



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2024 – 12:12 am GMT

PDB ID : 5FDV  
Title : Crystal structure of the Pyrrhocoricin 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 : 2.80 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](mailto: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>.

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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  
buster-report : 1.1.7 (2018)  
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

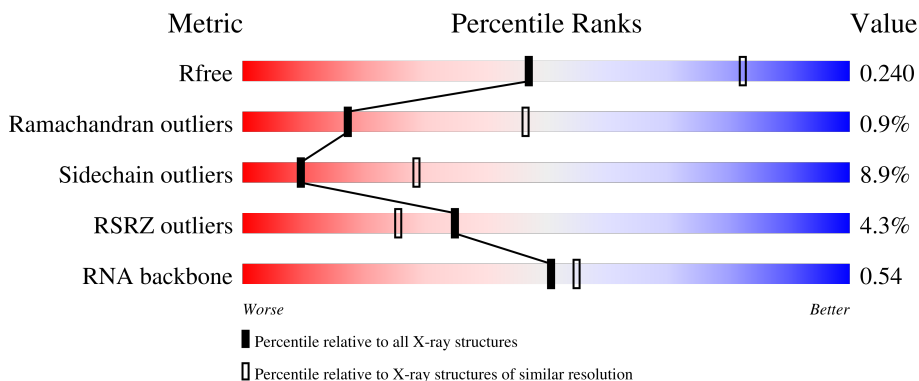
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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  $\geq 3$ , 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	

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Mol	Chain	Length	Quality of chain
3	1D	275	92% 8%
3	2D	275	91% 9%
4	1E	204	91% 8%
4	2E	204	91% 9%
5	1F	203	87% 13%
5	2F	203	91% 9%
6	1G	181	92% 7%
6	2G	181	8% 93% 7%
7	1H	174	93% 7%
7	2H	174	16% 92% 7%
8	1I	147	88% 11%
8	2I	147	3% 90% 8%
9	1N	140	88% 12%
9	2N	140	90% 10%
10	1O	122	92% 7%
10	2O	122	93% 7%
11	1P	149	94% 6%
11	2P	149	2% 93% 7%
12	1Q	141	94% 6%
12	2Q	141	94% 6%
13	1R	118	87% 11%
13	2R	118	87% 13%
14	1S	110	88% 11%
14	2S	110	3% 91% 9%
15	1T	131	92% 8%

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Mol	Chain	Length	Quality of chain
15	2T	131	95% 5%
16	1U	116	85% 14%
16	2U	116	95% 5%
17	1V	101	90% 8%
17	2V	101	91% 8%
18	1W	112	2% 90% 8%
18	2W	112	93% 6%
19	1X	95	94% 6%
19	2X	95	% 94% 5%
20	1Y	107	% 94% 6%
20	2Y	107	11% 95% 5%
21	1Z	203	91% 9%
21	2Z	203	% 91% 8%
22	10	77	91% 9%
22	20	77	3% 94% 6%
23	11	97	% 93% 7%
23	21	97	% 91% 7%
24	12	70	94% 6%
24	22	70	99%
25	13	59	95% 5%
25	23	59	3% 93% 7%
26	14	69	17% 84% 14%
26	24	69	30% 81% 19%
27	15	59	86% 12%
27	25	59	92% 8%

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Mol	Chain	Length	Quality of chain
28	16	53	83% 17%
28	26	53	92% 8%
29	17	48	92% 6% .
29	27	48	96% .
30	18	64	84% 16%
30	28	64	92% 8%
31	19	37	92% 5% .
31	29	37	3% 100%
32	1a	1521	4% 52% 38% 8% .
32	2a	1521	4% 57% 35% 8% .
33	1x	97	% 95% 5%
33	2x	97	41% 89% 10% .
34	1b	231	8% 84% 14% .
34	2b	231	6% 87% 12% .
35	1c	206	6% 98% .
35	2c	206	8% 91% 9% .
36	1d	208	% 91% 9% .
36	2d	208	% 91% 9% .
37	1e	148	93% 7%
37	2e	148	94% 6%
38	1f	100	96% .
38	2f	100	94% 6%
39	1g	155	3% 95% 5% .
39	2g	155	9% 94% 6% .
40	1h	137	% 94% 6% .

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Mol	Chain	Length	Quality of chain
40	2h	137	96% .
41	1i	127	6% 92% 8%
41	2i	127	27% 90% 9% .
42	1j	97	21% 91% 9%
42	2j	97	20% 92% 7% .
43	1k	114	96% .
43	2k	114	% 91% 9%
44	1l	122	2% 95% 5%
44	2l	122	% 90% 8% .
45	1m	116	7% 91% 9%
45	2m	116	9% 88% 10% .
46	1n	60	7% 90% 8% .
46	2n	60	17% 95% . .
47	1o	88	% 93% 7%
47	2o	88	% 93% 7%
48	1p	82	4% 89% 11%
48	2p	82	2% 87% 13%
49	1q	99	2% 96% .
49	2q	99	93% 6% .
50	1r	68	7% 91% 9%
50	2r	68	3% 94% 6%
51	1s	83	19% 88% 12%
51	2s	83	39% 90% 8% .
52	1t	98	3% 90% 7% . .
52	2t	98	% 89% 11%

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Mol	Chain	Length	Quality of chain
53	1u	23	
53	2u	23	
54	1y	16	
54	2y	16	

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	1A	3062	-	-	-	X
55	MG	1A	3095	-	-	-	X
55	MG	1A	3174	-	-	-	X
55	MG	1A	3213	-	-	-	X
55	MG	1A	3219	-	-	-	X
55	MG	1A	3254	-	-	-	X
55	MG	1A	3514	-	-	-	X
55	MG	1A	3700	-	-	-	X
55	MG	1A	3724	-	-	-	X
55	MG	1A	3757	-	-	-	X
55	MG	1A	3758	-	-	-	X
55	MG	1A	3898	-	-	-	X
55	MG	1A	3904	-	-	-	X
55	MG	1D	303	-	-	-	X
55	MG	1a	3038	-	-	-	X
55	MG	1a	3039	-	-	-	X
55	MG	1a	3049	-	-	-	X
55	MG	1a	3057	-	-	-	X
55	MG	1a	3058	-	-	-	X
55	MG	1a	3063	-	-	-	X
55	MG	1a	3074	-	-	-	X
55	MG	1a	3077	-	-	-	X
55	MG	1a	3078	-	-	-	X
55	MG	1a	3136	-	-	-	X
55	MG	28	101	-	-	-	X
55	MG	2A	3011	-	-	-	X
55	MG	2A	3028	-	-	-	X
55	MG	2A	3041	-	-	-	X
55	MG	2A	3042	-	-	-	X
55	MG	2A	3049	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2A	3109	-	-	-	X
55	MG	2A	3128	-	-	-	X
55	MG	2A	3131	-	-	-	X
55	MG	2A	3132	-	-	-	X
55	MG	2A	3133	-	-	-	X
55	MG	2A	3136	-	-	-	X
55	MG	2A	3138	-	-	-	X
55	MG	2A	3141	-	-	-	X
55	MG	2A	3151	-	-	-	X
55	MG	2A	3183	-	-	-	X
55	MG	2A	3188	-	-	-	X
55	MG	2A	3255	-	-	-	X
55	MG	2A	3411	-	-	-	X
55	MG	2A	3416	-	-	-	X
55	MG	2A	3454	-	-	-	X
55	MG	2A	3475	-	-	-	X
55	MG	2A	3506	-	-	-	X
55	MG	2A	3513	-	-	-	X
55	MG	2A	3533	-	-	-	X
55	MG	2A	3549	-	-	-	X
55	MG	2A	3554	-	-	-	X
55	MG	2A	3555	-	-	-	X
55	MG	2A	3562	-	-	-	X
55	MG	2A	3631	-	-	-	X
55	MG	2A	3727	-	-	-	X
55	MG	2A	3752	-	-	-	X
55	MG	2A	3765	-	-	-	X
55	MG	2A	3791	-	-	-	X
55	MG	2A	3795	-	-	-	X
55	MG	2A	3811	-	-	-	X
55	MG	2A	3813	-	-	-	X
55	MG	2A	3815	-	-	-	X
55	MG	2D	304	-	-	-	X
55	MG	2N	201	-	-	-	X
55	MG	2Q	204	-	-	-	X
55	MG	2X	102	-	-	-	X
55	MG	2a	1603	-	-	-	X
55	MG	2a	1620	-	-	-	X
55	MG	2a	1641	-	-	-	X
55	MG	2a	1654	-	-	-	X
55	MG	2a	1733	-	-	-	X
55	MG	2a	1741	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
55	MG	2l	201	-	-	-	X
55	MG	2n	502	-	-	-	X
58	A	2A	3816	-	-	-	X

## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 293583 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
			Total	C	N	O	S			
5	1F	203	Total 1584	C 1009	N 298	O 275	S 2	0	0	1
5	2F	203	Total 1580	C 1007	N 297	O 274	S 2	0	0	1

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	1W	112	Total 886	C 557	N 174	O 153	S 2	0	0	0
18	2W	112	Total 886	C 557	N 174	O 153	S 2	0	0	0

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

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

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

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

- 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 Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	2x	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			
33	1x	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
34	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
35	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
36	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

- Molecule 37 is a protein called 30S ribosomal protein S5.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
37	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
38	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
39	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
40	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
41	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	2j	96	710	442	137	131	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	1k	114	834	520	156	155	3	0	0	0
43	2k	114	833	519	156	155	3	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1l	122	932	586	185	159	2	0	0	0
44	2l	122	932	586	185	159	2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	1m	116	914	564	189	159	2	0	0	0
45	2m	114	895	550	186	157	2	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	1n	60	492	312	104	72	4	0	0	0
46	2n	60	492	312	104	72	4	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	1o	88	728	456	144	126	2	0	0	0
47	2o	88	728	456	144	126	2	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
48	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
49	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
50	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
51	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
52	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

- Molecule 53 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
53	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 54 is a protein called Pyrrhocoricin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	1y	16	Total	C	N	O	0	0	0
			120	79	20	21			
54	2y	16	Total	C	N	O	0	0	0
			120	79	20	21			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1A	945	Total	Mg	0	0
			945	945		
55	1B	26	Total	Mg	0	0
			26	26		
55	1D	14	Total	Mg	0	0
			14	14		
55	1E	5	Total	Mg	0	0
			5	5		
55	1F	12	Total	Mg	0	0
			12	12		
55	1G	3	Total	Mg	0	0
			3	3		
55	1H	2	Total	Mg	0	0
			2	2		
55	1N	4	Total	Mg	0	0
			4	4		
55	1P	2	Total	Mg	0	0
			2	2		
55	1Q	4	Total	Mg	0	0
			4	4		
55	1R	3	Total	Mg	0	0
			3	3		
55	1U	3	Total	Mg	0	0
			3	3		
55	1V	1	Total	Mg	0	0
			1	1		
55	1W	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1X	1	Total Mg 1 1	0	0
55	1Y	1	Total Mg 1 1	0	0
55	10	7	Total Mg 7 7	0	0
55	11	3	Total Mg 3 3	0	0
55	13	1	Total Mg 1 1	0	0
55	15	4	Total Mg 4 4	0	0
55	17	2	Total Mg 2 2	0	0
55	18	3	Total Mg 3 3	0	0
55	19	2	Total Mg 2 2	0	0
55	1a	226	Total Mg 226 226	0	0
55	1b	1	Total Mg 1 1	0	0
55	1d	5	Total Mg 5 5	0	0
55	1e	1	Total Mg 1 1	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	1o	1	Total Mg 1 1	0	0
55	1t	1	Total Mg 1 1	0	0
55	1y	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	2A	837	Total Mg 837 837	0	0
55	2B	18	Total Mg 18 18	0	0
55	2D	10	Total Mg 10 10	0	0
55	2E	4	Total Mg 4 4	0	0
55	2F	9	Total Mg 9 9	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	2	Total Mg 2 2	0	0
55	2S	1	Total Mg 1 1	0	0
55	2U	2	Total Mg 2 2	0	0
55	2V	3	Total Mg 3 3	0	0
55	2W	1	Total Mg 1 1	0	0
55	2X	3	Total Mg 3 3	0	0
55	20	5	Total Mg 5 5	0	0
55	21	2	Total Mg 2 2	0	0
55	25	3	Total Mg 3 3	0	0
55	27	2	Total Mg 2 2	0	0
55	28	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	2a	197	Total Mg 197 197	0	0
55	2b	1	Total Mg 1 1	0	0
55	2d	3	Total Mg 3 3	0	0
55	2e	2	Total Mg 2 2	0	0
55	2f	1	Total Mg 1 1	0	0
55	2g	1	Total Mg 1 1	0	0
55	2h	2	Total Mg 2 2	0	0
55	2l	2	Total Mg 2 2	0	0
55	2n	1	Total Mg 1 1	0	0
55	2o	1	Total Mg 1 1	0	0
55	2q	1	Total Mg 1 1	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

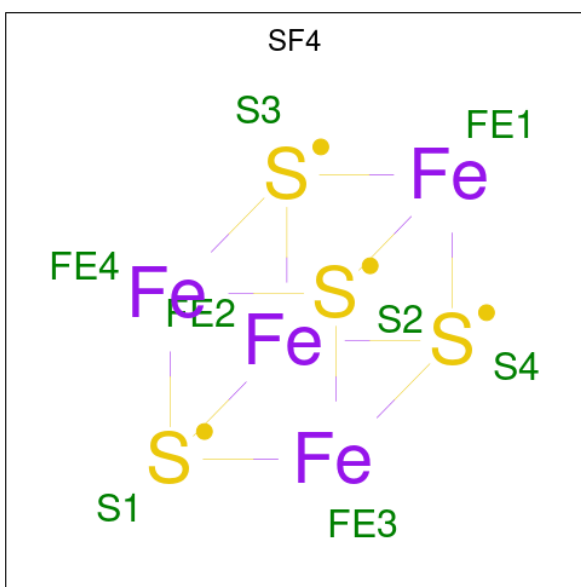
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1Y	1	Total Zn 1 1	0	0
56	14	1	Total Zn 1 1	0	0
56	15	1	Total Zn 1 1	0	0
56	16	1	Total Zn 1 1	0	0
56	19	1	Total Zn 1 1	0	0
56	1n	1	Total Zn 1 1	0	0
56	2Y	1	Total Zn 1 1	0	0
56	24	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	25	1	Total Zn 1 1	0	0
56	26	1	Total Zn 1 1	0	0
56	29	1	Total Zn 1 1	0	0
56	2n	1	Total Zn 1 1	0	0

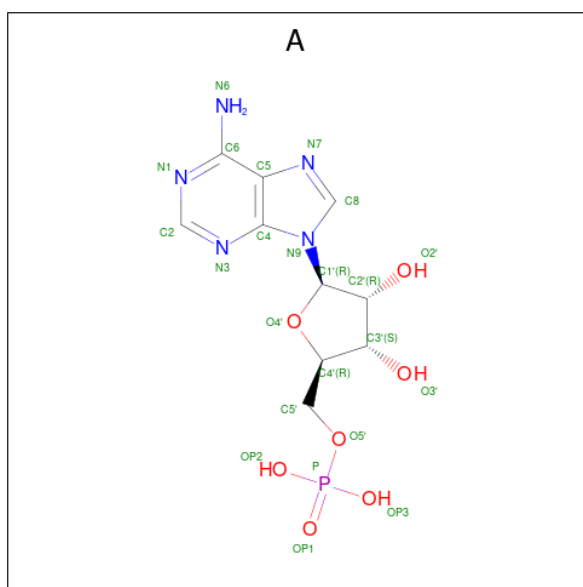
- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1d	1	Total Fe S 8 4 4	0	0
57	2d	1	Total Fe S 8 4 4	0	0

- Molecule 58 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	2A	1	Total P 1 1	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1740	Total O 1740 1740	0	0
59	1B	43	Total O 43 43	0	0
59	1D	16	Total O 16 16	0	0
59	1E	17	Total O 17 17	0	0
59	1F	9	Total O 9 9	0	0
59	1G	2	Total O 2 2	0	0
59	1H	3	Total O 3 3	0	0
59	1N	8	Total O 8 8	0	0
59	1P	13	Total O 13 13	0	0
59	1Q	7	Total O 7 7	0	0
59	1R	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1T	5	Total 5	O 5	0	0
59	1U	5	Total 5	O 5	0	0
59	1V	3	Total 3	O 3	0	0
59	1W	2	Total 2	O 2	0	0
59	1X	4	Total 4	O 4	0	0
59	1Y	4	Total 4	O 4	0	0
59	10	5	Total 5	O 5	0	0
59	11	3	Total 3	O 3	0	0
59	13	1	Total 1	O 1	0	0
59	15	2	Total 2	O 2	0	0
59	16	2	Total 2	O 2	0	0
59	17	2	Total 2	O 2	0	0
59	18	9	Total 9	O 9	0	0
59	19	2	Total 2	O 2	0	0
59	1a	395	Total 395	O 395	0	0
59	1d	10	Total 10	O 10	0	0
59	1e	2	Total 2	O 2	0	0
59	1f	1	Total 1	O 1	0	0
59	1h	1	Total 1	O 1	0	0
59	1j	1	Total 1	O 1	0	0
59	1l	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1m	2	Total O 2 2	0	0
59	1n	1	Total O 1 1	0	0
59	1p	1	Total O 1 1	0	0
59	1q	1	Total O 1 1	0	0
59	1t	1	Total O 1 1	0	0
59	1y	2	Total O 2 2	0	0
59	2A	1667	Total O 1667 1667	0	0
59	2B	35	Total O 35 35	0	0
59	2D	14	Total O 14 14	0	0
59	2E	16	Total O 16 16	0	0
59	2F	11	Total O 11 11	0	0
59	2G	2	Total O 2 2	0	0
59	2H	2	Total O 2 2	0	0
59	2N	2	Total O 2 2	0	0
59	2P	11	Total O 11 11	0	0
59	2Q	4	Total O 4 4	0	0
59	2R	4	Total O 4 4	0	0
59	2T	2	Total O 2 2	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

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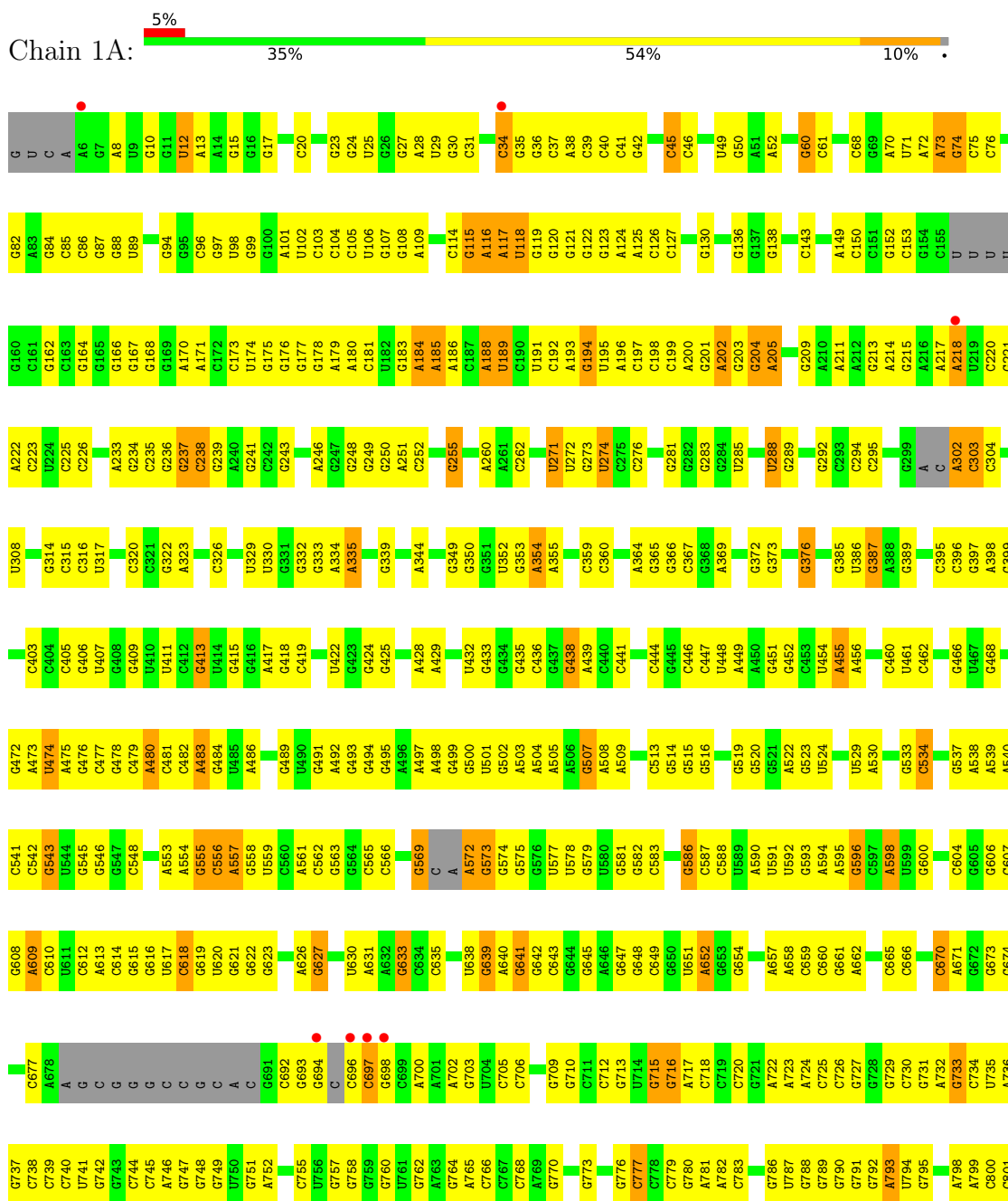
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2X	5	Total 5	O 5	0	0
59	2Y	3	Total 3	O 3	0	0
59	20	7	Total 7	O 7	0	0
59	21	2	Total 2	O 2	0	0
59	23	2	Total 2	O 2	0	0
59	25	1	Total 1	O 1	0	0
59	26	2	Total 2	O 2	0	0
59	27	1	Total 1	O 1	0	0
59	28	6	Total 6	O 6	0	0
59	2a	387	Total 387	O 387	0	0
59	2c	1	Total 1	O 1	0	0
59	2d	6	Total 6	O 6	0	0
59	2e	4	Total 4	O 4	0	0
59	2f	1	Total 1	O 1	0	0
59	2h	1	Total 1	O 1	0	0
59	2j	1	Total 1	O 1	0	0
59	2l	3	Total 3	O 3	0	0
59	2m	2	Total 2	O 2	0	0
59	2o	1	Total 1	O 1	0	0
59	2t	1	Total 1	O 1	0	0
59	2y	1	Total 1	O 1	0	0

