	1a	3190	1/1	0.99	0.04	79,79,79,79	0
55	MG	1A	3306	1/1	0.99	0.12	14,14,14,14	0
55	MG	1A	3152	1/1	0.99	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3224	1/1	0.99	0.07	73,73,73,73	0
57	ZN	1Y	501	1/1	0.99	0.13	61,61,61,61	0
55	MG	1A	3197	1/1	0.99	0.13	25,25,25,25	0
57	ZN	15	106	1/1	0.99	0.16	47,47,47,47	0
57	ZN	16	101	1/1	0.99	0.12	44,44,44,44	0
55	MG	2A	3466	1/1	0.99	0.10	37,37,37,37	0
55	MG	1A	3732	1/1	0.99	0.09	21,21,21,21	0
55	MG	2A	3683	1/1	0.99	0.06	60,60,60,60	0
57	ZN	25	104	1/1	0.99	0.11	54,54,54,54	0
55	MG	2a	1685	1/1	0.99	0.15	56,56,56,56	0
55	MG	2A	3079	1/1	0.99	0.28	50,50,50,50	0
55	MG	2A	3003	1/1	0.99	0.11	31,31,31,31	0
58	SF4	1d	501	8/8	0.99	0.14	65,70,75,78	0
58	SF4	2d	501	8/8	0.99	0.12	65,69,77,88	0
57	ZN	19	102	1/1	1.00	0.12	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.