### 3 Residue-property plots

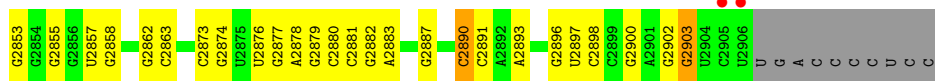
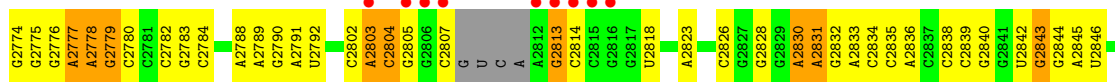
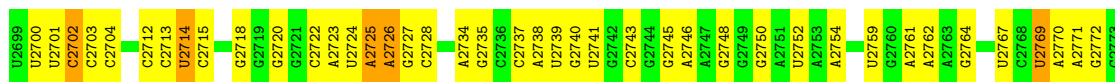
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

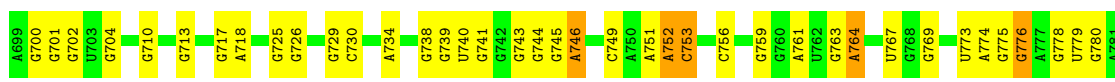
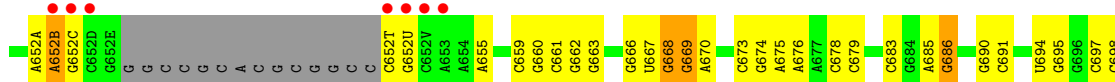
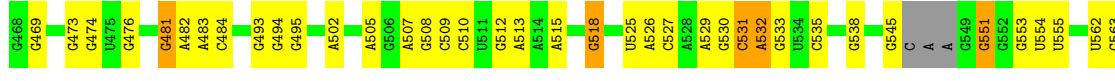
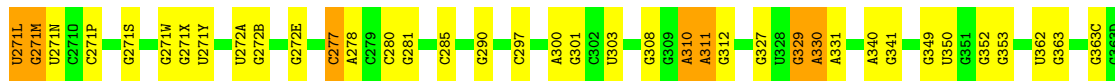
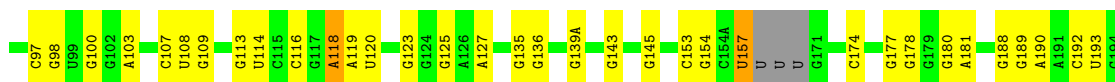
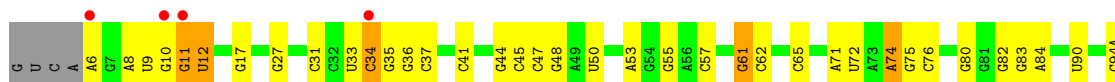


G1676	G1683	G1684	G1685	G1686	G1687	G1688	G1689	G1690	G1691	G1692	G1693	G1694	G1695	G1696	G1697	G1700	G1701	G1702	G1705	G1706	G1707	G1708	G1709	G1710	G1711	G1714	G1715	G1716	G1717	G1718	G1719	G1720	G1721	G1722	G1723	G1724	G1725	G1726	G1727	G1728	G1729	G1735	G1736	G1739	G1740	G1741	G1742	G1743	G1746										
G1614	G1615	G1616	G1617	G1618	G1619	G1620	G1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628	G1629	G1630	G1631	G1632	G1633	G1634	G1635	G1636	G1637	G1640	G1641	G1642	G1643	G1644	G1645	G1646	G1647	G1648	G1649	G1650	G1651	G1652	G1653	G1654	G1655	G1656	G1657	G1658	G1659	G1660	G1661	G1662	G1663	G1664	G1665	G1666	G1667	G1668	G1669	G1670	G1671	G1672	G1673	G1674	G1675
C1539	U1543	C1548	C1549	C1550	A1554	C1555	C1556	A1557	C1558	C1559	U1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	U1569	G1570	G1571	G1572	G1573	A1574	A1575	A1576	C1577	C1578	C1579	U	A	C	G1584	G1588	A1589	C1590	C1593	C1594	C1595	C1598	G1599	A1600	A1601	G1602	C1603	C1604	A1605	G1606	G1607	G1608	C1611	C1612	A1613					
G1467	G1470	G1471	G1472	G1473	G1474	G1475	C1478	G1479	A1480	G1481	G1482	A1485	G1486	G1487	A1491	C1492	C1493	G1494	G1495	G1496	G1497	A1500	A1504	C1505	G1506	A1507	G1508	C1511	G1512	G1513	C1514	C1515	A1518	A1519	G1520	C1521	G1522	C1523	A1524	G1525	G1526	G1527	G1528	G1529	A1532	G1533	A1536	G1537	G1538										
G1401	G1402	G1403	G1404	A1405	A1406	G1407	C1408	C1409	G1410	G1411	G1412	G1413	G1414	G1417	G1418	G1419	G1420	C1421	C1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	A1430	G1431	C1432	G1433	G1434	U1437	A1438	A1439	U1440	A1441	U1442	G1447	G1448	C1449	C1450	U1451	U1452	C1453	C1454	C1455	G1456	C1457	A1458	U1461	G1462	C1463	G1464	G1465	G1466				
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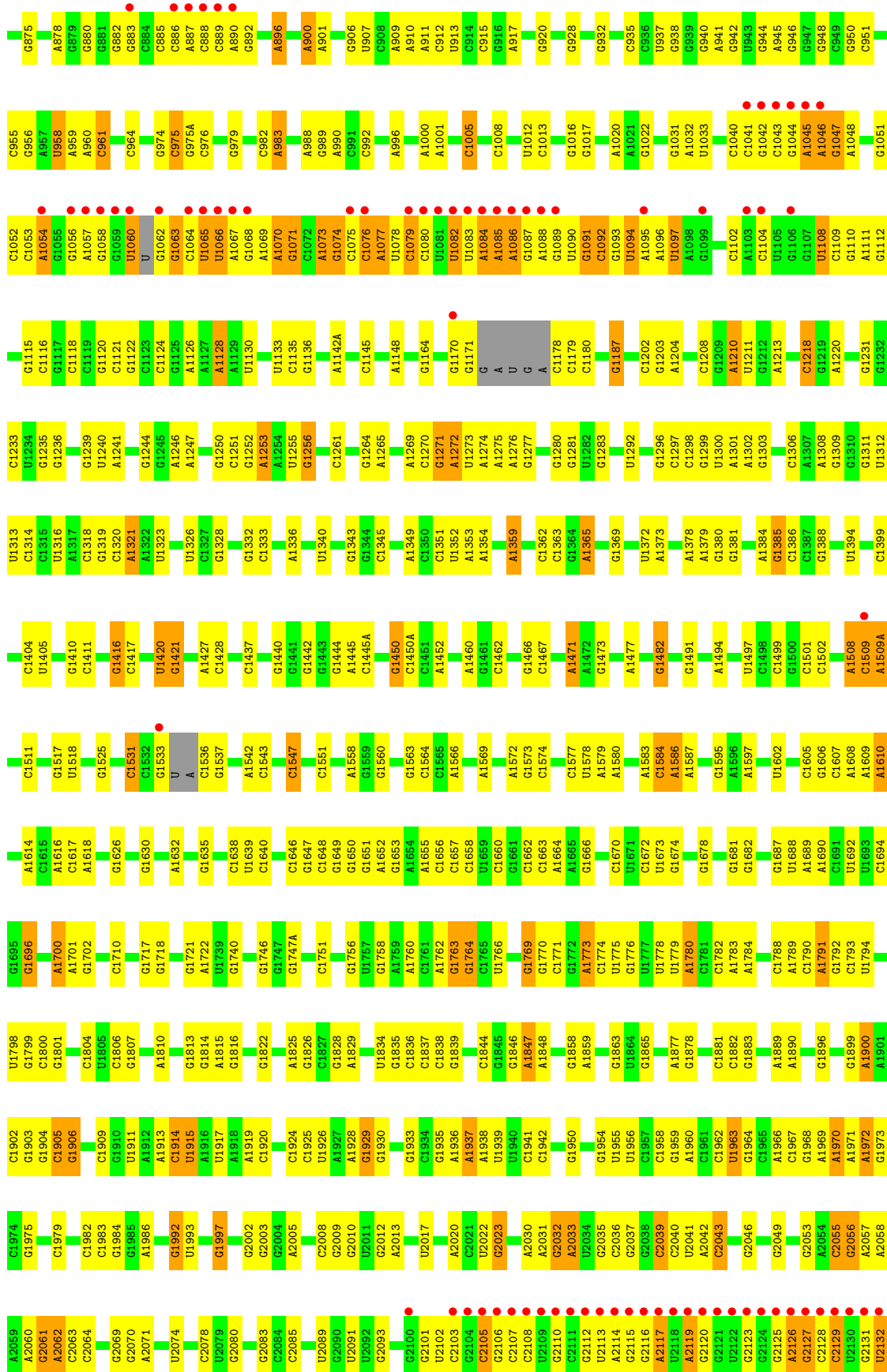
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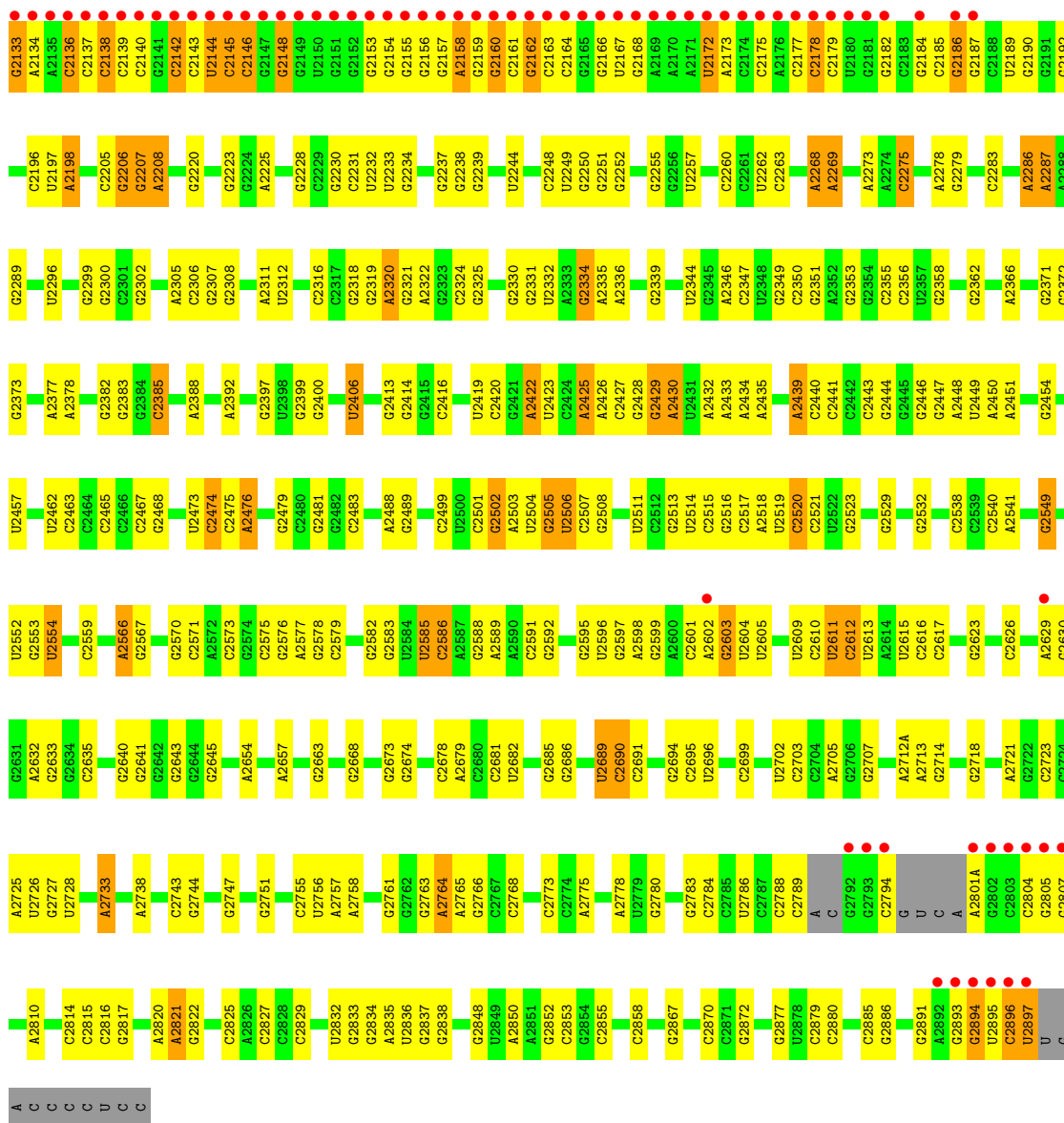


• Molecule 1: 23S ribosomal RNA

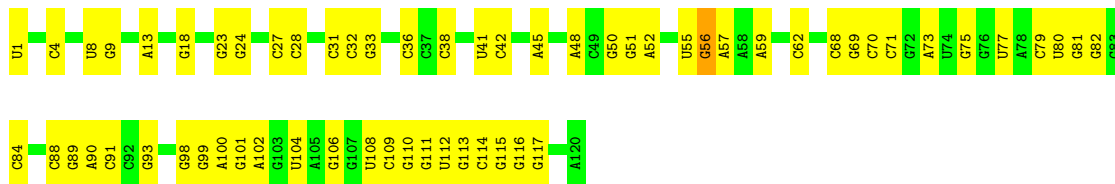




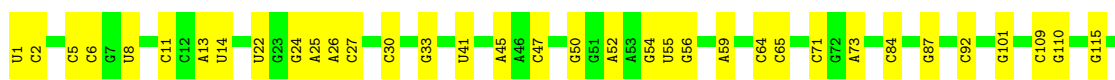




• Molecule 2: 5S ribosomal RNA

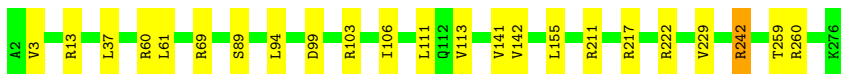


• Molecule 2: 5S ribosomal RNA



A120

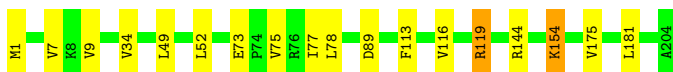
- Molecule 3: 50S ribosomal protein L2

Chain 1D:  92% 8%

- Molecule 3: 50S ribosomal protein L2

Chain 2D:  91% 9%

- Molecule 4: 50S ribosomal protein L3

Chain 1E:  91% 8%

- Molecule 4: 50S ribosomal protein L3

Chain 2E:  91% 9%

- Molecule 5: 50S ribosomal protein L4

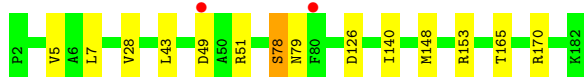
Chain 1F:  % 87% 13%

- Molecule 5: 50S ribosomal protein L4

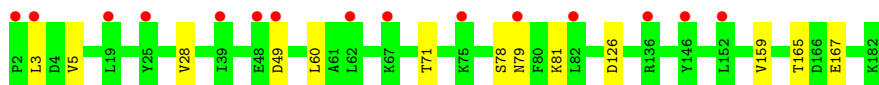
Chain 2F:  91% 9%

- Molecule 6: 50S ribosomal protein L5

Chain 1G:  % 92% 7%



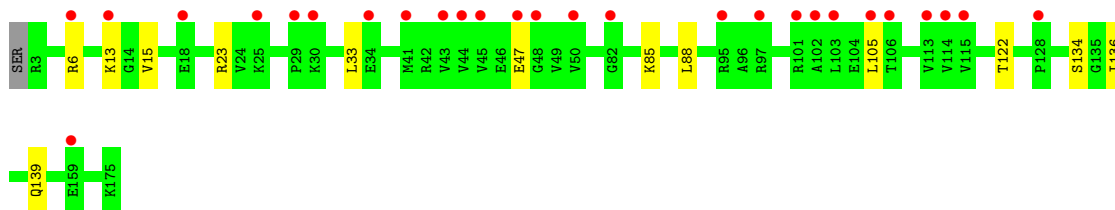
- Molecule 6: 50S ribosomal protein L5



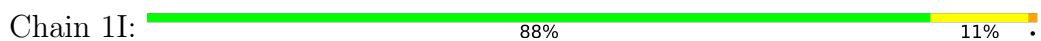
- Molecule 7: 50S ribosomal protein L6



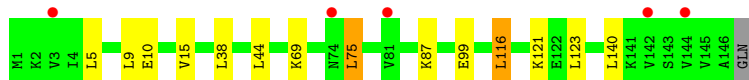
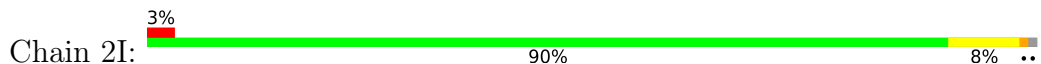
- Molecule 7: 50S ribosomal protein L6



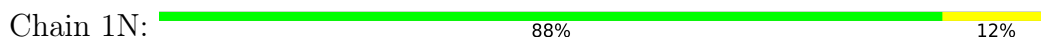
- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13

Chain 2N:  90% 10%



- Molecule 10: 50S ribosomal protein L14

Chain 1O:  92% 7%



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  93% 7%

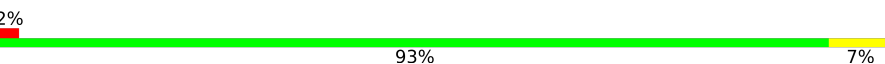


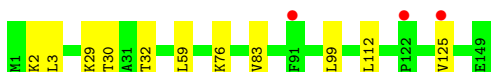
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  94% 6%



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  93% 7% 2%



- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  94% 6%




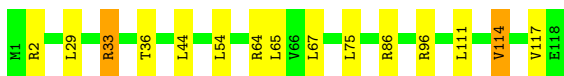
- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  94% 6%




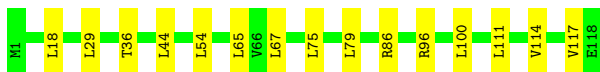
- Molecule 13: 50S ribosomal protein L17

Chain 1R:  87% 11%




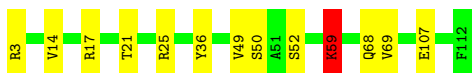
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  87% 13%

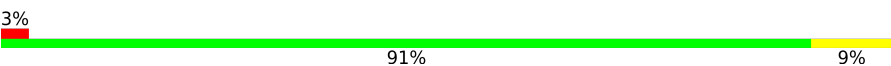


- Molecule 14: 50S ribosomal protein L18

Chain 1S:  88% 11%



- Molecule 14: 50S ribosomal protein L18

Chain 2S:  3% 91% 9%



- Molecule 15: 50S ribosomal protein L19

Chain 1T:  1% 92% 8%




- Molecule 15: 50S ribosomal protein L19

Chain 2T:  95% 5%



- Molecule 16: 50S ribosomal protein L20

Chain 1U:  85% 14%



- Molecule 16: 50S ribosomal protein L20

Chain 2U:  95% 5%



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  90% 8%



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  91% 8%



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  90% 8%



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  93% 6%



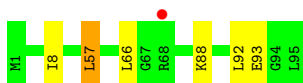
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  94% 6%

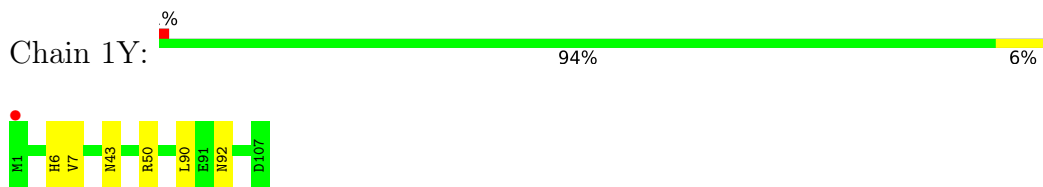


- Molecule 19: 50S ribosomal protein L23

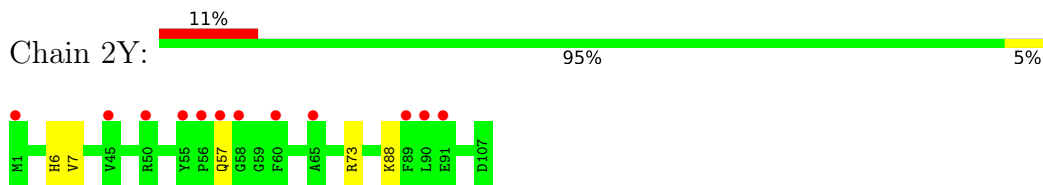
Chain 2X:  94% 5%



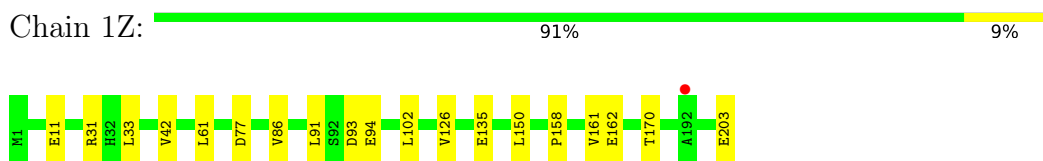
- Molecule 20: 50S ribosomal protein L24



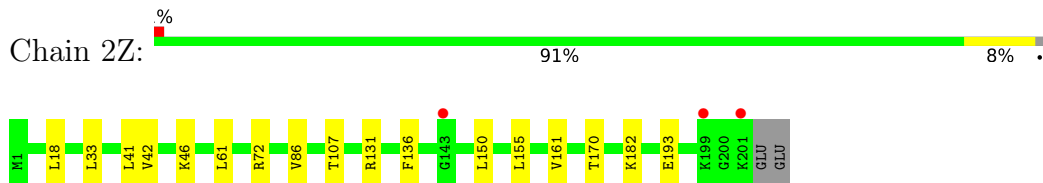
- Molecule 20: 50S ribosomal protein L24



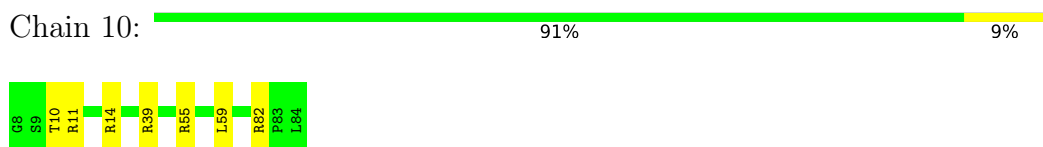
- Molecule 21: 50S ribosomal protein L25



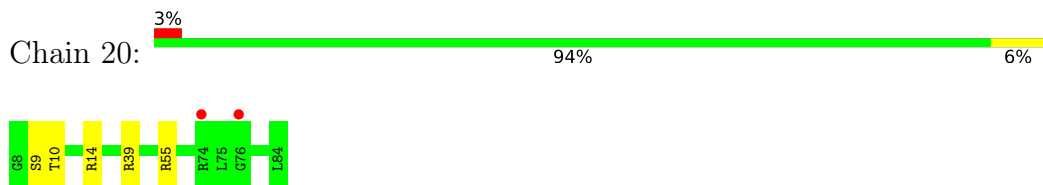
- Molecule 21: 50S ribosomal protein L25



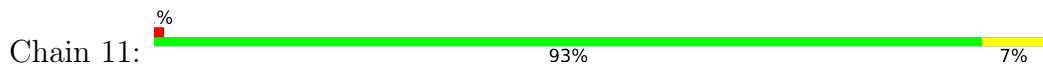
- Molecule 22: 50S ribosomal protein L27



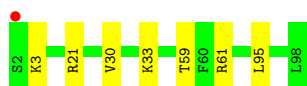
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28







- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



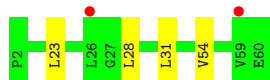
- Molecule 24: 50S ribosomal protein L29



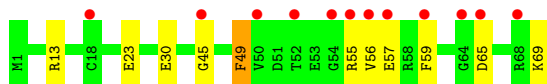
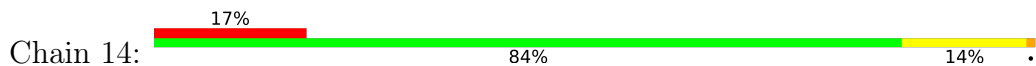
- Molecule 25: 50S ribosomal protein L30



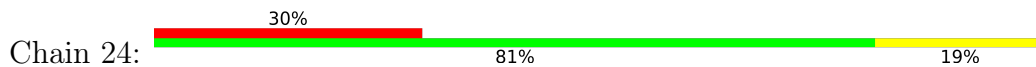
- Molecule 25: 50S ribosomal protein L30

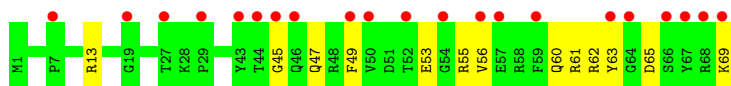


- Molecule 26: 50S ribosomal protein L31



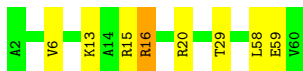
- Molecule 26: 50S ribosomal protein L31





- Molecule 27: 50S ribosomal protein L32

Chain 15: 86% 12%



- Molecule 27: 50S ribosomal protein L32

Chain 25: 92% 8%



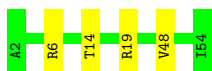
- Molecule 28: 50S ribosomal protein L33

Chain 16: 83% 17%



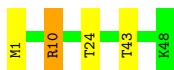
- Molecule 28: 50S ribosomal protein L33

Chain 26: 92% 8%



- Molecule 29: 50S ribosomal protein L34

Chain 17: 92% 6%



- Molecule 29: 50S ribosomal protein L34

Chain 27: 96%



- Molecule 30: 50S ribosomal protein L35

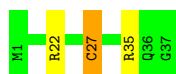
Chain 18: 84% 16%



- Molecule 30: 50S ribosomal protein L35



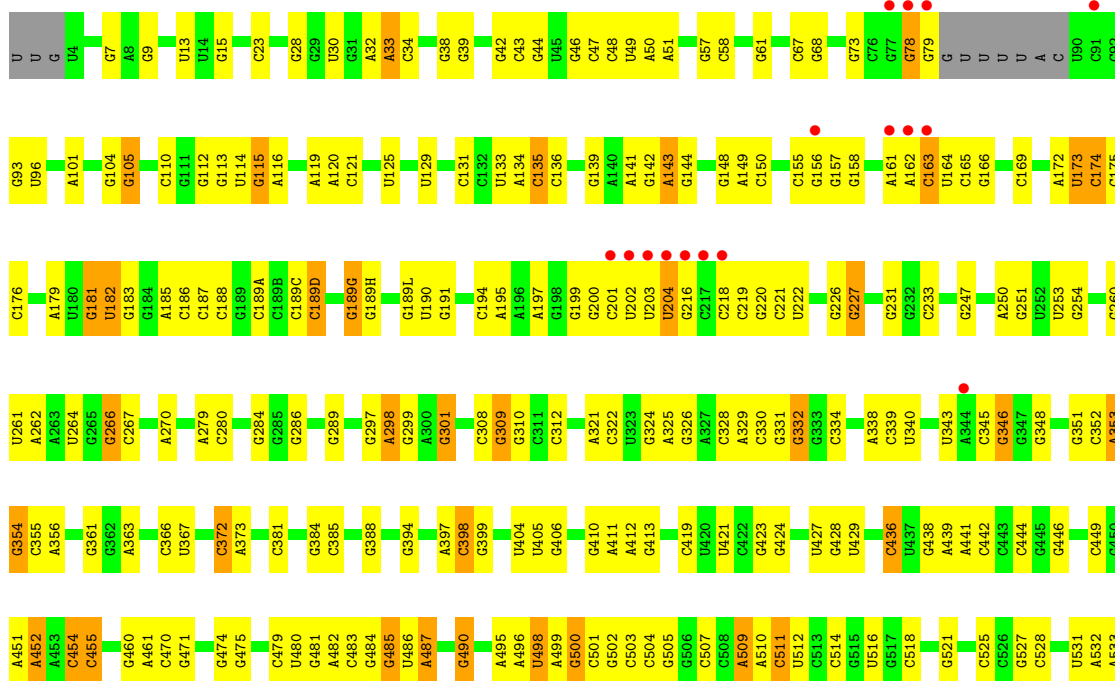
- Molecule 31: 50S ribosomal protein L36

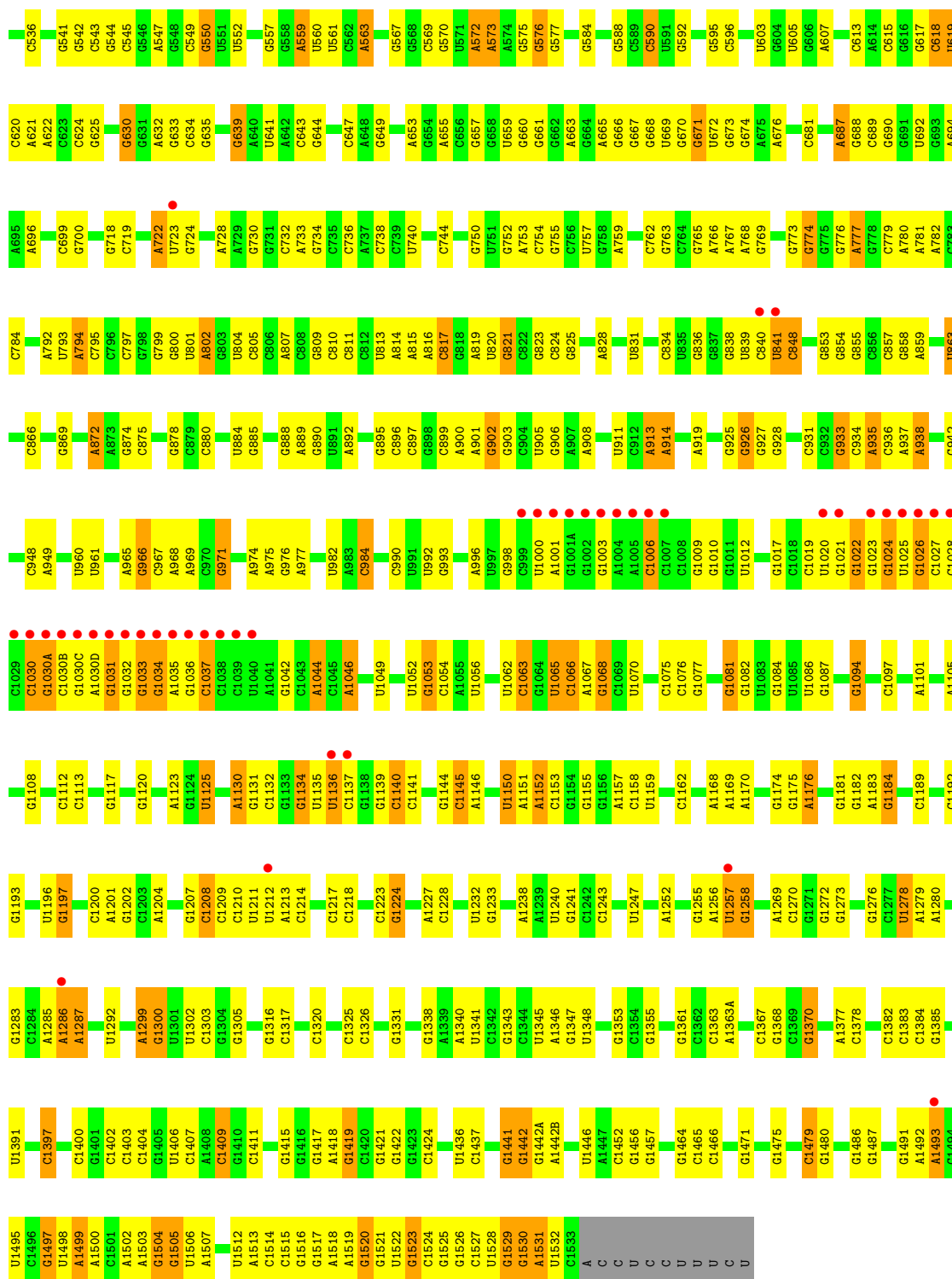


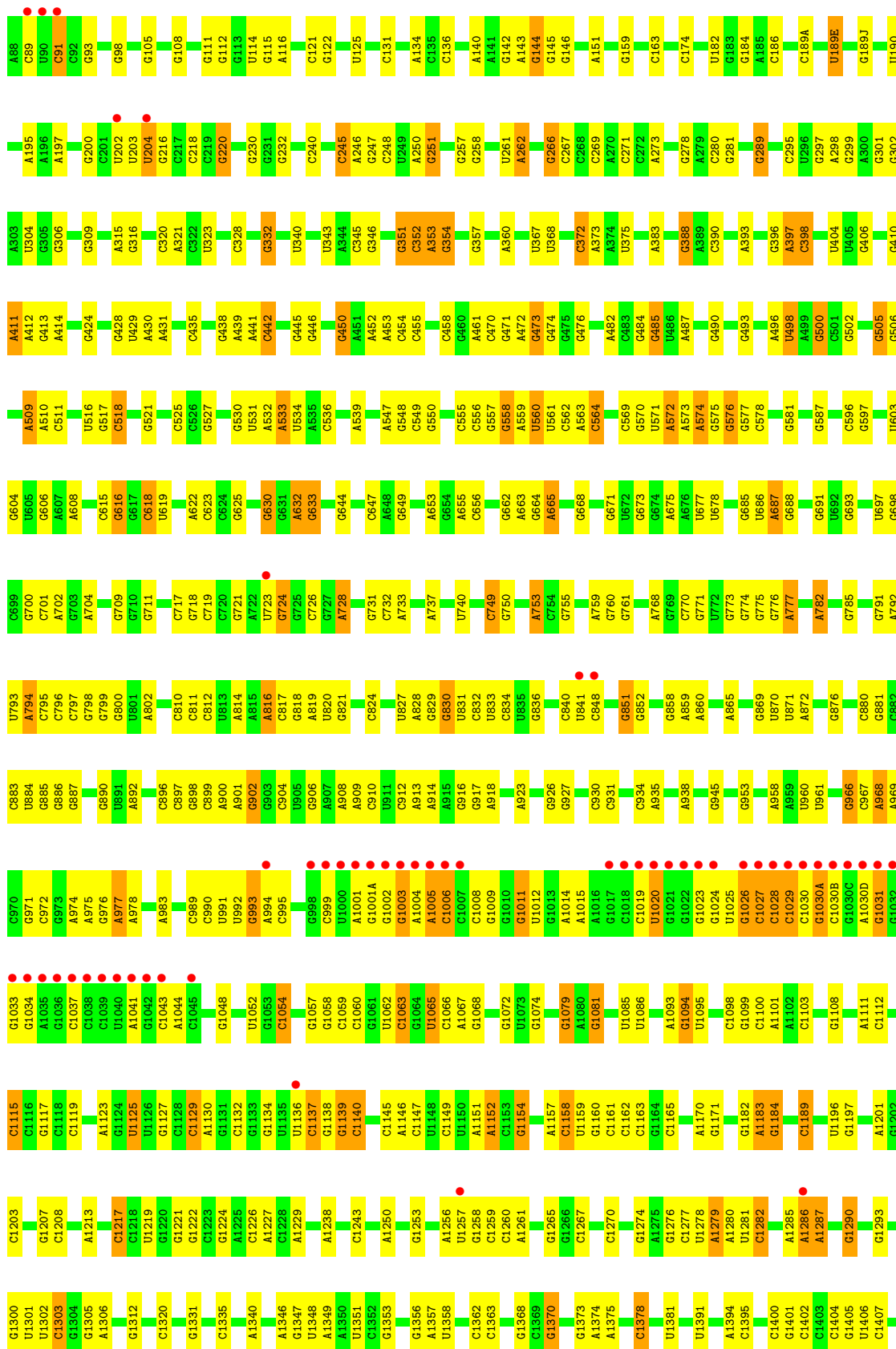
- Molecule 31: 50S ribosomal protein L36

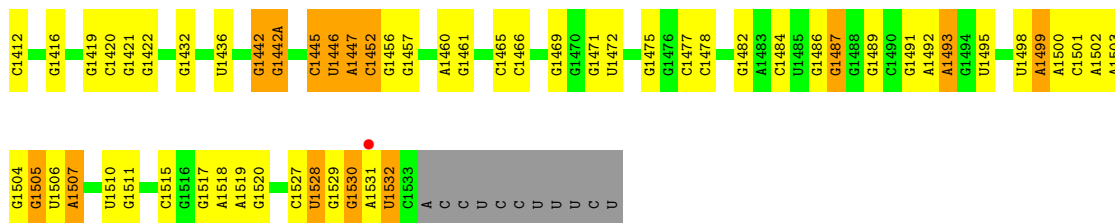


- Molecule 32: 16S ribosomal RNA

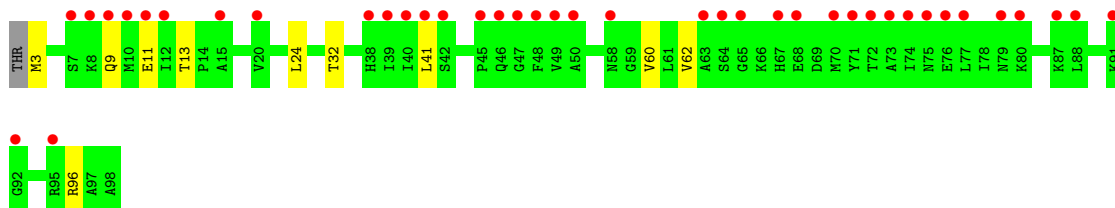
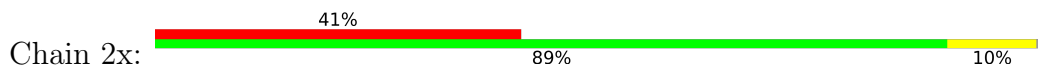








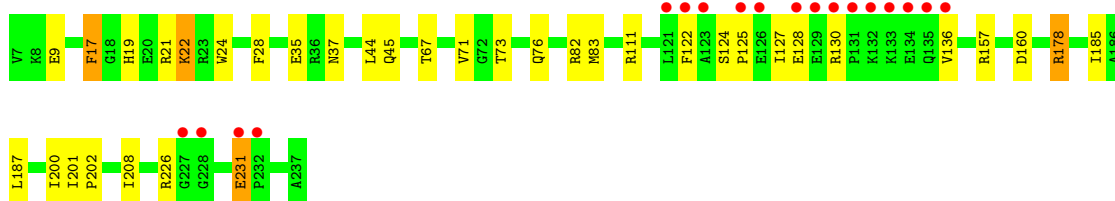
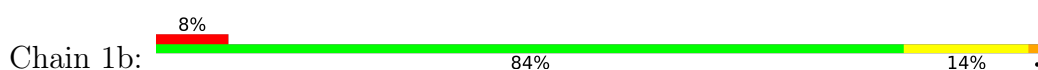
• Molecule 33: Ribosome-associated inhibitor A



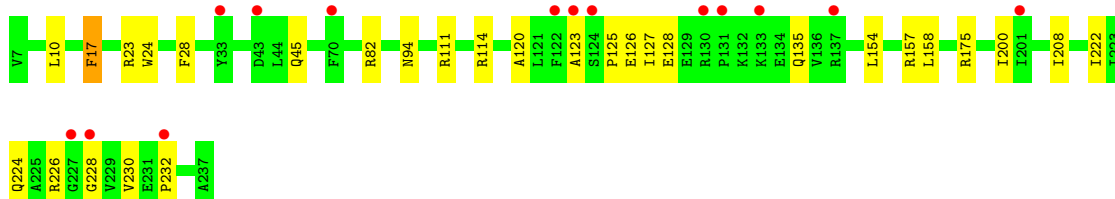
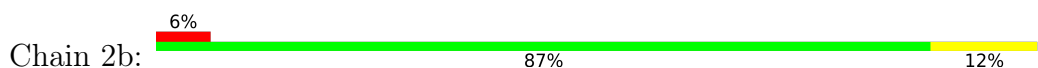
• Molecule 33: Ribosome-associated inhibitor A



• Molecule 34: 30S ribosomal protein S2



• Molecule 34: 30S ribosomal protein S2

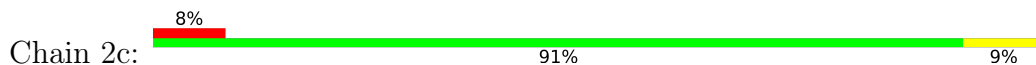


• Molecule 35: 30S ribosomal protein S3

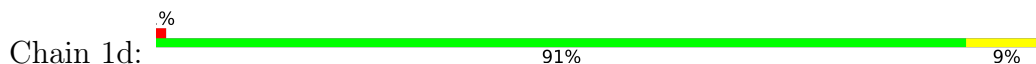




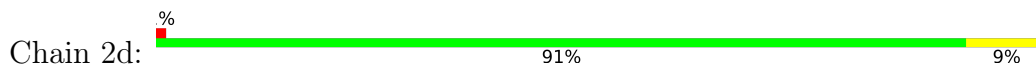
- Molecule 35: 30S ribosomal protein S3



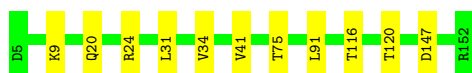
- Molecule 36: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S4



- Molecule 37: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S5



- Molecule 38: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S6

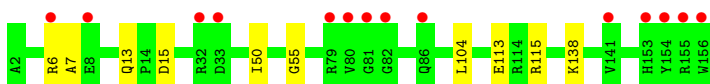




- Molecule 39: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S7



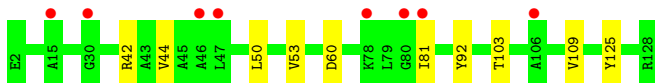
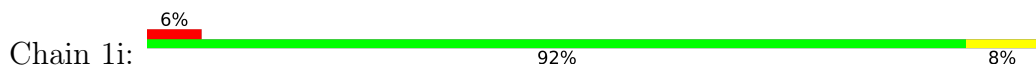
- Molecule 40: 30S ribosomal protein S8



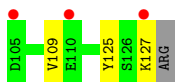
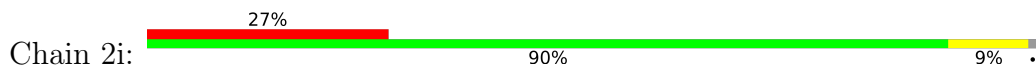
- Molecule 40: 30S ribosomal protein S8



- Molecule 41: 30S ribosomal protein S9

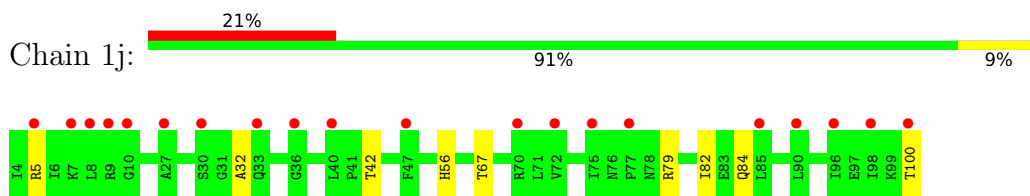


- Molecule 41: 30S ribosomal protein S9

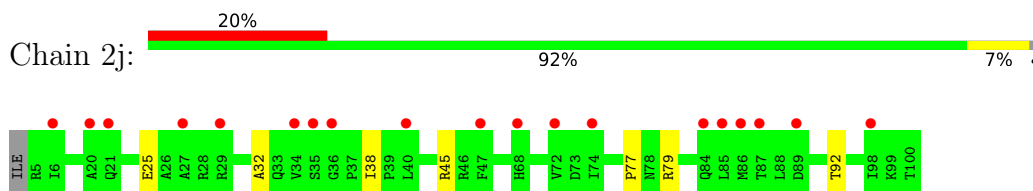




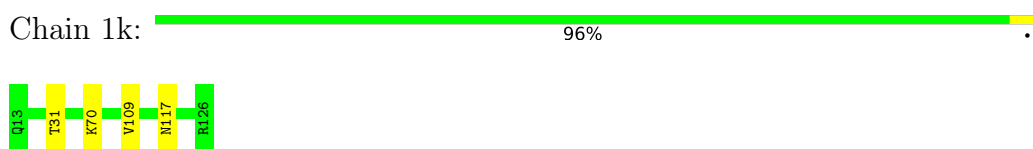
- Molecule 42: 30S ribosomal protein S10



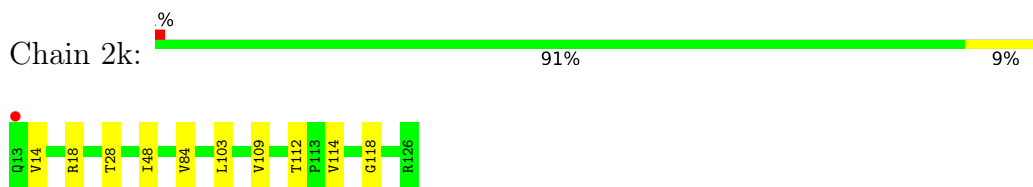
- Molecule 42: 30S ribosomal protein S10



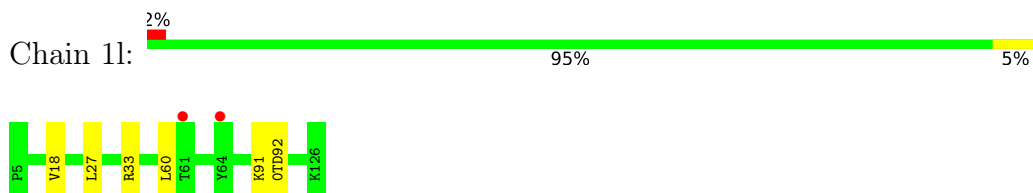
- Molecule 43: 30S ribosomal protein S11



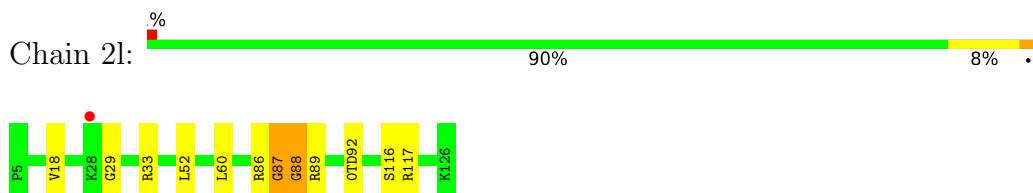
- Molecule 43: 30S ribosomal protein S11



- Molecule 44: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S12

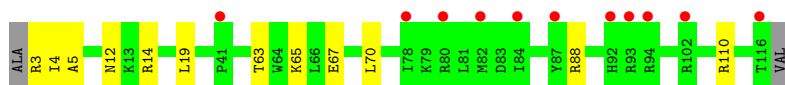
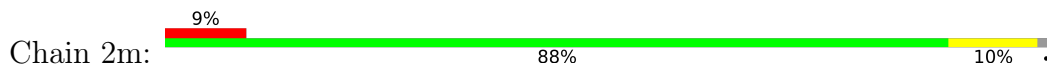


- Molecule 45: 30S ribosomal protein S13

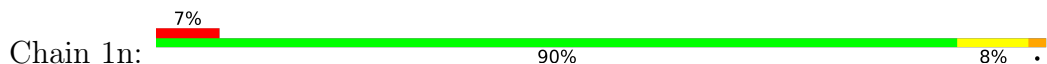




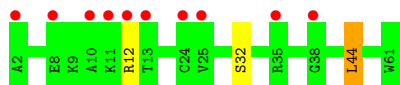
- Molecule 45: 30S ribosomal protein S13



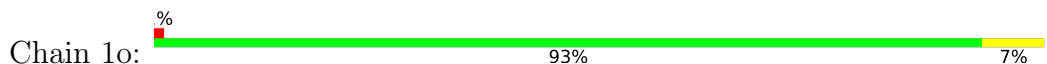
- Molecule 46: 30S ribosomal protein S14 type Z



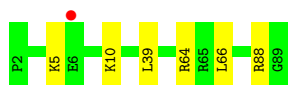
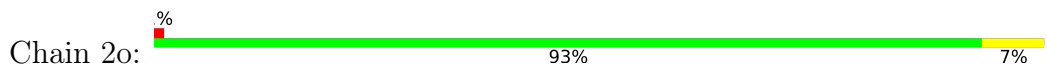
- Molecule 46: 30S ribosomal protein S14 type Z



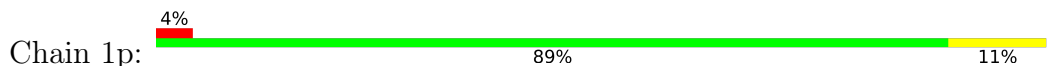
- Molecule 47: 30S ribosomal protein S15



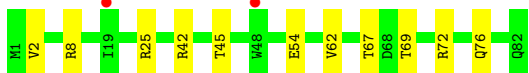
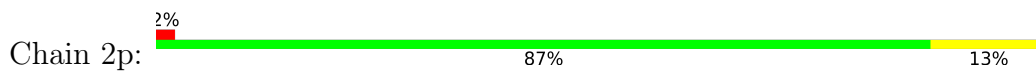
- Molecule 47: 30S ribosomal protein S15



- Molecule 48: 30S ribosomal protein S16



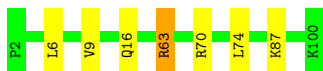
- Molecule 48: 30S ribosomal protein S16



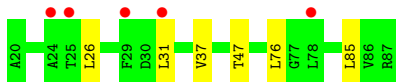
- Molecule 49: 30S ribosomal protein S17



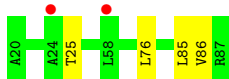
- Molecule 49: 30S ribosomal protein S17



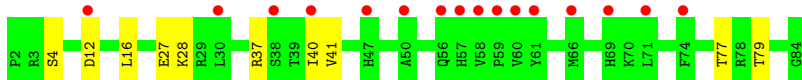
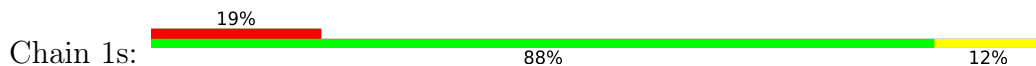
- Molecule 50: 30S ribosomal protein S18



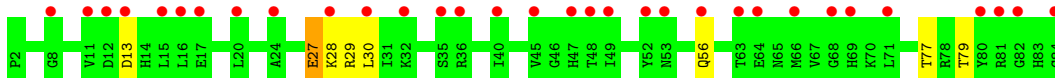
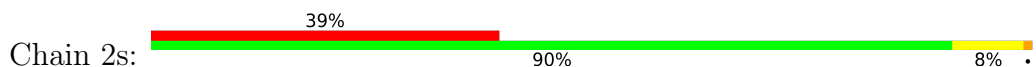
- Molecule 50: 30S ribosomal protein S18



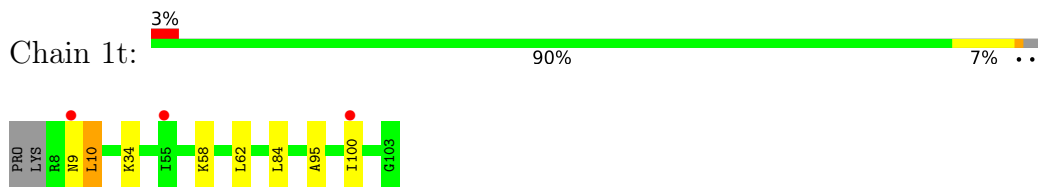
- Molecule 51: 30S ribosomal protein S19



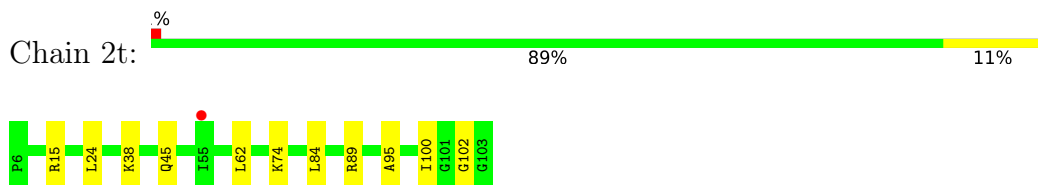
- Molecule 51: 30S ribosomal protein S19



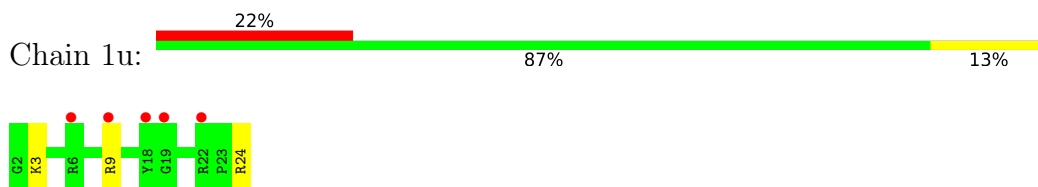
- Molecule 52: 30S ribosomal protein S20



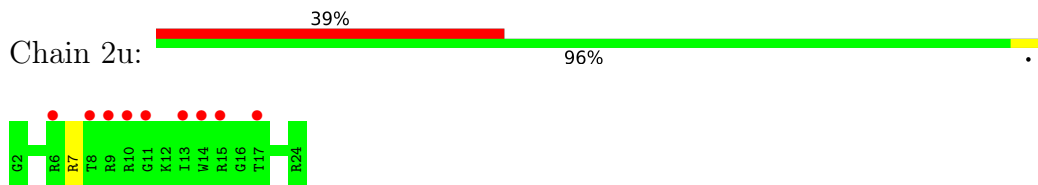
- Molecule 52: 30S ribosomal protein S20



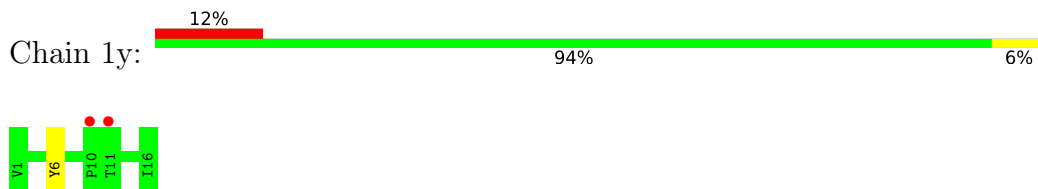
- Molecule 53: 30S ribosomal protein Thx



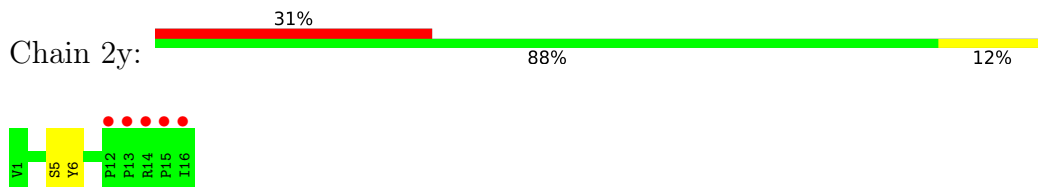
- Molecule 53: 30S ribosomal protein Thx



- Molecule 54: Pyrrhocoricin



- Molecule 54: Pyrrhocoricin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.94Å 450.10Å 622.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.80 49.81 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.81-2.80) 99.9 (49.81-2.59)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 2.58Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.189 , 0.240 0.190 , 0.240	Depositor DCC
$R_{free}$ test set	88568 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.2	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	293583	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, MA6, PSU, OMC, M2G, UR3, 2MA, G7M, 0TD, OMU, 4OC, OMG, 5MC, ZN, 5MU, MG, SF4

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	1.57	577/69022 (0.8%)	2.06	3825/107739 (3.6%)
1	2A	1.21	119/68893 (0.2%)	1.72	1783/107533 (1.7%)
2	1B	1.15	4/2879 (0.1%)	1.89	110/4490 (2.4%)
2	2B	1.02	1/2874 (0.0%)	1.58	50/4482 (1.1%)
3	1D	0.93	0/2181	1.00	4/2940 (0.1%)
3	2D	0.78	0/2186	0.87	1/2944 (0.0%)
4	1E	0.99	0/1592	1.02	3/2149 (0.1%)
4	2E	0.79	0/1592	0.91	2/2149 (0.1%)
5	1F	0.95	0/1619	0.96	4/2193 (0.2%)
5	2F	0.73	0/1615	0.85	0/2188
6	1G	0.70	0/1451	0.86	0/1961
6	2G	0.78	1/1449 (0.1%)	0.86	0/1957
7	1H	0.80	0/1356	0.89	0/1834
7	2H	0.77	0/1350	0.85	0/1826
8	1I	0.77	2/1109 (0.2%)	0.92	2/1512 (0.1%)
8	2I	0.67	0/1091	0.87	2/1490 (0.1%)
9	1N	0.93	1/1148 (0.1%)	0.97	3/1547 (0.2%)
9	2N	0.64	0/1144	0.83	0/1543
10	1O	1.02	0/943	1.00	2/1269 (0.2%)
10	2O	0.81	0/943	0.86	1/1269 (0.1%)
11	1P	0.89	0/1152	0.96	2/1533 (0.1%)
11	2P	0.68	0/1152	0.83	0/1533
12	1Q	0.94	0/1143	0.94	0/1527
12	2Q	0.68	0/1143	0.83	0/1527
13	1R	0.94	0/982	1.08	7/1312 (0.5%)
13	2R	0.70	0/982	0.90	1/1312 (0.1%)
14	1S	0.79	1/887 (0.1%)	0.98	2/1180 (0.2%)
14	2S	0.68	0/880	0.85	0/1172
15	1T	0.88	1/1105 (0.1%)	1.06	4/1477 (0.3%)
15	2T	0.73	0/1097	0.91	2/1468 (0.1%)
16	1U	1.08	2/977 (0.2%)	1.05	7/1301 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.73	0/977	0.83	0/1301
17	1V	0.94	0/786	0.98	2/1053 (0.2%)
17	2V	0.67	0/782	0.84	0/1049
18	1W	1.04	0/897	1.02	4/1205 (0.3%)
18	2W	0.83	0/897	0.84	1/1205 (0.1%)
19	1X	0.95	0/764	0.96	1/1025 (0.1%)
19	2X	0.76	0/764	0.86	2/1025 (0.2%)
20	1Y	0.86	0/823	0.96	1/1099 (0.1%)
20	2Y	0.79	0/823	0.92	0/1100
21	1Z	0.73	0/1620	0.83	1/2200 (0.0%)
21	2Z	0.70	0/1590	0.84	1/2162 (0.0%)
22	10	0.88	0/616	0.94	0/821
22	20	0.68	0/616	0.86	0/821
23	11	1.01	1/761 (0.1%)	0.96	1/1013 (0.1%)
23	21	0.79	0/766	0.92	2/1018 (0.2%)
24	12	0.87	0/590	0.94	0/781
24	22	0.77	0/594	0.81	0/785
25	13	0.92	0/474	0.94	0/635
25	23	0.62	0/469	0.80	1/630 (0.2%)
26	14	0.89	0/559	0.89	0/754
26	24	1.06	0/549	0.97	0/741
27	15	1.08	3/473 (0.6%)	1.07	6/639 (0.9%)
27	25	0.83	0/469	0.97	2/635 (0.3%)
28	16	0.98	2/460 (0.4%)	1.04	1/613 (0.2%)
28	26	0.68	0/456	0.80	0/608
29	17	1.08	0/426	1.08	1/561 (0.2%)
29	27	0.81	0/426	0.88	0/561
30	18	0.96	1/525 (0.2%)	0.95	2/691 (0.3%)
30	28	0.72	0/525	0.79	0/691
31	19	0.96	1/310 (0.3%)	1.09	2/407 (0.5%)
31	29	0.70	0/310	0.79	0/407
32	1a	1.14	55/35795 (0.2%)	1.70	881/55864 (1.6%)
32	2a	1.10	48/35890 (0.1%)	1.65	737/56012 (1.3%)
33	1x	0.66	0/776	0.79	0/1048
33	2x	0.72	0/761	0.79	0/1030
34	1b	0.77	0/1876	0.93	3/2533 (0.1%)
34	2b	0.78	0/1860	0.89	0/2518
35	1c	0.72	0/1582	0.80	0/2137
35	2c	0.81	0/1566	0.81	0/2119
36	1d	0.71	0/1695	0.84	0/2274
36	2d	0.70	0/1698	0.85	0/2277
37	1e	0.66	0/1149	0.88	0/1548
37	2e	0.68	0/1149	0.87	0/1548

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1f	0.72	0/827	0.81	0/1120
38	2f	0.70	0/829	0.84	0/1123
39	1g	0.71	1/1254 (0.1%)	0.77	0/1683
39	2g	0.73	0/1248	0.76	0/1676
40	1h	0.67	0/1118	0.83	0/1506
40	2h	0.61	0/1108	0.83	0/1494
41	1i	0.77	0/1005	0.82	0/1351
41	2i	0.84	0/985	0.88	0/1329
42	1j	0.79	0/732	0.84	0/993
42	2j	0.81	0/723	0.76	0/984
43	1k	0.73	0/849	0.85	0/1150
43	2k	0.67	0/848	0.86	1/1149 (0.1%)
44	1l	0.69	0/937	0.83	0/1260
44	2l	0.68	0/937	0.95	3/1260 (0.2%)
45	1m	0.68	0/924	0.83	0/1242
45	2m	0.76	0/905	0.82	0/1217
46	1n	0.74	0/501	0.93	2/664 (0.3%)
46	2n	0.75	0/501	0.82	1/664 (0.2%)
47	1o	0.72	0/739	0.86	0/985
47	2o	0.65	0/739	0.79	0/985
48	1p	0.69	0/697	0.85	0/939
48	2p	0.70	0/693	0.90	0/935
49	1q	0.73	0/836	0.86	0/1117
49	2q	0.67	0/836	0.85	1/1117 (0.1%)
50	1r	0.70	0/560	0.87	1/746 (0.1%)
50	2r	0.70	0/560	0.81	0/746
51	1s	0.73	0/663	0.81	0/895
51	2s	0.81	0/660	0.79	1/893 (0.1%)
52	1t	0.68	0/734	0.86	0/969
52	2t	0.64	0/736	0.85	0/976
53	1u	0.69	0/203	0.83	0/266
53	2u	0.73	0/203	0.87	0/266
54	1y	0.83	0/125	0.82	0/173
54	2y	0.69	0/125	0.74	0/173
All	All	1.17	821/310171 (0.3%)	1.62	7479/463547 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
19	1X	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	2X	0	1
30	18	0	1
44	2l	0	1
All	All	0	4

All (821) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2026	G	N7-C5	-11.28	1.32	1.39
1	1A	2040	G	P-OP2	-11.24	1.29	1.49
1	1A	354	A	N9-C4	-10.67	1.31	1.37
1	1A	1814	A	N3-C4	-10.29	1.28	1.34
1	2A	1046	A	N9-C4	9.81	1.43	1.37
1	1A	2040	G	P-OP1	-9.48	1.32	1.49
32	2a	1034	G	C6-N1	9.40	1.46	1.39
28	16	13	CYS	CB-SG	9.24	1.98	1.82
32	2a	343	U	C2-N3	-9.16	1.31	1.37
1	1A	1820	A	N9-C4	-9.09	1.32	1.37
1	1A	854	U	C2-N3	8.70	1.43	1.37
1	1A	782	A	N3-C4	-8.47	1.29	1.34
1	1A	572	A	N9-C4	8.29	1.42	1.37
1	1A	1994	A	N9-C4	-8.23	1.32	1.37
1	1A	2042	A	C6-N6	-8.23	1.27	1.33
1	1A	2803	A	N9-C4	8.22	1.42	1.37
1	1A	1092	A	N9-C4	8.18	1.42	1.37
32	1a	1493	A	N9-C4	8.12	1.42	1.37
32	2a	1003	G	N9-C4	8.09	1.44	1.38
1	1A	1132	A	N9-C4	8.05	1.42	1.37
1	1A	492	A	C6-N6	-8.03	1.27	1.33
1	1A	835	A	N7-C5	-8.01	1.34	1.39
1	1A	1144	A	N9-C4	7.92	1.42	1.37
1	1A	1280	U	C2-N3	-7.87	1.32	1.37
1	1A	13	A	N7-C5	-7.86	1.34	1.39
1	1A	1272	A	N9-C4	-7.83	1.33	1.37
32	1a	250	A	N9-C4	7.71	1.42	1.37
1	1A	251	A	N9-C4	-7.70	1.33	1.37
1	1A	609	A	N3-C4	-7.62	1.30	1.34
1	1A	2803	A	N3-C4	7.56	1.39	1.34
1	1A	813	C	N1-C6	-7.56	1.32	1.37
1	1A	986	A	N7-C5	-7.55	1.34	1.39
28	16	16	CYS	CB-SG	-7.53	1.69	1.82
1	1A	1222	A	N9-C4	7.52	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2612	A	C6-N1	-7.50	1.30	1.35
1	1A	2272	C	N3-C4	-7.46	1.28	1.33
32	1a	163	C	N1-C6	7.43	1.41	1.37
1	1A	1846	A	N3-C4	-7.42	1.30	1.34
1	1A	886	U	C4-O4	-7.41	1.17	1.23
1	1A	2697	G	C6-N1	-7.41	1.34	1.39
1	1A	2331	G	N9-C4	-7.41	1.32	1.38
1	1A	731	G	C6-N1	-7.36	1.34	1.39
1	1A	537	G	C5-C4	-7.36	1.33	1.38
1	1A	716	G	C2-N3	-7.34	1.26	1.32
1	1A	1283	A	N3-C4	-7.34	1.30	1.34
1	1A	1795	G	N7-C5	-7.34	1.34	1.39
1	1A	409	G	C6-N1	-7.33	1.34	1.39
1	1A	752	A	C5-C6	-7.27	1.34	1.41
32	1a	161	A	N9-C4	7.25	1.42	1.37
32	2a	1034	G	N9-C4	7.25	1.43	1.38
1	1A	2778	A	N7-C5	-7.24	1.34	1.39
1	1A	1001	G	C6-N1	-7.23	1.34	1.39
1	2A	2805	G	N9-C4	7.23	1.43	1.38
1	1A	36	G	N7-C5	-7.22	1.34	1.39
1	1A	700	A	N3-C4	7.20	1.39	1.34
32	1a	1003	G	N9-C4	7.19	1.43	1.38
32	2a	1279	A	N9-C4	7.18	1.42	1.37
1	1A	989	G	C6-N1	-7.16	1.34	1.39
2	1B	1	U	C2-N3	7.16	1.42	1.37
1	1A	2454	C	N1-C2	-7.10	1.33	1.40
1	1A	827	G	N9-C8	-7.10	1.32	1.37
1	2A	2117	A	N9-C4	7.09	1.42	1.37
1	1A	476	G	C6-O6	-7.09	1.17	1.24
1	1A	2040	G	P-O5'	-7.08	1.52	1.59
1	1A	178	G	N7-C5	-7.03	1.35	1.39
1	1A	2630	G	N7-C5	-7.02	1.35	1.39
1	1A	724	A	C6-N1	-7.01	1.30	1.35
1	1A	1679	A	N7-C5	-6.99	1.35	1.39
1	1A	1377	A	N3-C4	-6.98	1.30	1.34
1	1A	2082	A	N9-C4	-6.97	1.33	1.37
1	1A	101	A	C6-N6	6.97	1.39	1.33
1	1A	2039	U	O3'-P	-6.96	1.52	1.61
1	1A	2633	A	C5-C6	-6.96	1.34	1.41
1	1A	1833	A	C5-C6	-6.94	1.34	1.41
1	2A	1091	G	N9-C4	6.94	1.43	1.38
1	1A	2331	G	N3-C4	-6.93	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1113	A	N9-C4	6.92	1.42	1.37
1	2A	529	A	N9-C4	-6.91	1.33	1.37
1	1A	1741	C	N1-C6	-6.91	1.33	1.37
1	1A	670	C	N1-C6	6.90	1.41	1.37
1	1A	1067	A	N3-C4	-6.89	1.30	1.34
2	1B	75	G	N1-C2	6.85	1.43	1.37
1	1A	2600	G	C6-N1	-6.85	1.34	1.39
1	1A	218	A	N9-C4	6.83	1.42	1.37
1	1A	776	G	N3-C4	-6.81	1.30	1.35
1	1A	199	C	C2-N3	-6.80	1.30	1.35
1	1A	554	A	C6-N1	6.80	1.40	1.35
1	1A	2600	G	N3-C4	-6.78	1.30	1.35
1	1A	1834	A	N3-C4	-6.78	1.30	1.34
32	1a	148	G	N9-C4	6.78	1.43	1.38
1	1A	1130	A	C5-C6	6.77	1.47	1.41
1	1A	27	G	C6-N1	-6.77	1.34	1.39
1	1A	987	G	N7-C5	-6.77	1.35	1.39
1	1A	2591	C	N1-C6	-6.76	1.33	1.37
1	1A	186	A	C2-N3	-6.75	1.27	1.33
1	1A	731	G	N1-C2	-6.74	1.32	1.37
1	1A	1312	G	N7-C5	-6.74	1.35	1.39
1	1A	476	G	N9-C8	-6.72	1.33	1.37
1	1A	2697	G	N1-C2	-6.72	1.32	1.37
1	1A	1669	G	C6-N1	-6.71	1.34	1.39
32	2a	1030(D)	A	N9-C4	6.71	1.41	1.37
1	1A	2883	A	C6-N1	-6.71	1.30	1.35
32	2a	1034	G	C2-N3	6.70	1.38	1.32
1	1A	720	C	N3-C4	6.70	1.38	1.33
1	1A	1313	U	P-OP1	-6.70	1.37	1.49
1	1A	1822	A	N3-C4	-6.69	1.30	1.34
1	1A	2069	U	C4-O4	-6.68	1.18	1.23
1	1A	2106	C	N3-C4	-6.68	1.29	1.33
1	1A	2442	A	N9-C4	-6.67	1.33	1.37
1	1A	2251	G	N1-C2	-6.67	1.32	1.37
1	1A	1422	C	N3-C4	-6.65	1.29	1.33
1	1A	840	A	C5-C6	-6.62	1.35	1.41
1	2A	2805	G	N3-C4	6.62	1.40	1.35
1	1A	2658	C	N3-C4	-6.61	1.29	1.33
1	1A	2035	A	N7-C5	-6.61	1.35	1.39
1	1A	722	A	C5-C6	-6.60	1.35	1.41
1	2A	2030	A	N9-C4	-6.59	1.33	1.37
1	1A	1672	G	C6-N1	-6.58	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	848	G	C6-N1	-6.58	1.34	1.39
1	1A	835	A	N9-C8	-6.57	1.32	1.37
1	1A	717	A	N7-C5	-6.54	1.35	1.39
32	2a	1026	G	N9-C8	6.53	1.42	1.37
1	1A	823	G	C6-N1	-6.53	1.34	1.39
1	2A	1533	G	C5-C4	6.52	1.43	1.38
1	2A	1054	A	N9-C4	6.52	1.41	1.37
1	1A	1305	G	C6-N1	-6.51	1.34	1.39
1	1A	2460	A	C5-C4	-6.51	1.34	1.38
1	1A	1259	A	N9-C8	-6.49	1.32	1.37
1	1A	1135	G	N9-C4	6.49	1.43	1.38
1	1A	1130	A	N7-C5	6.48	1.43	1.39
32	2a	1436	U	C2-N3	6.48	1.42	1.37
1	1A	2006	G	C6-N1	-6.47	1.35	1.39
1	1A	1175	A	C6-N1	-6.46	1.31	1.35
1	1A	2510	C	N3-C4	-6.46	1.29	1.33
1	1A	1271	G	N3-C4	-6.46	1.30	1.35
1	1A	354	A	C5-C6	-6.45	1.35	1.41
32	2a	1034	G	N3-C4	6.44	1.40	1.35
1	1A	1405	A	N7-C5	6.43	1.43	1.39
1	1A	1822	A	N9-C4	-6.43	1.33	1.37
1	1A	1298	G	N9-C4	-6.42	1.32	1.38
1	1A	1113	A	N3-C4	6.41	1.38	1.34
1	1A	1838	G	N9-C4	-6.41	1.32	1.38
1	1A	1010	C	N3-C4	-6.40	1.29	1.33
1	1A	2260	C	C4-N4	-6.40	1.28	1.33
1	2A	1378	A	N9-C4	-6.39	1.34	1.37
1	1A	164	G	C2-N3	6.38	1.37	1.32
1	1A	1394	G	N9-C8	-6.38	1.33	1.37
1	1A	2261	U	C4-O4	-6.38	1.18	1.23
1	1A	1690	G	N3-C4	-6.38	1.30	1.35
1	1A	2777	A	N9-C4	-6.38	1.34	1.37
1	1A	742	G	N1-C2	-6.37	1.32	1.37
1	1A	1727	U	C4-O4	-6.34	1.18	1.23
32	1a	1492	A	N9-C4	6.34	1.41	1.37
1	1A	1822	A	C6-N1	-6.34	1.31	1.35
1	1A	2376	C	N1-C6	-6.33	1.33	1.37
1	1A	125	A	C6-N6	-6.32	1.28	1.33
32	1a	1493	A	N3-C4	6.32	1.38	1.34
2	2B	1	U	N1-C2	6.31	1.44	1.38
1	1A	557	A	C6-N1	-6.30	1.31	1.35
1	2A	1721	G	N3-C4	6.28	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	859	C	C4-N4	-6.28	1.28	1.33
1	1A	1091	A	C5-C6	6.27	1.46	1.41
1	2A	2897	U	C2-N3	6.27	1.42	1.37
1	2A	2775	A	N9-C4	-6.27	1.34	1.37
1	1A	1117	G	N9-C4	6.26	1.43	1.38
1	1A	1102	G	N3-C4	6.26	1.39	1.35
1	1A	1660	A	N7-C5	-6.26	1.35	1.39
1	1A	474	U	C4-O4	-6.26	1.18	1.23
1	1A	2033	U	C2-O2	-6.25	1.16	1.22
1	1A	1829	U	C4-O4	-6.25	1.18	1.23
1	1A	2034	G	C6-N1	-6.25	1.35	1.39
32	1a	1286	A	N9-C4	6.25	1.41	1.37
32	1a	1034	G	C6-N1	6.25	1.44	1.39
1	2A	1913	A	N9-C4	6.25	1.41	1.37
1	1A	839	G	C6-N1	-6.25	1.35	1.39
32	1a	204	U	N1-C2	6.24	1.44	1.38
1	2A	1070	A	N9-C4	6.23	1.41	1.37
1	1A	1701	A	C8-N7	-6.22	1.27	1.31
1	1A	2451	A	N7-C5	-6.22	1.35	1.39
1	1A	555	G	N1-C2	-6.22	1.32	1.37
1	2A	645	C	N1-C6	6.22	1.40	1.37
1	2A	1652	A	N9-C4	-6.21	1.34	1.37
1	1A	2554	A	N9-C4	-6.21	1.34	1.37
1	1A	598	A	N3-C4	-6.21	1.31	1.34
32	2a	759	A	N9-C4	-6.21	1.34	1.37
1	1A	815	G	N3-C4	-6.21	1.31	1.35
16	1U	9	VAL	CB-CG1	-6.21	1.39	1.52
1	1A	1653	C	N1-C6	-6.21	1.33	1.37
1	1A	1479	U	C4-O4	-6.20	1.18	1.23
1	2A	1345	C	N1-C6	-6.20	1.33	1.37
1	1A	2331	G	N9-C8	6.20	1.42	1.37
1	1A	731	G	C5-C4	-6.20	1.34	1.38
1	1A	2584	A	C5-C4	-6.20	1.34	1.38
1	1A	1148	C	N1-C2	6.19	1.46	1.40
1	1A	2073	A	N3-C4	-6.19	1.31	1.34
1	1A	1507	A	N3-C4	6.19	1.38	1.34
1	1A	537	G	N7-C5	-6.18	1.35	1.39
1	1A	1132	A	N3-C4	6.18	1.38	1.34
31	19	27	CYS	CB-SG	6.17	1.92	1.82
1	1A	2605	U	C2-N3	-6.17	1.33	1.37
1	2A	1963	U	N1-C2	6.17	1.44	1.38
1	1A	2187	G	N3-C4	6.17	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	827	G	N7-C5	-6.16	1.35	1.39
32	2a	1157	A	N9-C4	6.16	1.41	1.37
1	1A	2112	G	C6-N1	-6.15	1.35	1.39
1	1A	2443	U	N1-C6	-6.15	1.32	1.38
1	1A	1724	A	N3-C4	-6.14	1.31	1.34
1	1A	2134	G	N9-C4	6.13	1.42	1.38
1	2A	1794	U	C2-N3	-6.13	1.33	1.37
32	2a	1026	G	C8-N7	6.12	1.34	1.30
1	1A	1475	G	N1-C2	-6.12	1.32	1.37
1	1A	2453	C	N1-C6	-6.12	1.33	1.37
1	1A	1076	G	N7-C5	-6.11	1.35	1.39
1	1A	1658	C	N1-C6	-6.11	1.33	1.37
1	1A	1705	C	N1-C6	6.11	1.40	1.37
1	1A	2625	U	C2-N3	-6.11	1.33	1.37
32	1a	1044	A	N9-C4	6.10	1.41	1.37
1	1A	2280	A	N7-C5	-6.09	1.35	1.39
1	1A	2612	A	N3-C4	-6.08	1.31	1.34
1	1A	1718	U	C4-O4	-6.07	1.18	1.23
1	2A	1082	U	N1-C2	6.07	1.44	1.38
1	1A	1293	A	C6-N6	-6.06	1.29	1.33
1	1A	1356	G	N1-C2	-6.06	1.32	1.37
1	1A	2093	A	C5-C4	-6.06	1.34	1.38
1	1A	2294	G	C6-N1	-6.05	1.35	1.39
1	1A	878	G	C8-N7	-6.05	1.27	1.30
16	1U	15	LYS	CE-NZ	6.05	1.64	1.49
1	1A	1121	C	N1-C2	6.05	1.46	1.40
1	1A	1235	G	N7-C5	-6.04	1.35	1.39
1	1A	724	A	N7-C5	-6.03	1.35	1.39
1	1A	2836	A	C5-C6	-6.03	1.35	1.41
1	1A	1015	C	N3-C4	-6.03	1.29	1.33
1	1A	1026	A	N9-C4	-6.03	1.34	1.37
1	1A	2634	C	C4-N4	-6.02	1.28	1.33
1	1A	1304	C	N3-C4	-6.02	1.29	1.33
1	2A	2244	U	C2-N3	-6.01	1.33	1.37
1	1A	1711	A	N7-C5	-6.00	1.35	1.39
32	1a	1436	U	C2-N3	6.00	1.42	1.37
1	1A	1700	G	C6-N1	-6.00	1.35	1.39
1	1A	2024	G	C8-N7	-6.00	1.27	1.30
1	1A	729	G	C6-N1	-5.99	1.35	1.39
1	1A	1666	G	C6-N1	-5.99	1.35	1.39
1	1A	1221	G	N7-C5	5.99	1.42	1.39
1	1A	2828	G	C6-N1	-5.99	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2441	G	N7-C5	-5.98	1.35	1.39
1	1A	553	A	N9-C4	5.98	1.41	1.37
1	1A	554	A	C2-N3	5.98	1.39	1.33
1	1A	832	G	N9-C4	-5.97	1.33	1.38
1	1A	2775	G	C5-C4	-5.97	1.34	1.38
1	1A	2075	G	N7-C5	-5.97	1.35	1.39
1	1A	2738	A	N9-C4	-5.97	1.34	1.37
1	2A	792	G	N1-C2	-5.97	1.32	1.37
1	1A	2467	G	C2-N2	-5.96	1.28	1.34
1	1A	2517	G	C2-N3	-5.95	1.27	1.32
1	1A	1282	G	C5-C4	-5.95	1.34	1.38
1	1A	180	A	N9-C8	-5.94	1.32	1.37
1	2A	1721	G	C2-N3	5.94	1.37	1.32
1	2A	2153	G	C5-C4	5.94	1.42	1.38
1	1A	1853	G	C6-N1	-5.94	1.35	1.39
32	1a	1030(A)	G	N9-C4	5.93	1.42	1.38
1	1A	1690	G	C5-C4	-5.93	1.34	1.38
1	1A	833	C	N3-C4	-5.93	1.29	1.33
1	1A	876	A	N7-C5	-5.92	1.35	1.39
1	1A	2466	G	N7-C5	-5.92	1.35	1.39
8	1I	10	GLU	CB-CG	5.92	1.63	1.52
1	1A	2530	A	N7-C5	-5.92	1.35	1.39
1	1A	1368	A	N7-C5	-5.92	1.35	1.39
1	1A	1080	G	C5-C4	-5.91	1.34	1.38
1	1A	1109	G	N3-C4	5.91	1.39	1.35
1	1A	2342	G	C8-N7	5.91	1.34	1.30
6	2G	167	GLU	CG-CD	5.91	1.60	1.51
1	2A	570	G	C6-O6	-5.90	1.18	1.24
1	1A	2405	A	N7-C5	-5.90	1.35	1.39
1	1A	417	A	N9-C4	-5.90	1.34	1.37
1	1A	2611	G	N3-C4	-5.90	1.31	1.35
1	1A	2442	A	C8-N7	-5.90	1.27	1.31
1	1A	2006	G	C2-N3	-5.89	1.28	1.32
1	1A	952	G	C8-N7	5.89	1.34	1.30
1	1A	962	G	N7-C5	-5.89	1.35	1.39
1	1A	1014	U	C4-O4	-5.88	1.19	1.23
1	1A	1035	G	C5-C4	-5.88	1.34	1.38
1	1A	1299	A	C5-C4	-5.87	1.34	1.38
1	1A	2600	G	C5-C4	-5.86	1.34	1.38
1	1A	2358	A	N7-C5	-5.86	1.35	1.39
1	1A	2037	A	C8-N7	-5.85	1.27	1.31
1	1A	798	A	N7-C5	-5.85	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2506	G	C2-N3	-5.85	1.28	1.32
27	15	6	VAL	CB-CG2	-5.85	1.40	1.52
32	2a	1370	G	N3-C4	5.85	1.39	1.35
1	1A	2014	G	C5-C4	-5.85	1.34	1.38
1	1A	2780	C	N3-C4	-5.85	1.29	1.33
32	1a	1030(A)	G	C5-C4	5.84	1.42	1.38
32	1a	1030(A)	G	N3-C4	5.84	1.39	1.35
32	2a	404	U	N1-C2	5.84	1.43	1.38
1	1A	2251	G	C6-N1	-5.83	1.35	1.39
1	1A	2003	A	C6-N6	-5.83	1.29	1.33
1	2A	2578	G	N3-C4	-5.83	1.31	1.35
1	1A	709	G	N9-C8	-5.82	1.33	1.37
1	1A	2093	A	N7-C5	-5.82	1.35	1.39
1	1A	2451	A	C8-N7	-5.82	1.27	1.31
1	1A	1221	G	C6-N1	5.81	1.43	1.39
1	2A	2113	U	C2-N3	5.81	1.41	1.37
1	1A	2030	C	C2-O2	-5.81	1.19	1.24
1	2A	2805	G	C2-N3	5.81	1.37	1.32
1	1A	1417	G	N7-C5	-5.81	1.35	1.39
32	2a	1447	A	N9-C4	5.81	1.41	1.37
1	2A	1051	G	C6-N1	5.80	1.43	1.39
1	1A	2491	G	N7-C5	-5.80	1.35	1.39
1	1A	1411	A	N9-C8	-5.80	1.33	1.37
1	1A	2037	A	N9-C4	-5.80	1.34	1.37
1	1A	829	A	C5-C4	-5.79	1.34	1.38
1	1A	174	U	C2-O2	-5.79	1.17	1.22
1	2A	2821	A	N9-C4	-5.79	1.34	1.37
32	2a	1134	G	N9-C4	5.79	1.42	1.38
1	1A	515	G	N3-C4	-5.79	1.31	1.35
1	2A	652(B)	A	N9-C4	5.79	1.41	1.37
1	1A	1394	G	C5-C4	-5.79	1.34	1.38
1	1A	25	U	C4-C5	-5.79	1.38	1.43
1	1A	2004	C	N3-C4	-5.78	1.29	1.33
1	1A	1840	A	C6-N6	-5.78	1.29	1.33
1	1A	833	C	C4-N4	-5.77	1.28	1.33
1	1A	1301	U	C2-O2	-5.77	1.17	1.22
1	1A	1133	G	N3-C4	5.76	1.39	1.35
1	1A	1413	A	N7-C5	-5.76	1.35	1.39
1	1A	2828	G	N9-C8	-5.76	1.33	1.37
30	18	56	GLU	CG-CD	5.76	1.60	1.51
1	1A	731	G	C6-O6	-5.76	1.19	1.24
1	1A	800	C	N3-C4	-5.76	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	575	G	C6-N1	-5.75	1.35	1.39
1	1A	2187	G	N9-C4	5.75	1.42	1.38
32	1a	1024	G	N3-C4	5.75	1.39	1.35
1	1A	185	A	N3-C4	-5.75	1.31	1.34
1	1A	811	A	N3-C4	-5.75	1.31	1.34
1	2A	1041	C	N1-C6	5.75	1.40	1.37
32	1a	1035	A	N9-C4	5.75	1.41	1.37
1	2A	673	C	C2-N3	5.75	1.40	1.35
1	2A	2009	G	N3-C4	-5.75	1.31	1.35
1	1A	1829	U	C2-N3	-5.74	1.33	1.37
1	1A	495	G	N9-C8	-5.74	1.33	1.37
1	2A	1508	A	N3-C4	5.74	1.38	1.34
1	1A	239	G	N3-C4	-5.73	1.31	1.35
32	2a	791	G	N9-C4	-5.73	1.33	1.38
1	1A	505	A	N3-C4	-5.73	1.31	1.34
32	2a	848	C	N1-C6	5.73	1.40	1.37
1	1A	1394	G	N1-C2	-5.72	1.33	1.37
1	2A	776	G	N7-C5	-5.72	1.35	1.39
1	1A	354	A	N9-C8	5.71	1.42	1.37
1	1A	1427	G	N1-C2	-5.71	1.33	1.37
1	1A	2440	G	N7-C5	-5.71	1.35	1.39
1	1A	1149	A	N9-C4	5.71	1.41	1.37
1	1A	1720	U	N1-C2	-5.71	1.33	1.38
1	1A	645	G	N9-C8	-5.71	1.33	1.37
1	1A	986	A	N9-C4	-5.71	1.34	1.37
39	1g	90	GLU	CG-CD	5.71	1.60	1.51
1	1A	747	G	N9-C8	-5.71	1.33	1.37
1	1A	1537	G	N9-C8	-5.70	1.33	1.37
1	1A	836	A	N7-C5	-5.70	1.35	1.39
1	1A	1296	G	N1-C2	-5.70	1.33	1.37
1	1A	1248	G	N7-C5	-5.69	1.35	1.39
1	1A	225	C	C2-O2	-5.69	1.19	1.24
1	1A	460	C	N3-C4	-5.69	1.29	1.33
1	1A	2171	G	N7-C5	5.69	1.42	1.39
1	1A	713	G	C5-C4	-5.68	1.34	1.38
1	1A	2076	A	N7-C5	-5.68	1.35	1.39
32	2a	530	G	C2-N3	5.68	1.37	1.32
1	1A	2134	G	N3-C4	5.68	1.39	1.35
1	1A	1307	C	C4-N4	-5.68	1.28	1.33
1	1A	2187	G	N7-C5	5.68	1.42	1.39
1	1A	609	A	N9-C4	-5.68	1.34	1.37
1	1A	2134	G	C2-N3	5.68	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2579	G	N3-C4	-5.68	1.31	1.35
1	1A	473	A	N3-C4	-5.67	1.31	1.34
1	2A	2140	C	N1-C6	5.67	1.40	1.37
1	1A	218	A	C5-C4	5.67	1.42	1.38
32	2a	190	U	C2-N3	5.67	1.41	1.37
23	11	33	LYS	CE-NZ	5.67	1.63	1.49
1	1A	2638	C	C4-N4	-5.66	1.28	1.33
1	2A	741	G	N3-C4	-5.66	1.31	1.35
1	1A	2555	G	C6-N1	-5.65	1.35	1.39
1	1A	2579	G	C5-C4	-5.65	1.34	1.38
1	1A	2735	G	N3-C4	5.65	1.39	1.35
32	1a	821	G	N7-C5	-5.65	1.35	1.39
1	1A	2586	G	N1-C2	-5.65	1.33	1.37
1	2A	2160	G	C5-C4	5.65	1.42	1.38
1	1A	1807	G	C6-N1	-5.64	1.35	1.39
1	1A	2582	G	N9-C4	-5.64	1.33	1.38
1	2A	2119	A	N9-C4	5.64	1.41	1.37
1	1A	1600	A	N7-C5	-5.64	1.35	1.39
1	2A	2160	G	N9-C4	5.64	1.42	1.38
1	1A	1809	U	C4-O4	-5.64	1.19	1.23
32	1a	965	A	N9-C4	-5.63	1.34	1.37
32	1a	1030(D)	A	N9-C4	5.63	1.41	1.37
1	1A	2652	G	N3-C4	-5.63	1.31	1.35
1	1A	2443	U	N3-C4	-5.62	1.33	1.38
1	1A	1665	G	N9-C8	-5.62	1.33	1.37
1	1A	716	G	N1-C2	-5.62	1.33	1.37
1	1A	2191	A	N7-C5	5.62	1.42	1.39
1	1A	2587	C	C4-N4	-5.62	1.28	1.33
1	1A	700	A	N9-C4	5.61	1.41	1.37
1	1A	2102	G	N9-C8	-5.61	1.33	1.37
1	2A	639	U	C2-N3	-5.61	1.33	1.37
1	1A	2636	G	C2-N3	5.61	1.37	1.32
8	1I	10	GLU	CG-CD	5.61	1.60	1.51
1	1A	1395	A	N3-C4	5.61	1.38	1.34
1	1A	218	A	N3-C4	5.61	1.38	1.34
1	1A	932	C	N1-C6	5.61	1.40	1.37
1	1A	1375	U	C2-O2	-5.60	1.17	1.22
1	1A	561	A	N3-C4	-5.60	1.31	1.34
1	1A	1181	G	N9-C8	-5.60	1.33	1.37
1	2A	2589	A	N9-C4	-5.60	1.34	1.37
32	1a	346	G	N9-C4	5.60	1.42	1.38
1	2A	729	G	N3-C4	-5.60	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1091	A	N3-C4	5.59	1.38	1.34
1	1A	1674	G	N7-C5	-5.59	1.35	1.39
1	1A	2752	U	N1-C6	-5.59	1.32	1.38
1	1A	1305	G	C8-N7	5.59	1.34	1.30
1	1A	2086	C	N1-C6	-5.58	1.33	1.37
1	2A	2153	G	N3-C4	5.58	1.39	1.35
32	1a	814	A	N9-C4	-5.58	1.34	1.37
1	1A	1816	A	C6-N1	-5.58	1.31	1.35
1	1A	2654	G	N1-C2	-5.58	1.33	1.37
1	1A	215	G	C2-N3	-5.57	1.28	1.32
1	1A	2261	U	C2-O2	-5.57	1.17	1.22
1	1A	839	G	N1-C2	-5.57	1.33	1.37
1	1A	1241	C	N1-C6	-5.57	1.33	1.37
1	1A	1863	C	C2-O2	-5.57	1.19	1.24
1	1A	811	A	C5-C4	-5.56	1.34	1.38
1	1A	1112	U	C2-N3	5.56	1.41	1.37
32	1a	1026	G	C5-C4	5.56	1.42	1.38
1	2A	1536	C	N3-C4	5.56	1.37	1.33
1	1A	1404	G	N7-C5	-5.55	1.35	1.39
32	2a	1405	G	N7-C5	-5.55	1.35	1.39
1	1A	1017	G	C8-N7	-5.55	1.27	1.30
1	2A	2249	U	C2-N3	-5.55	1.33	1.37
1	1A	2256	U	C2-N3	-5.54	1.33	1.37
1	1A	365	G	N1-C2	-5.54	1.33	1.37
1	1A	2426	G	N3-C4	-5.54	1.31	1.35
32	1a	346	G	N7-C5	5.54	1.42	1.39
1	2A	1274	A	N7-C5	-5.54	1.35	1.39
1	2A	1972	A	N9-C4	-5.54	1.34	1.37
32	1a	630	G	N3-C4	5.54	1.39	1.35
1	1A	1831	C	N1-C6	-5.54	1.33	1.37
1	1A	2561	G	N3-C4	-5.53	1.31	1.35
1	1A	594	A	C5-C4	-5.53	1.34	1.38
1	1A	1175	A	C6-N6	-5.53	1.29	1.33
32	2a	1029	C	N1-C6	5.53	1.40	1.37
1	1A	2446	A	N7-C5	-5.52	1.35	1.39
1	1A	2456	G	C8-N7	5.52	1.34	1.30
1	1A	109	A	C6-N6	-5.52	1.29	1.33
1	1A	2516	U	C4-O4	-5.51	1.19	1.23
32	2a	346	G	C6-N1	5.51	1.43	1.39
1	1A	607	C	C2-O2	-5.51	1.19	1.24
1	1A	556	C	P-OP2	-5.51	1.39	1.49
1	1A	860	U	C4-O4	-5.51	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	592	U	C2-O2	-5.51	1.17	1.22
1	1A	1873	G	C6-O6	-5.51	1.19	1.24
1	1A	2139	A	N9-C4	5.51	1.41	1.37
1	1A	1296	G	C6-N1	-5.50	1.35	1.39
32	1a	155	C	N1-C6	5.50	1.40	1.37
1	2A	1074	G	N7-C5	5.50	1.42	1.39
1	1A	2431	U	C2-N3	-5.50	1.33	1.37
32	2a	1026	G	C5-C4	5.50	1.42	1.38
1	1A	1441	A	C5-C6	-5.50	1.36	1.41
1	2A	1584	C	N3-C4	5.50	1.37	1.33
32	2a	1030(D)	A	C5-C4	5.50	1.42	1.38
1	1A	1786	A	N7-C5	-5.49	1.35	1.39
1	2A	1537	G	N9-C4	5.49	1.42	1.38
1	1A	2001	C	C2-O2	-5.49	1.19	1.24
1	2A	2106	G	C5-C4	5.49	1.42	1.38
1	1A	1952	G	C6-N1	-5.49	1.35	1.39
1	2A	450	G	C6-O6	-5.49	1.19	1.24
1	1A	456	A	C6-N1	-5.48	1.31	1.35
1	1A	1728	G	N3-C4	-5.48	1.31	1.35
32	2a	51	A	N7-C5	-5.48	1.35	1.39
1	1A	780	G	C6-N1	-5.47	1.35	1.39
1	2A	1086	A	N9-C4	5.47	1.41	1.37
1	1A	2448	G	C5-C4	-5.47	1.34	1.38
1	1A	694	G	C5-C4	5.47	1.42	1.38
1	1A	1092	A	N3-C4	5.47	1.38	1.34
1	1A	2738	A	N3-C4	-5.47	1.31	1.34
1	1A	1293	A	N9-C4	-5.46	1.34	1.37
1	1A	1394	G	N7-C5	-5.46	1.35	1.39
1	1A	1411	A	C8-N7	-5.46	1.27	1.31
1	1A	2157	A	N9-C4	5.46	1.41	1.37
32	1a	1003	G	C5-C4	5.46	1.42	1.38
1	1A	504	A	C6-N6	-5.46	1.29	1.33
1	1A	843	C	C2-O2	-5.46	1.19	1.24
1	1A	1427	G	C2-N3	-5.46	1.28	1.32
1	1A	1537	G	C5-C4	-5.46	1.34	1.38
1	1A	1313	U	C2-O2	-5.46	1.17	1.22
1	1A	1042	A	C5-C4	-5.45	1.34	1.38
1	2A	2106	G	N9-C4	5.45	1.42	1.38
1	1A	13	A	C8-N7	-5.45	1.27	1.31
1	1A	2082	A	C6-N1	-5.45	1.31	1.35
1	1A	934	A	N7-C5	5.45	1.42	1.39
1	1A	1661	C	C4-N4	-5.45	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	78	G	C6-N1	5.44	1.43	1.39
1	1A	215	G	N3-C4	-5.44	1.31	1.35
1	1A	1439	A	N3-C4	-5.44	1.31	1.34
1	1A	2017	U	N1-C2	-5.44	1.33	1.38
1	1A	2538	G	N9-C8	-5.44	1.34	1.37
1	2A	1359	A	N9-C4	5.44	1.41	1.37
1	1A	1012	C	C4-N4	-5.44	1.29	1.33
1	2A	2296	U	N1-C2	5.44	1.43	1.38
1	1A	2009	G	C2-N3	-5.43	1.28	1.32
1	2A	2319	G	N9-C8	5.43	1.41	1.37
1	1A	1080	G	N9-C8	-5.43	1.34	1.37
1	1A	2639	G	C5-C4	-5.43	1.34	1.38
1	1A	2057	G	N9-C4	-5.43	1.33	1.38
1	1A	237	G	N1-C2	-5.42	1.33	1.37
1	1A	2277	U	N1-C6	-5.42	1.33	1.38
1	1A	1993	A	N9-C4	-5.42	1.34	1.37
1	1A	2001	C	C4-N4	-5.42	1.29	1.33
1	1A	841	G	N9-C8	-5.42	1.34	1.37
1	1A	2601	A	N9-C4	-5.42	1.34	1.37
32	1a	346	G	C6-N1	5.42	1.43	1.39
1	1A	543	G	C8-N7	5.42	1.34	1.30
1	1A	724	A	N9-C8	-5.42	1.33	1.37
1	1A	1189	A	N3-C4	-5.41	1.31	1.34
1	1A	1507	A	N9-C4	5.41	1.41	1.37
1	1A	2639	G	N7-C5	-5.41	1.36	1.39
32	1a	1000	U	C2-N3	5.41	1.41	1.37
1	1A	2724	U	C4-C5	-5.40	1.38	1.43
1	1A	865	G	N7-C5	-5.40	1.36	1.39
1	1A	1382	A	N1-C2	-5.40	1.29	1.34
1	2A	2805	G	C5-C6	5.40	1.47	1.42
1	1A	1669	G	C5-C4	-5.40	1.34	1.38
32	1a	1134	G	C5-C4	5.39	1.42	1.38
1	1A	2883	A	C8-N7	-5.39	1.27	1.31
32	2a	1149	C	N1-C6	5.39	1.40	1.37
1	1A	1248	G	C5-C6	-5.39	1.36	1.42
1	2A	2893	G	N3-C4	5.39	1.39	1.35
32	2a	1001	A	C5-C6	5.39	1.45	1.41
1	2A	1076	C	N1-C2	5.39	1.45	1.40
32	2a	1030	C	N1-C2	5.39	1.45	1.40
1	1A	845	G	N1-C2	-5.39	1.33	1.37
1	1A	2740	G	N7-C5	-5.39	1.36	1.39
1	1A	38	A	C5-C4	-5.38	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1059	C	C4-N4	-5.38	1.29	1.33
1	1A	1119	A	N9-C4	5.38	1.41	1.37
1	1A	2454	C	C2-N3	-5.38	1.31	1.35
1	2A	1587	A	N9-C4	5.38	1.41	1.37
1	1A	2028	C	N1-C2	-5.38	1.34	1.40
1	1A	2752	U	N3-C4	-5.38	1.33	1.38
1	1A	168	G	N3-C4	-5.38	1.31	1.35
1	1A	2514	G	C6-N1	-5.38	1.35	1.39
1	1A	97	G	N7-C5	-5.38	1.36	1.39
32	1a	1257	U	N1-C2	5.37	1.43	1.38
1	2A	2450	A	N9-C4	-5.37	1.34	1.37
1	1A	1674	G	N1-C2	-5.37	1.33	1.37
1	1A	1814	A	N9-C4	-5.36	1.34	1.37
1	1A	2094	G	N7-C5	-5.36	1.36	1.39
1	2A	1846	G	N9-C4	-5.36	1.33	1.38
32	2a	1034	G	N7-C5	5.36	1.42	1.39
1	1A	2521	G	C5-C4	-5.36	1.34	1.38
1	2A	1626	G	C6-N1	-5.36	1.35	1.39
1	1A	2660	C	N1-C6	-5.35	1.33	1.37
1	1A	1752	G	C6-N1	-5.35	1.35	1.39
1	1A	2299	A	N9-C4	-5.35	1.34	1.37
1	2A	1074	G	N3-C4	5.35	1.39	1.35
32	2a	990	C	N1-C2	5.35	1.45	1.40
32	2a	1129	C	N3-C4	5.35	1.37	1.33
32	1a	1035	A	N3-C4	5.34	1.38	1.34
1	2A	2801(A)	A	N9-C4	5.34	1.41	1.37
1	1A	418	G	C5-C4	-5.33	1.34	1.38
1	1A	809	U	C4-O4	-5.33	1.19	1.23
1	1A	1232	G	C6-O6	-5.33	1.19	1.24
1	1A	2068	G	C5-C4	-5.33	1.34	1.38
1	1A	1403	U	C2-N3	-5.33	1.34	1.37
1	1A	1449	C	N1-C6	-5.33	1.33	1.37
1	1A	478	G	C5-C4	-5.33	1.34	1.38
1	1A	495	G	C2-N3	-5.32	1.28	1.32
1	1A	118	U	N1-C2	-5.32	1.33	1.38
1	1A	1707	C	N3-C4	-5.32	1.30	1.33
1	1A	1316	C	N3-C4	-5.32	1.30	1.33
1	1A	2041	A	N7-C5	-5.32	1.36	1.39
1	2A	1650	G	N1-C2	-5.32	1.33	1.37
1	1A	2179	G	C5-C6	5.32	1.47	1.42
1	1A	779	C	N3-C4	-5.31	1.30	1.33
1	1A	869	U	C2-O2	-5.31	1.17	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	840	A	C6-N1	-5.31	1.31	1.35
1	2A	1460	A	N9-C4	5.31	1.41	1.37
1	2A	2160	G	N3-C4	5.31	1.39	1.35
1	1A	1394	G	C6-N1	-5.31	1.35	1.39
27	15	59	GLU	CB-CG	5.30	1.62	1.52
32	2a	1530	G	N7-C5	5.30	1.42	1.39
1	1A	2633	A	C5-C4	-5.30	1.35	1.38
1	1A	2556	G	N3-C4	-5.30	1.31	1.35
32	1a	767	A	N9-C4	-5.29	1.34	1.37
32	1a	1003	G	N3-C4	5.29	1.39	1.35
1	1A	999	G	C6-N1	-5.29	1.35	1.39
32	2a	1014	A	N9-C4	5.28	1.41	1.37
1	1A	795	G	C6-N1	-5.28	1.35	1.39
1	2A	2129	C	N1-C6	5.27	1.40	1.37
1	1A	365	G	C6-N1	-5.27	1.35	1.39
1	1A	821	A	N1-C2	-5.27	1.29	1.34
1	1A	115	G	N9-C8	-5.27	1.34	1.37
32	2a	250	A	N9-C4	5.27	1.41	1.37
1	1A	178	G	C5-C4	-5.26	1.34	1.38
1	2A	213	A	N9-C4	-5.26	1.34	1.37
1	2A	1084	A	N3-C4	5.26	1.38	1.34
1	2A	2598	A	N3-C4	-5.26	1.31	1.34
1	1A	1398	U	C4-C5	-5.26	1.38	1.43
15	1T	5	ALA	CA-CB	-5.26	1.41	1.52
1	1A	1110	C	N1-C2	5.26	1.45	1.40
1	1A	2203	G	C6-N1	5.26	1.43	1.39
1	1A	2443	U	P-OP2	-5.26	1.40	1.49
32	1a	1036	G	N3-C4	5.26	1.39	1.35
1	2A	507	A	N7-C5	5.26	1.42	1.39
1	1A	825	G	N1-C2	-5.26	1.33	1.37
32	2a	1357	A	N9-C4	5.26	1.41	1.37
1	1A	123	G	N1-C2	-5.25	1.33	1.37
1	1A	791	G	N9-C8	-5.25	1.34	1.37
1	1A	591	U	C4-O4	-5.25	1.19	1.23
1	1A	2138	G	C5-C4	5.25	1.42	1.38
1	2A	686	G	N7-C5	-5.25	1.36	1.39
1	1A	398	A	N9-C4	-5.25	1.34	1.37
32	1a	1530	G	C6-N1	5.24	1.43	1.39
1	1A	582	G	N7-C5	-5.24	1.36	1.39
32	1a	250	A	C5-C4	5.24	1.42	1.38
1	2A	2177	C	N1-C6	5.24	1.40	1.37
32	1a	1030(C)	G	N9-C4	5.23	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2153	G	C6-N1	5.23	1.43	1.39
1	1A	2171	G	C6-N1	5.23	1.43	1.39
1	1A	2187	G	C2-N3	5.23	1.36	1.32
1	1A	540	A	N9-C4	-5.23	1.34	1.37
1	1A	446	C	C2-O2	-5.23	1.19	1.24
1	1A	1846	A	N9-C4	-5.23	1.34	1.37
1	1A	2245	U	C2-O2	-5.22	1.17	1.22
32	1a	156	G	N9-C8	5.22	1.41	1.37
1	2A	1536	C	C2-N3	5.22	1.40	1.35
1	2A	2162	G	C5-C4	5.22	1.42	1.38
1	1A	1255	A	C5-C4	-5.22	1.35	1.38
1	1A	2063	U	C2-O2	-5.22	1.17	1.22
1	1A	369	A	C6-N6	-5.22	1.29	1.33
1	1A	1149	A	N3-C4	5.21	1.38	1.34
1	1A	1112	U	N1-C6	5.21	1.42	1.38
1	1A	2068	G	N7-C5	-5.21	1.36	1.39
1	1A	221	G	N7-C5	-5.21	1.36	1.39
1	1A	1669	G	N1-C2	-5.21	1.33	1.37
32	2a	1030(A)	G	N3-C4	5.21	1.39	1.35
32	2a	1446	U	N1-C2	5.21	1.43	1.38
1	2A	1041	C	N1-C2	5.20	1.45	1.40
1	2A	1788	C	N1-C6	-5.20	1.34	1.37
1	1A	747	G	N1-C2	-5.20	1.33	1.37
1	1A	2129	C	N1-C6	5.20	1.40	1.37
1	1A	579	G	N3-C4	-5.20	1.31	1.35
1	1A	2453	C	N3-C4	-5.20	1.30	1.33
1	2A	6	A	N9-C4	5.20	1.41	1.37
1	2A	2613	U	C2-N3	-5.20	1.34	1.37
1	1A	538	A	N7-C5	-5.20	1.36	1.39
1	1A	2565	G	N9-C8	-5.20	1.34	1.37
1	1A	845	G	N7-C5	-5.19	1.36	1.39
1	1A	1665	G	C8-N7	-5.19	1.27	1.30
1	1A	2450	U	C4-O4	-5.19	1.19	1.23
1	1A	166	G	C6-N1	-5.19	1.35	1.39
1	2A	675	A	N9-C4	-5.19	1.34	1.37
1	1A	428	A	N3-C4	-5.19	1.31	1.34
1	2A	2132	U	C2-N3	5.19	1.41	1.37
1	1A	1304	C	C2-N3	-5.18	1.31	1.35
1	2A	229	A	C5-C4	5.18	1.42	1.38
1	2A	2517	C	N1-C6	-5.18	1.34	1.37
32	2a	1031	G	N9-C4	5.18	1.42	1.38
1	1A	1669	G	N3-C4	-5.18	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	484	G	C6-N1	-5.18	1.35	1.39
1	1A	23	G	C6-O6	5.18	1.28	1.24
1	2A	1092	C	N1-C6	5.18	1.40	1.37
1	1A	2623	U	C2-O2	-5.17	1.17	1.22
1	1A	2576	A	C5-C6	-5.17	1.36	1.41
1	2A	2064	C	C2-O2	-5.17	1.19	1.24
1	1A	2092	G	C6-N1	-5.17	1.35	1.39
1	1A	2137	G	N9-C4	5.17	1.42	1.38
1	1A	2258	G	N1-C2	-5.17	1.33	1.37
1	1A	2069	U	C2-N3	5.17	1.41	1.37
32	2a	1374	A	N9-C4	5.16	1.41	1.37
1	1A	2560	G	C8-N7	5.16	1.34	1.30
1	1A	1143	U	C2-N3	5.16	1.41	1.37
1	1A	2256	U	C2-O2	-5.16	1.17	1.22
1	1A	1846	A	C5-C4	-5.16	1.35	1.38
1	1A	2879	G	N7-C5	-5.16	1.36	1.39
32	1a	1024	G	N9-C4	5.16	1.42	1.38
1	2A	2167	U	N1-C2	5.15	1.43	1.38
1	1A	1390	G	C2-N3	-5.15	1.28	1.32
14	1S	107	GLU	CG-CD	5.15	1.59	1.51
32	1a	144	G	N9-C4	5.15	1.42	1.38
1	1A	323	A	C6-N1	-5.15	1.31	1.35
1	1A	1141	A	C5-C4	5.15	1.42	1.38
32	1a	1276	G	C5-C4	5.15	1.42	1.38
1	2A	2113	U	N1-C2	5.15	1.43	1.38
1	1A	176	G	N7-C5	-5.14	1.36	1.39
1	1A	794	U	C4-O4	5.14	1.27	1.23
1	2A	2177	C	C2-N3	5.14	1.39	1.35
32	1a	1026	G	N3-C4	5.14	1.39	1.35
1	1A	1356	G	C6-N1	-5.14	1.35	1.39
1	1A	1959	A	N3-C4	-5.14	1.31	1.34
1	1A	751	G	N3-C4	-5.13	1.31	1.35
1	1A	1666	G	N1-C2	-5.13	1.33	1.37
1	1A	1873	G	C6-N1	-5.13	1.35	1.39
1	2A	1655	A	N9-C8	-5.13	1.33	1.37
1	1A	2828	G	C5-C4	-5.13	1.34	1.38
1	2A	883	G	N7-C5	5.13	1.42	1.39
32	2a	204	U	N1-C2	5.12	1.43	1.38
1	1A	1371	G	N9-C8	-5.12	1.34	1.37
1	1A	2834	C	C4-C5	-5.12	1.38	1.43
1	2A	2635	C	N1-C6	-5.12	1.34	1.37
1	1A	891	C	N1-C6	-5.12	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1306	G	N3-C4	-5.12	1.31	1.35
1	1A	1816	A	C5-C6	-5.12	1.36	1.41
1	1A	29	U	C2-N3	-5.12	1.34	1.37
1	1A	255	G	C5-C6	-5.12	1.37	1.42
1	1A	1690	G	C2-N3	-5.12	1.28	1.32
32	2a	1033	G	C6-N1	5.12	1.43	1.39
1	1A	2689	G	N1-C2	-5.12	1.33	1.37
1	1A	608	G	C8-N7	5.12	1.34	1.30
1	1A	2271	G	N1-C2	-5.12	1.33	1.37
1	2A	792	G	C5-C4	-5.12	1.34	1.38
1	1A	1668	G	O3'-P	-5.11	1.55	1.61
1	1A	617	U	C2-N3	-5.11	1.34	1.37
1	1A	1177	G	C6-N1	-5.11	1.35	1.39
1	2A	2454	G	C6-N1	-5.11	1.35	1.39
1	1A	2639	G	C5-C6	-5.11	1.37	1.42
1	1A	2071	G	N1-C2	-5.11	1.33	1.37
1	1A	2440	G	C8-N7	5.11	1.34	1.30
32	2a	306	G	N7-C5	5.11	1.42	1.39
1	1A	1993	A	C6-N1	-5.10	1.31	1.35
1	1A	2348	A	C8-N7	-5.10	1.27	1.31
9	1N	14	VAL	CB-CG1	-5.10	1.42	1.52
1	2A	568	U	C4-O4	-5.10	1.19	1.23
1	2A	1509	C	N1-C2	5.10	1.45	1.40
1	1A	792	G	N1-C2	-5.10	1.33	1.37
1	2A	1079	C	N1-C2	5.10	1.45	1.40
1	2A	2114	A	C5-C4	5.10	1.42	1.38
1	1A	1109	G	N7-C5	5.10	1.42	1.39
1	1A	1133	G	N9-C4	5.10	1.42	1.38
1	1A	1475	G	C2-N3	-5.10	1.28	1.32
1	1A	2061	C	C4-C5	-5.10	1.38	1.43
1	1A	2857	U	C2-N3	-5.10	1.34	1.37
32	2a	1027	C	N1-C2	5.09	1.45	1.40
1	1A	495	G	N7-C5	-5.09	1.36	1.39
1	1A	1726	U	C2-O2	-5.09	1.17	1.22
1	1A	1997	G	C8-N7	-5.09	1.27	1.30
1	1A	271	U	N1-C6	5.08	1.42	1.38
1	1A	631	A	N3-C4	-5.08	1.31	1.34
1	1A	1724	A	C8-N7	-5.08	1.27	1.31
1	1A	2158	C	N1-C2	5.08	1.45	1.40
32	1a	189(L)	G	N9-C4	5.08	1.42	1.38
1	1A	122	G	N1-C2	-5.08	1.33	1.37
1	1A	885	C	C2-O2	-5.08	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2042	A	N9-C4	-5.08	1.34	1.37
1	1A	2341	G	N9-C4	-5.08	1.33	1.38
1	1A	2205	C	N1-C6	5.07	1.40	1.37
1	2A	2727	G	N7-C5	-5.07	1.36	1.39
32	2a	908	A	N7-C5	-5.07	1.36	1.39
1	1A	541	C	N1-C2	-5.07	1.35	1.40
1	1A	933	C	N1-C2	5.07	1.45	1.40
1	1A	1357	G	N1-C2	-5.07	1.33	1.37
1	1A	2113	U	C2-O2	-5.07	1.17	1.22
1	2A	459	U	C2-N3	-5.07	1.34	1.37
1	1A	1702	A	C8-N7	5.07	1.35	1.31
1	1A	848	G	P-OP2	-5.07	1.40	1.49
1	1A	1172	A	C5-C4	-5.06	1.35	1.38
1	1A	2187	G	C5-C6	5.06	1.47	1.42
1	1A	2724	U	N1-C6	-5.06	1.33	1.38
1	1A	479	C	C4-C5	5.06	1.47	1.43
1	1A	872	C	C4-C5	-5.06	1.39	1.43
1	1A	2823	A	C6-N1	-5.05	1.32	1.35
1	1A	810	G	N1-C2	-5.05	1.33	1.37
32	1a	156	G	N9-C4	5.05	1.42	1.38
32	1a	1285	A	C5-C4	5.05	1.42	1.38
1	1A	1203	G	C8-N7	-5.05	1.27	1.30
1	2A	744	G	N1-C2	-5.05	1.33	1.37
1	2A	2553	G	N9-C8	-5.05	1.34	1.37
27	15	59	GLU	CG-CD	5.04	1.59	1.51
32	1a	1286	A	C5-C4	5.04	1.42	1.38
1	1A	123	G	N3-C4	-5.04	1.31	1.35
1	2A	2128	C	N3-C4	5.04	1.37	1.33
1	1A	1197	G	N7-C5	5.04	1.42	1.39
32	1a	1001	A	C5-C4	5.04	1.42	1.38
1	2A	1950	G	N7-C5	-5.04	1.36	1.39
1	1A	1117	G	C5-C4	5.04	1.41	1.38
1	1A	1240	G	N3-C4	-5.04	1.31	1.35
32	1a	1525	G	C8-N7	5.04	1.33	1.30
1	1A	1380	G	N3-C4	-5.04	1.31	1.35
1	1A	477	C	C2-O2	-5.03	1.20	1.24
1	1A	715	G	N9-C8	-5.03	1.34	1.37
1	1A	2093	A	C6-N1	-5.03	1.32	1.35
1	1A	1676	G	C2-N3	-5.03	1.28	1.32
1	2A	2156	G	N9-C4	5.03	1.42	1.38
1	1A	1650	C	N1-C6	-5.03	1.34	1.37
1	1A	2013	U	N1-C2	-5.03	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2457	G	C6-N1	-5.03	1.36	1.39
1	1A	2610	A	C5-C4	-5.03	1.35	1.38
2	1B	98	G	N7-C5	-5.03	1.36	1.39
1	2A	652(A)	A	N9-C4	5.03	1.40	1.37
1	1A	1555	C	N1-C6	5.03	1.40	1.37
32	1a	1134	G	N9-C4	5.03	1.42	1.38
1	1A	1970	G	C2-N3	-5.02	1.28	1.32
1	1A	2043	C	N1-C6	-5.02	1.34	1.37
1	2A	2604	U	C2-N3	-5.02	1.34	1.37
32	2a	993	G	N9-C4	5.02	1.42	1.38
1	1A	1330	A	N3-C4	5.02	1.37	1.34
32	1a	298	A	N3-C4	-5.02	1.31	1.34
1	2A	1678	G	N7-C5	-5.02	1.36	1.39
1	1A	1661	C	N3-C4	-5.02	1.30	1.33
1	1A	1092	A	C5-C4	5.01	1.42	1.38
1	2A	1256	G	C8-N7	-5.01	1.27	1.30
1	1A	104	C	N3-C4	-5.01	1.30	1.33
1	1A	2006	G	N1-C2	-5.01	1.33	1.37
1	2A	741	G	N1-C2	-5.01	1.33	1.37
32	2a	1030(A)	G	C6-N1	5.01	1.43	1.39
1	1A	872	C	N3-C4	-5.01	1.30	1.33
1	1A	2818	U	N3-C4	5.01	1.43	1.38
2	1B	1	U	N3-C4	5.01	1.43	1.38
32	1a	73	G	N7-C5	5.01	1.42	1.39
1	1A	2048	C	N1-C6	-5.01	1.34	1.37
1	1A	2535	G	C6-N1	-5.01	1.36	1.39
1	1A	2818	U	C2-N3	5.01	1.41	1.37
1	2A	2160	G	C6-N1	5.01	1.43	1.39
1	2A	2794	C	N1-C6	5.01	1.40	1.37
32	1a	1278	U	N1-C6	5.00	1.42	1.38
1	1A	2180	A	N7-C5	5.00	1.42	1.39

All (7479) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1208	C	O5'-P-OP1	-33.37	70.65	110.70
32	1a	1520	G	O5'-P-OP1	-31.38	73.04	110.70
32	1a	1520	G	O5'-P-OP2	26.23	142.18	110.70
32	1a	1520	G	OP1-P-OP2	-24.67	82.60	119.60
32	2a	1208	C	OP1-P-OP2	-24.65	82.62	119.60
1	1A	354	A	C2-N3-C4	-20.05	100.57	110.60
1	1A	543	G	O5'-P-OP2	-18.52	88.47	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1208	C	O5'-P-OP2	17.85	132.12	110.70
1	1A	2045	G	O5'-P-OP1	-17.16	90.10	110.70
1	1A	2624	C	O5'-P-OP2	-16.87	90.45	110.70
1	1A	1847	G	O5'-P-OP1	-16.84	90.49	110.70
1	1A	2091	G	O5'-P-OP2	-16.80	90.54	110.70
32	2a	343	U	N3-C4-O4	-16.62	107.77	119.40
1	1A	991	G	O5'-P-OP1	-16.43	90.91	105.70
1	1A	2596	U	O5'-P-OP2	-16.28	91.05	105.70
32	2a	438	G	O5'-P-OP2	-16.24	91.09	105.70
1	2A	2603	G	O5'-P-OP2	-16.23	91.10	105.70
1	1A	1006	C	O5'-P-OP2	-16.15	91.17	105.70
32	2a	343	U	C2-N1-C1'	-15.59	98.99	117.70
32	1a	343	U	C2-N1-C1'	-14.61	100.17	117.70
1	2A	2554	U	O5'-P-OP1	-14.55	92.60	105.70
32	1a	533	A	N1-C6-N6	14.45	127.27	118.60
1	1A	834	U	O5'-P-OP1	-14.30	92.83	105.70
1	1A	2453	C	C2-N3-C4	-14.22	112.79	119.90
32	2a	404	U	N1-C2-O2	14.19	132.74	122.80
1	1A	1562	U	O5'-P-OP2	-14.19	92.93	105.70
1	1A	2331	G	N3-C4-N9	-14.14	117.52	126.00
1	1A	2598	C	N1-C2-O2	-13.95	110.53	118.90
1	1A	295	C	O5'-P-OP2	-13.93	93.16	105.70
1	2A	1272	A	O5'-P-OP2	-13.86	93.23	105.70
32	1a	343	U	N3-C4-O4	-13.78	109.76	119.40
1	1A	1054	C	C6-N1-C2	-13.75	114.80	120.30
32	1a	1530	G	C5-C6-O6	-13.73	120.36	128.60
1	1A	832	G	O5'-P-OP2	-13.72	93.35	105.70
32	2a	1207	2MG	OP2-P-O3'	-13.67	75.14	105.20
32	2a	1207	2MG	OP1-P-O3'	13.64	135.22	105.20
1	1A	1042	A	O5'-P-OP1	-13.50	93.55	105.70
1	1A	2194	U	C5-C4-O4	13.40	133.94	125.90
32	2a	1003	G	N3-C4-C5	-13.39	121.91	128.60
32	2a	1034	G	C5-C6-O6	-13.38	120.57	128.60
1	1A	2697	G	N1-C6-O6	-13.35	111.89	119.90
1	1A	82	G	N9-C4-C5	-13.35	100.06	105.40
32	1a	1530	G	N1-C6-O6	13.23	127.83	119.90
1	1A	2639	G	C5-C6-O6	-13.22	120.67	128.60
1	1A	1316	C	C6-N1-C2	13.10	125.54	120.30
32	1a	404	U	N1-C2-O2	13.07	131.95	122.80
1	1A	2620	G	C5-C6-O6	-12.86	120.88	128.60
1	1A	918	U	C5-C4-O4	-12.86	118.19	125.90
1	1A	2331	G	N3-C4-C5	12.86	135.03	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	194	G	C8-N9-C4	12.81	111.52	106.40
1	1A	354	A	N3-C4-C5	12.75	135.72	126.80
1	2A	2413	G	O5'-P-OP2	-12.60	94.36	105.70
32	2a	1003	G	C8-N9-C4	-12.59	101.36	106.40
1	1A	205	A	O5'-P-OP1	-12.50	94.45	105.70
1	2A	518	G	O5'-P-OP2	-12.46	94.49	105.70
1	1A	641	G	O5'-P-OP2	-12.43	94.52	105.70
1	1A	537	G	O4'-C1'-N9	12.33	118.07	108.20
32	1a	902	G	O5'-P-OP2	-12.29	94.64	105.70
1	1A	2102	G	O5'-P-OP2	-12.21	94.71	105.70
1	1A	1571	G	O5'-P-OP2	-12.19	94.73	105.70
1	1A	2566	U	O5'-P-OP1	-12.12	94.80	105.70
1	1A	2402	U	O5'-P-OP1	-12.07	94.84	105.70
1	1A	575	G	N1-C6-O6	-12.05	112.67	119.90
1	1A	1743	G	O5'-P-OP2	-12.04	94.86	105.70
1	1A	2440	G	C8-N9-C4	-12.03	101.59	106.40
1	1A	1695	C	O5'-P-OP1	-12.02	94.88	105.70
1	2A	1639	U	O5'-P-OP2	-12.02	94.88	105.70
32	2a	343	U	C5-C4-O4	12.01	133.10	125.90
32	2a	404	U	N3-C2-O2	-12.01	113.80	122.20
1	2A	2566	A	O5'-P-OP2	-11.96	94.94	105.70
1	2A	1063	G	C8-N9-C4	-11.95	101.62	106.40
1	1A	1425	A	N1-C6-N6	11.95	125.77	118.60
1	1A	1237	G	C8-N9-C4	11.95	111.18	106.40
1	2A	906	G	C5-C6-O6	11.94	135.76	128.60
2	1B	108	U	O5'-P-OP2	-11.93	94.97	105.70
1	1A	1666	G	N1-C6-O6	-11.92	112.75	119.90
1	1A	2331	G	C5-N7-C8	-11.87	98.36	104.30
1	2A	2575	C	O5'-P-OP2	-11.87	95.02	105.70
1	2A	2378	A	N1-C6-N6	11.86	125.72	118.60
32	1a	42	G	O5'-P-OP1	-11.81	95.07	105.70
32	1a	533	A	C5-C6-N6	-11.77	114.29	123.70
1	1A	2027	A	O5'-P-OP1	-11.77	95.11	105.70
1	1A	1318	A	O5'-P-OP2	-11.76	95.12	105.70
1	1A	2436	C	O5'-P-OP2	-11.76	95.11	105.70
2	1B	75	G	C6-N1-C2	-11.75	118.05	125.10
1	2A	1071	G	C8-N9-C4	-11.71	101.72	106.40
1	2A	481	G	O5'-P-OP2	-11.69	95.18	105.70
1	2A	1597	A	O5'-P-OP2	-11.68	95.18	105.70
2	1B	56	G	O5'-P-OP2	-11.68	95.19	105.70
1	1A	1986	G	N9-C4-C5	-11.67	100.73	105.40
1	2A	2145	C	C5-C6-N1	11.65	126.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	266	G	C8-N9-C4	-11.64	101.74	106.40
32	2a	299	G	C5-C6-O6	-11.62	121.63	128.60
32	1a	1137	C	C6-N1-C2	-11.62	115.65	120.30
2	1B	57	A	N9-C4-C5	-11.59	101.17	105.80
1	1A	2599	A	O5'-P-OP2	-11.58	95.28	105.70
1	1A	322	G	O5'-P-OP2	-11.52	95.33	105.70
1	2A	751	A	O5'-P-OP1	-11.49	95.36	105.70
1	1A	1787	G	O5'-P-OP2	-11.46	95.39	105.70
1	1A	1270	C	C6-N1-C2	11.40	124.86	120.30
1	1A	1358	U	C5-C4-O4	11.40	132.74	125.90
1	1A	36	G	O5'-P-OP2	-11.40	95.44	105.70
32	1a	343	U	C5-C4-O4	11.40	132.74	125.90
1	1A	2612	A	N1-C6-N6	-11.35	111.79	118.60
32	2a	1003	G	C2-N3-C4	11.34	117.57	111.90
1	2A	2612	C	C6-N1-C2	11.34	124.84	120.30
1	1A	2443	U	C5-C6-N1	-11.30	117.05	122.70
1	1A	49	U	O5'-P-OP1	-11.30	95.53	105.70
1	1A	2735	G	C8-N9-C4	11.28	110.91	106.40
32	2a	343	U	C6-N1-C1'	11.24	136.93	121.20
1	1A	1298	G	O5'-P-OP1	-11.23	95.59	105.70
1	1A	2640	C	C6-N1-C2	11.21	124.78	120.30
1	1A	2511	C	N3-C4-C5	-11.20	117.42	121.90
1	1A	2331	G	C2-N3-C4	-11.20	106.30	111.90
1	1A	1442	U	O5'-P-OP1	-11.17	95.64	105.70
1	1A	2586	G	N1-C6-O6	-11.17	113.20	119.90
1	2A	467	G	C8-N9-C4	11.13	110.85	106.40
1	2A	555	U	O5'-P-OP2	-11.12	95.70	105.70
1	1A	2067	C	C5-C6-N1	-11.11	115.44	121.00
1	1A	1237	G	N7-C8-N9	-11.09	107.56	113.10
1	1A	1720	U	N1-C2-O2	-11.05	115.06	122.80
1	1A	418	G	C6-N1-C2	-11.04	118.48	125.10
1	1A	575	G	C5-C6-O6	11.03	135.22	128.60
1	1A	2578	A	O5'-P-OP2	-11.03	95.78	105.70
1	1A	2014	G	N7-C8-N9	-11.01	107.60	113.10
32	1a	855	G	O5'-P-OP1	-11.00	95.80	105.70
1	1A	2006	G	C5-C6-O6	10.98	135.19	128.60
1	1A	1015	C	C5-C6-N1	-10.97	115.51	121.00
1	1A	1434	G	O5'-P-OP2	-10.95	95.85	105.70
1	1A	720	C	C2-N3-C4	-10.93	114.44	119.90
1	1A	2326	C	O5'-P-OP2	-10.92	95.87	105.70
1	1A	101	A	C5-C6-N1	-10.92	112.24	117.70
1	2A	205	G	O5'-P-OP2	-10.88	95.91	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	194	G	N9-C4-C5	-10.86	101.06	105.40
1	1A	1382	A	O5'-P-OP2	-10.85	95.93	105.70
1	1A	1569	U	O5'-P-OP2	10.85	123.72	110.70
2	1B	55	U	O5'-P-OP1	-10.85	95.94	105.70
1	1A	841	G	N1-C6-O6	-10.84	113.39	119.90
1	1A	2475	C	N3-C4-C5	10.83	126.23	121.90
1	2A	1673	U	O5'-P-OP1	-10.83	95.95	105.70
1	2A	752	A	P-O3'-C3'	10.78	132.63	119.70
1	2A	807	U	C2-N3-C4	-10.75	120.55	127.00
1	1A	2014	G	C8-N9-C4	10.74	110.69	106.40
1	1A	1700	G	C5-C6-O6	10.72	135.03	128.60
1	1A	2623	U	O5'-P-OP1	-10.71	96.06	105.70
28	16	13	CYS	CA-CB-SG	10.69	133.24	114.00
1	1A	1425	A	N9-C4-C5	-10.67	101.53	105.80
1	1A	1569	U	O5'-P-OP1	-10.66	96.10	105.70
1	1A	652	A	O5'-P-OP2	-10.66	96.11	105.70
1	2A	2023	G	O5'-P-OP1	-10.66	96.11	105.70
1	1A	101	A	C4-C5-C6	10.63	122.31	117.00
1	2A	1992	G	N3-C4-C5	-10.62	123.29	128.60
32	1a	226	G	C8-N9-C4	10.61	110.64	106.40
1	1A	2348	A	C8-N9-C4	10.60	110.04	105.80
1	1A	409	G	N1-C6-O6	-10.59	113.55	119.90
1	1A	1069	U	O5'-P-OP2	-10.59	96.17	105.70
1	1A	581	G	C5-C6-O6	10.56	134.94	128.60
1	1A	2348	A	N9-C4-C5	-10.56	101.58	105.80
32	1a	343	U	C6-N1-C1'	10.56	135.99	121.20
32	2a	697	U	O5'-P-OP2	-10.56	96.19	105.70
2	1B	75	G	N3-C2-N2	-10.54	112.53	119.90
32	1a	442	C	C6-N1-C2	-10.53	116.09	120.30
32	1a	1465	C	C2-N3-C4	-10.53	114.64	119.90
1	1A	537	G	N1-C6-O6	10.49	126.19	119.90
1	1A	449	A	O5'-P-OP2	-10.48	96.27	105.70
1	1A	1472	G	C5-C6-O6	-10.47	122.32	128.60
1	2A	912	C	C6-N1-C2	-10.46	116.11	120.30
1	2A	869	G	O5'-P-OP2	-10.44	96.30	105.70
1	1A	436	C	O5'-P-OP1	-10.44	96.31	105.70
1	1A	101	A	C2-N3-C4	-10.43	105.39	110.60
1	1A	2257	U	C2-N3-C4	-10.43	120.74	127.00
32	1a	1436	U	C2-N3-C4	-10.43	120.74	127.00
1	1A	1995	G	O5'-P-OP2	-10.41	96.33	105.70
32	1a	533	A	C6-C5-N7	-10.40	125.02	132.30
1	1A	2521	G	N1-C6-O6	-10.39	113.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1753	U	O5'-P-OP1	-10.37	96.36	105.70
1	1A	82	G	C4-C5-N7	10.35	114.94	110.80
1	2A	467	G	N7-C8-N9	-10.34	107.93	113.10
1	2A	2145	C	C6-N1-C2	-10.33	116.17	120.30
32	2a	1028	C	C6-N1-C2	-10.33	116.17	120.30
1	2A	510	C	O5'-P-OP2	-10.32	96.41	105.70
1	1A	2464	C	N1-C2-O2	-10.31	112.71	118.90
1	1A	1291	G	N1-C6-O6	-10.31	113.72	119.90
1	1A	1700	G	N1-C6-O6	-10.29	113.73	119.90
1	1A	2735	G	N9-C4-C5	-10.29	101.28	105.40
1	1A	849	A	O5'-P-OP1	-10.29	96.44	105.70
1	1A	2858	G	O4'-C1'-N9	10.28	116.42	108.20
32	2a	1530	G	C8-N9-C4	10.28	110.51	106.40
1	2A	2318	G	O4'-C1'-N9	10.27	116.42	108.20
1	1A	1052	C	C5-C6-N1	-10.25	115.87	121.00
1	1A	255	G	C5-C6-O6	-10.25	122.45	128.60
1	1A	354	A	C5-N7-C8	-10.24	98.78	103.90
1	2A	1071	G	N7-C8-N9	10.23	118.22	113.10
1	2A	2467	C	C6-N1-C2	-10.23	116.21	120.30
1	2A	749	C	O5'-P-OP2	-10.23	96.50	105.70
1	1A	1035	G	C5-C6-N1	10.22	116.61	111.50
1	2A	2549	G	O5'-P-OP2	-10.21	96.51	105.70
1	1A	593	G	C5-C6-O6	-10.21	122.47	128.60
1	1A	1099	C	C2-N3-C4	10.20	125.00	119.90
1	1A	1210	G	C5-C6-O6	10.19	134.71	128.60
1	1A	1216	G	C8-N9-C4	-10.19	102.33	106.40
1	1A	1621	C	O5'-P-OP2	-10.18	96.53	105.70
1	2A	1063	G	N7-C8-N9	10.18	118.19	113.10
1	1A	1425	A	C8-N9-C4	10.17	109.87	105.80
1	1A	2100	C	C2-N3-C4	-10.17	114.81	119.90
1	1A	1093	G	O5'-P-OP2	-10.16	96.56	105.70
1	1A	1386	U	C2-N3-C4	-10.14	120.91	127.00
32	1a	1502	A	O5'-P-OP2	-10.13	96.58	105.70
1	1A	31	C	O5'-P-OP1	-10.12	96.59	105.70
1	1A	1319	U	N3-C4-O4	-10.12	112.32	119.40
1	1A	1959	A	N1-C2-N3	10.11	134.35	129.30
1	1A	2582	G	C5-C6-O6	10.10	134.66	128.60
1	1A	1847	G	O5'-P-OP2	10.10	122.82	110.70
1	1A	1959	A	N1-C6-N6	-10.09	112.55	118.60
1	1A	2697	G	C5-C6-O6	10.09	134.66	128.60
1	2A	1187	G	O5'-P-OP2	-10.08	96.63	105.70
1	2A	948	G	O5'-P-OP1	-10.06	96.65	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2576	G	O5'-P-OP1	-10.04	96.66	105.70
1	2A	807	U	C5-C4-O4	-10.03	119.88	125.90
1	1A	2335	G	C4-C5-N7	10.03	114.81	110.80
1	1A	1425	A	C5-C6-N6	-10.02	115.68	123.70
2	2B	115	G	C8-N9-C4	10.02	110.41	106.40
1	1A	848	G	C5-C6-O6	10.01	134.61	128.60
1	2A	1092	C	N1-C2-O2	10.01	124.91	118.90
1	1A	1620	G	C5-C6-O6	-10.01	122.60	128.60
1	1A	2638	C	N3-C4-C5	9.99	125.90	121.90
32	1a	1137	C	C5-C6-N1	9.98	125.99	121.00
1	1A	2440	G	N9-C4-C5	9.97	109.39	105.40
1	1A	40	C	N1-C2-O2	-9.97	112.92	118.90
1	1A	45	C	O5'-P-OP1	-9.97	96.73	105.70
1	1A	1299	A	C5-N7-C8	9.95	108.88	103.90
1	1A	1723	A	N7-C8-N9	-9.95	108.82	113.80
32	2a	266	G	N3-C4-C5	-9.95	123.62	128.60
1	1A	1766	G	C4-C5-N7	9.95	114.78	110.80
1	1A	856	G	N1-C6-O6	-9.94	113.94	119.90
1	1A	952	G	N9-C4-C5	9.94	109.37	105.40
1	2A	856	C	C6-N1-C2	-9.93	116.33	120.30
1	1A	1245	C	N1-C2-O2	-9.93	112.94	118.90
1	1A	2610	A	N7-C8-N9	-9.93	108.84	113.80
1	2A	2105	C	C5-C6-N1	9.93	125.96	121.00
1	2A	2105	C	C6-N1-C2	-9.92	116.33	120.30
1	1A	1347	A	O5'-P-OP2	-9.91	96.78	105.70
32	2a	246	A	O5'-P-OP2	-9.91	96.78	105.70
1	1A	2596	U	C5-C4-O4	9.91	131.84	125.90
1	2A	1913	A	C8-N9-C4	-9.90	101.84	105.80
1	2A	2172	U	O4'-C1'-N1	9.90	116.12	108.20
1	1A	472	G	C4-C5-N7	9.90	114.76	110.80
1	1A	1048	G	O5'-P-OP2	-9.89	96.80	105.70
1	1A	2453	C	N3-C4-C5	9.89	125.85	121.90
1	2A	2430	A	O5'-P-OP2	-9.88	96.81	105.70
1	1A	874	U	C5-C6-N1	-9.87	117.77	122.70
1	1A	2439	C	C6-N1-C2	9.87	124.25	120.30
1	2A	2554	U	O5'-P-OP2	9.86	122.53	110.70
1	1A	1669	G	N1-C6-O6	-9.86	113.98	119.90
1	1A	752	A	N1-C6-N6	9.85	124.51	118.60
1	1A	1357	G	O5'-P-OP2	-9.85	96.84	105.70
1	2A	1536	C	N3-C4-C5	-9.84	117.96	121.90
32	2a	30	U	O5'-P-OP2	-9.81	96.87	105.70
1	1A	1148	C	N1-C2-O2	9.80	124.78	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2022	U	O5'-P-OP1	-9.79	96.89	105.70
1	1A	1439	A	N1-C6-N6	-9.78	112.73	118.60
1	1A	2383	G	C5-C6-O6	-9.78	122.73	128.60
1	1A	1316	C	C5-C6-N1	-9.78	116.11	121.00
1	1A	2238	C	C6-N1-C2	9.77	124.21	120.30
1	1A	1299	A	N7-C8-N9	-9.77	108.92	113.80
2	2B	24	G	C5-C6-O6	-9.77	122.74	128.60
1	1A	101	A	N1-C2-N3	9.77	134.18	129.30
1	1A	1181	G	C8-N9-C4	9.76	110.31	106.40
32	2a	1158	C	C6-N1-C2	-9.75	116.40	120.30
1	2A	673	C	C2-N3-C4	-9.75	115.03	119.90
32	2a	295	C	C6-N1-C2	9.75	124.20	120.30
1	1A	2257	U	N3-C4-C5	9.73	120.44	114.60
1	1A	2029	C	N3-C4-N4	-9.72	111.20	118.00
1	1A	2521	G	C5-C6-O6	9.72	134.43	128.60
1	1A	2630	G	N9-C4-C5	9.70	109.28	105.40
1	1A	2702	C	O5'-P-OP1	-9.70	96.97	105.70
32	2a	1495	U	N1-C2-O2	9.70	129.59	122.80
1	1A	1995	G	N1-C6-O6	-9.69	114.09	119.90
2	2B	6	C	C6-N1-C2	9.69	124.18	120.30
32	1a	1512	U	C5-C4-O4	9.68	131.71	125.90
32	2a	1034	G	C2-N3-C4	9.68	116.74	111.90
1	1A	1218	G	O4'-C1'-N9	9.67	115.94	108.20
1	1A	1294	G	N9-C4-C5	-9.67	101.53	105.40
1	1A	842	C	N1-C2-O2	9.67	124.70	118.90
1	2A	529	A	C5-N7-C8	-9.66	99.07	103.90
1	1A	537	G	C5-C6-O6	-9.66	122.81	128.60
1	1A	843	C	C2-N3-C4	-9.65	115.07	119.90
1	1A	246	A	O5'-P-OP2	-9.65	97.02	105.70
1	1A	790	G	N1-C6-O6	-9.64	114.11	119.90
32	1a	366	C	O5'-P-OP2	-9.64	97.02	105.70
32	2a	558	G	O5'-P-OP1	-9.64	97.03	105.70
1	1A	127	C	O5'-P-OP2	-9.62	97.04	105.70
1	1A	2272	C	C5-C6-N1	-9.62	116.19	121.00
1	1A	735	U	C5-C6-N1	-9.61	117.90	122.70
1	1A	2434	A	C8-N9-C4	-9.60	101.96	105.80
1	1A	417	A	C8-N9-C4	9.60	109.64	105.80
32	2a	1125	U	C5-C4-O4	9.59	131.65	125.90
1	1A	354	A	N3-C4-N9	-9.59	119.73	127.40
1	1A	1665	G	C8-N9-C4	9.57	110.23	106.40
1	1A	2258	G	C8-N9-C4	9.57	110.23	106.40
1	2A	512	G	O4'-C1'-N9	9.57	115.85	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2112	G	N1-C6-O6	-9.56	114.16	119.90
1	1A	1807	G	O5'-P-OP2	-9.55	97.10	105.70
1	1A	1750	G	O5'-P-OP2	-9.55	97.11	105.70
1	1A	1150	C	C6-N1-C2	-9.54	116.48	120.30
1	1A	2630	G	C4-C5-N7	-9.53	106.99	110.80
32	1a	115	G	O5'-P-OP2	-9.51	97.14	105.70
1	1A	1707	C	O5'-P-OP2	-9.51	97.14	105.70
1	1A	2382	G	O5'-P-OP2	-9.50	97.15	105.70
1	1A	195	U	C5-C6-N1	-9.49	117.95	122.70
1	2A	2177	C	C5-C6-N1	9.48	125.74	121.00
1	1A	2703	C	C6-N1-C2	9.47	124.09	120.30
1	1A	1860	A	O5'-P-OP2	-9.47	97.18	105.70
32	2a	1034	G	N3-C4-N9	9.47	131.68	126.00
32	2a	1034	G	C5-C6-N1	9.46	116.23	111.50
1	1A	831	A	C8-N9-C4	9.46	109.58	105.80
1	1A	903	C	C6-N1-C2	-9.46	116.52	120.30
1	1A	20	C	C5-C6-N1	-9.46	116.27	121.00
1	1A	760	G	C2-N3-C4	-9.46	107.17	111.90
1	1A	1450	C	O5'-P-OP2	-9.46	97.19	105.70
32	2a	1420	C	C6-N1-C2	-9.46	116.52	120.30
1	1A	748	G	O5'-P-OP2	-9.45	97.20	105.70
1	1A	641	G	N1-C6-O6	-9.43	114.24	119.90
1	1A	765	A	N1-C6-N6	9.42	124.25	118.60
1	1A	702	A	C8-N9-C4	-9.42	102.03	105.80
1	1A	1216	G	N7-C8-N9	9.42	117.81	113.10
1	1A	1803	G	C8-N9-C4	9.42	110.17	106.40
1	1A	1015	C	C6-N1-C2	9.41	124.07	120.30
1	1A	1772	C	C6-N1-C2	-9.41	116.53	120.30
1	1A	1419	A	O5'-P-OP1	9.41	122.00	110.70
1	1A	726	C	O5'-P-OP1	-9.41	97.23	105.70
1	1A	1409	C	O5'-P-OP2	-9.40	97.24	105.70
32	1a	819	A	N1-C6-N6	9.40	124.24	118.60
1	1A	2088	C	C6-N1-C2	-9.40	116.54	120.30
1	1A	419	C	O5'-P-OP1	-9.39	97.25	105.70
32	1a	1424	C	O5'-P-OP2	-9.39	97.25	105.70
32	2a	902	G	O5'-P-OP2	-9.38	97.26	105.70
34	1b	178	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	1A	170	A	N1-C6-N6	-9.38	112.97	118.60
1	1A	2606	C	C5-C6-N1	-9.36	116.32	121.00
1	1A	1669	G	C5-C6-O6	9.36	134.22	128.60
1	1A	952	G	C5-C6-O6	9.36	134.21	128.60
1	1A	752	A	N9-C4-C5	-9.35	102.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	812	C	C6-N1-C2	-9.35	116.56	120.30
1	1A	98	U	N1-C2-O2	9.34	129.34	122.80
1	1A	710	G	O5'-P-OP2	-9.34	97.30	105.70
1	1A	2607	G	C5-C6-O6	9.33	134.20	128.60
1	1A	1724	A	N1-C2-N3	9.33	133.97	129.30
1	1A	2535	G	N1-C6-O6	-9.33	114.30	119.90
1	1A	405	C	N3-C4-C5	9.31	125.62	121.90
1	1A	183	G	C5-C6-O6	9.30	134.18	128.60
1	1A	1666	G	C5-C6-O6	9.30	134.18	128.60
32	1a	768	A	C8-N9-C4	9.30	109.52	105.80
1	1A	749	G	O5'-P-OP2	-9.30	97.33	105.70
1	1A	1865	U	O5'-P-OP1	-9.30	97.33	105.70
32	2a	1465	C	C2-N3-C4	-9.30	115.25	119.90
1	2A	249	C	C6-N1-C2	9.29	124.02	120.30
1	2A	474	G	C8-N9-C4	-9.29	102.68	106.40
1	1A	2030	C	C4-C5-C6	9.29	122.05	117.40
1	1A	1071	G	O5'-P-OP1	-9.28	97.35	105.70
2	1B	13	A	O5'-P-OP2	-9.28	97.35	105.70
1	1A	810	G	N3-C2-N2	9.28	126.39	119.90
1	2A	1780	A	O5'-P-OP1	-9.27	97.35	105.70
32	2a	297	G	O5'-P-OP2	-9.27	97.36	105.70
32	1a	533	A	N9-C4-C5	-9.27	102.09	105.80
1	1A	2700	U	N3-C4-O4	9.26	125.88	119.40
32	1a	204	U	C2-N1-C1'	9.26	128.81	117.70
1	1A	472	G	C5-C6-O6	-9.25	123.05	128.60
1	1A	1316	C	N3-C4-C5	9.25	125.60	121.90
1	1A	1354	A	O5'-P-OP2	-9.24	97.38	105.70
1	1A	1821	C	C5-C4-N4	-9.23	113.73	120.20
1	1A	716	G	C8-N9-C4	9.23	110.09	106.40
1	1A	1856	A	N1-C6-N6	-9.23	113.06	118.60
1	1A	2582	G	N1-C6-O6	-9.22	114.37	119.90
1	1A	241	G	C8-N9-C4	-9.21	102.71	106.40
1	1A	799	A	C2-N3-C4	-9.21	106.00	110.60
1	1A	852	G	C5-C6-N1	9.21	116.10	111.50
1	2A	2827	C	C6-N1-C2	9.21	123.98	120.30
1	2A	154	G	C8-N9-C4	9.21	110.08	106.40
1	1A	2450	U	C5-C6-N1	-9.20	118.10	122.70
1	1A	1462	G	O4'-C1'-N9	9.20	115.56	108.20
1	2A	1071	G	C6-C5-N7	-9.19	124.89	130.40
32	2a	1406	U	C2-N3-C4	-9.19	121.49	127.00
32	2a	299	G	C4-C5-N7	9.18	114.47	110.80
1	1A	109	A	N1-C6-N6	-9.18	113.09	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	751	G	C5-C6-O6	-9.18	123.09	128.60
1	1A	1766	G	C5-N7-C8	-9.16	99.72	104.30
1	1A	2025	G	N1-C6-O6	-9.16	114.40	119.90
1	2A	1076	C	N1-C2-O2	9.16	124.40	118.90
1	2A	1992	G	C8-N9-C4	-9.15	102.74	106.40
1	2A	2805	G	N3-C4-C5	-9.14	124.03	128.60
1	1A	365	G	C5-C6-O6	9.14	134.09	128.60
1	1A	2902	G	N1-C2-N3	-9.13	118.42	123.90
1	1A	642	G	O5'-P-OP2	-9.13	97.49	105.70
1	1A	238	C	C6-N1-C2	9.12	123.95	120.30
1	1A	1021	G	O5'-P-OP2	-9.12	97.49	105.70
1	1A	1995	G	C5-C6-O6	9.12	134.07	128.60
32	1a	1136	U	C5-C6-N1	9.12	127.26	122.70
1	1A	891	C	C5-C6-N1	-9.12	116.44	121.00
1	1A	1237	G	C5-N7-C8	9.12	108.86	104.30
1	1A	1701	A	N9-C4-C5	-9.11	102.16	105.80
1	1A	2331	G	O4'-C1'-N9	9.11	115.48	108.20
1	1A	1003	U	C6-N1-C2	-9.10	115.54	121.00
1	1A	125	A	C5-C6-N1	9.09	122.25	117.70
1	1A	82	G	C8-N9-C4	9.08	110.03	106.40
32	2a	665	A	O5'-P-OP2	-9.08	97.53	105.70
1	1A	1803	G	N7-C8-N9	-9.07	108.56	113.10
32	1a	884	U	O5'-P-OP2	-9.07	97.54	105.70
32	1a	1495	U	N1-C2-O2	9.06	129.14	122.80
1	1A	1814	A	C2-N3-C4	9.05	115.13	110.60
1	1A	598	A	O5'-P-OP1	-9.05	97.56	105.70
1	2A	1914	C	C6-N1-C2	-9.05	116.68	120.30
1	1A	2876	U	N1-C2-O2	9.04	129.13	122.80
1	1A	2158	C	C6-N1-C2	-9.04	116.69	120.30
1	2A	9	U	C2-N3-C4	9.04	132.42	127.00
1	2A	773	U	O5'-P-OP1	-9.03	97.57	105.70
1	2A	2699	C	C6-N1-C2	9.04	123.91	120.30
1	1A	96	C	O5'-P-OP2	-9.03	97.57	105.70
1	1A	354	A	C4-C5-N7	9.03	115.22	110.70
1	1A	1690	G	N1-C6-O6	-9.03	114.48	119.90
1	1A	2069	U	C5-C4-O4	-9.03	120.48	125.90
32	2a	487	A	C8-N9-C4	9.03	109.41	105.80
1	2A	33	U	N3-C2-O2	-9.03	115.88	122.20
1	1A	1060	U	O5'-P-OP2	-9.02	97.58	105.70
1	1A	2067	C	C6-N1-C2	9.02	123.91	120.30
1	1A	1980	C	N3-C4-C5	-9.01	118.29	121.90
1	1A	932	C	C6-N1-C2	-9.01	116.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2258	G	N7-C8-N9	-9.01	108.60	113.10
1	1A	2608	U	N1-C2-O2	-9.00	116.50	122.80
1	1A	1986	G	C8-N9-C4	9.00	110.00	106.40
1	1A	1655	A	N7-C8-N9	-9.00	109.30	113.80
1	1A	1826	C	C2-N3-C4	-8.99	115.40	119.90
32	1a	1530	G	N3-C4-C5	8.99	133.09	128.60
1	1A	1282	G	C8-N9-C4	8.98	109.99	106.40
1	2A	2502	G	O5'-P-OP2	-8.98	97.62	105.70
1	1A	1505	C	N3-C2-O2	-8.98	115.62	121.90
1	1A	2596	U	O5'-P-OP1	8.98	121.47	110.70
1	2A	1696	G	O5'-P-OP2	-8.98	97.62	105.70
1	2A	2306	C	N1-C2-O2	8.97	124.28	118.90
1	1A	493	G	O5'-P-OP2	-8.97	97.63	105.70
1	1A	1723	A	C8-N9-C4	8.97	109.39	105.80
1	2A	1913	A	C4-C5-C6	8.97	121.48	117.00
32	2a	1024	G	C2-N3-C4	8.97	116.38	111.90
1	2A	1614	A	O5'-P-OP1	-8.96	97.64	105.70
1	2A	906	G	N9-C4-C5	8.96	108.98	105.40
1	1A	2802	C	C2-N1-C1'	-8.95	108.95	118.80
32	1a	699	C	C6-N1-C2	-8.95	116.72	120.30
1	1A	2316	G	O5'-P-OP1	-8.95	97.64	105.70
1	1A	519	G	C8-N9-C4	-8.95	102.82	106.40
1	1A	1001	G	C2-N3-C4	-8.95	107.43	111.90
1	1A	2574	U	N3-C2-O2	-8.94	115.94	122.20
1	1A	20	C	C2-N3-C4	-8.93	115.43	119.90
1	1A	952	G	N1-C6-O6	-8.93	114.54	119.90
1	1A	581	G	N1-C6-O6	-8.93	114.54	119.90
1	1A	1346	U	P-O3'-C3'	8.92	130.41	119.70
1	2A	1906	G	O5'-P-OP1	-8.92	97.67	105.70
32	2a	1465	C	C5-C4-N4	-8.92	113.95	120.20
1	1A	2828	G	N1-C6-O6	-8.92	114.55	119.90
16	1U	33	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	1A	2561	G	O5'-P-OP2	-8.92	97.67	105.70
1	1A	1177	G	C5-C6-O6	8.91	133.95	128.60
1	1A	96	C	C6-N1-C2	-8.91	116.73	120.30
1	1A	1992	A	O5'-P-OP2	8.91	121.39	110.70
1	1A	2069	U	N3-C4-C5	8.91	119.95	114.60
1	1A	1427	G	C5-C6-O6	8.91	133.94	128.60
32	1a	825	G	N1-C6-O6	-8.91	114.56	119.90
32	2a	1436	U	C2-N3-C4	-8.90	121.66	127.00
1	1A	223	C	N1-C2-O2	8.90	124.24	118.90
1	2A	774	A	O5'-P-OP2	-8.89	97.69	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1278	U	C5-C6-N1	8.89	127.14	122.70
1	1A	1663	C	N1-C2-O2	-8.88	113.57	118.90
1	1A	2065	C	N1-C2-O2	-8.88	113.58	118.90
1	2A	832	G	O5'-P-OP2	8.87	121.35	110.70
1	1A	474	U	O5'-P-OP2	-8.87	97.72	105.70
1	1A	1958	A	O4'-C1'-N9	8.87	115.29	108.20
32	1a	1384	C	C6-N1-C2	-8.86	116.75	120.30
1	1A	365	G	N1-C6-O6	-8.86	114.58	119.90
1	1A	1148	C	O5'-P-OP1	8.86	121.33	110.70
1	2A	2855	C	C6-N1-C2	-8.85	116.76	120.30
1	1A	2630	G	C8-N9-C4	-8.84	102.86	106.40
1	1A	1705	C	C6-N1-C2	-8.84	116.76	120.30
1	1A	554	A	C6-N1-C2	-8.84	113.30	118.60
1	2A	1690	A	N1-C6-N6	8.84	123.90	118.60
1	1A	45	C	N3-C4-N4	-8.83	111.82	118.00
1	1A	2331	G	C8-N9-C4	-8.83	102.87	106.40
32	2a	1530	G	N3-C4-C5	8.82	133.01	128.60
1	1A	2251	G	N1-C6-O6	-8.82	114.61	119.90
1	2A	1776	G	O5'-P-OP2	-8.82	97.76	105.70
1	1A	733	G	C8-N9-C4	8.82	109.93	106.40
1	2A	2207	G	C6-C5-N7	-8.82	125.11	130.40
1	1A	848	G	N1-C6-O6	-8.81	114.61	119.90
32	2a	1495	U	N3-C2-O2	-8.81	116.03	122.20
1	1A	1747	A	O5'-P-OP1	-8.81	97.77	105.70
1	1A	121	G	O5'-P-OP2	-8.80	97.78	105.70
32	2a	472	A	C8-N9-C4	-8.80	102.28	105.80
1	1A	731	G	N1-C6-O6	-8.80	114.62	119.90
1	2A	1793	C	N3-C4-C5	8.80	125.42	121.90
1	1A	731	G	C2-N3-C4	8.80	116.30	111.90
1	1A	2858	G	C4-C5-N7	-8.80	107.28	110.80
32	1a	1530	G	C4-C5-N7	8.79	114.32	110.80
1	1A	874	U	C2-N3-C4	-8.79	121.73	127.00
1	1A	475	A	C8-N9-C4	8.78	109.31	105.80
1	2A	476	G	O5'-P-OP2	-8.78	97.80	105.70
1	1A	934	A	O4'-C1'-N9	8.78	115.22	108.20
1	1A	2611	G	N1-C6-O6	-8.78	114.64	119.90
1	2A	484	C	O5'-P-OP2	-8.78	97.80	105.70
1	2A	2167	U	N3-C2-O2	-8.77	116.06	122.20
32	1a	460	G	C8-N9-C4	-8.77	102.89	106.40
1	1A	799	A	C8-N9-C4	8.76	109.31	105.80
1	2A	2523	G	O5'-P-OP2	-8.76	97.82	105.70
1	1A	2674	A	C8-N9-C4	-8.76	102.30	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2245	U	N1-C2-N3	8.75	120.15	114.90
1	1A	2586	G	C5-C6-O6	8.75	133.85	128.60
1	2A	2207	G	N7-C8-N9	8.75	117.47	113.10
1	1A	1505	C	N1-C2-O2	8.74	124.14	118.90
1	1A	829	A	O5'-P-OP1	-8.73	97.84	105.70
32	1a	158	G	N9-C4-C5	8.73	108.89	105.40
1	1A	2034	G	C5-C6-O6	8.72	133.84	128.60
1	1A	809	U	C5-C4-O4	-8.72	120.67	125.90
1	2A	1187	G	C5-C6-O6	8.72	133.83	128.60
32	2a	884	U	O5'-P-OP2	-8.72	97.85	105.70
1	1A	1151	U	N1-C2-N3	-8.72	109.67	114.90
1	1A	2001	C	C2-N3-C4	-8.72	115.54	119.90
1	1A	1296	G	N1-C6-O6	-8.72	114.67	119.90
1	2A	1204	A	C8-N9-C4	8.71	109.28	105.80
1	1A	2425	G	O5'-P-OP2	-8.71	97.86	105.70
1	1A	1567	G	C8-N9-C4	-8.69	102.92	106.40
32	1a	404	U	N3-C2-O2	-8.69	116.11	122.20
1	2A	415	A	O5'-P-OP2	-8.69	97.88	105.70
1	1A	491	G	C6-N1-C2	-8.68	119.89	125.10
32	2a	530	G	N3-C4-C5	-8.68	124.26	128.60
1	1A	1725	G	C8-N9-C4	-8.68	102.93	106.40
1	1A	37	C	O5'-P-OP2	-8.67	97.89	105.70
1	1A	702	A	C5-N7-C8	-8.67	99.56	103.90
1	1A	1167	C	C6-N1-C2	-8.67	116.83	120.30
1	1A	102	U	C5-C4-O4	-8.67	120.70	125.90
1	1A	1769	G	N1-C6-O6	-8.67	114.70	119.90
1	1A	2047	C	N1-C2-O2	-8.66	113.70	118.90
1	1A	2046	G	C8-N9-C4	8.65	109.86	106.40
1	1A	2331	G	N7-C8-N9	8.65	117.43	113.10
1	2A	1926	U	C5-C4-O4	8.65	131.09	125.90
32	2a	1034	G	N3-C4-C5	-8.65	124.28	128.60
1	1A	1846	A	C6-N1-C2	-8.64	113.41	118.60
1	2A	1351	C	OP1-P-O3'	8.64	124.22	105.20
1	1A	735	U	C2-N3-C4	-8.64	121.81	127.00
2	2B	5	C	C6-N1-C2	8.64	123.76	120.30
1	1A	130	G	C4-C5-N7	-8.63	107.35	110.80
1	1A	1392	G	C5-C6-O6	8.63	133.78	128.60
1	1A	638	U	O5'-P-OP2	-8.62	97.94	105.70
32	1a	148	G	N3-C4-C5	-8.63	124.29	128.60
1	1A	747	G	N1-C6-O6	-8.62	114.73	119.90
1	1A	2579	G	N7-C8-N9	-8.62	108.79	113.10
1	1A	472	G	N1-C6-O6	8.61	125.07	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2612	A	C5-C6-N6	8.61	130.59	123.70
32	1a	135	C	O5'-P-OP1	8.61	121.03	110.70
1	1A	1245	C	C2-N3-C4	-8.61	115.60	119.90
1	1A	1620	G	N1-C6-O6	8.61	125.06	119.90
2	1B	70	C	O5'-P-OP2	-8.61	97.95	105.70
1	2A	2207	G	N1-C6-O6	8.61	125.07	119.90
32	1a	498	U	C5-C4-O4	8.60	131.06	125.90
1	2A	566	U	OP2-P-O3'	8.60	124.12	105.20
1	2A	1694	C	O5'-P-OP1	-8.60	97.96	105.70
1	1A	2802	C	N1-C2-O2	-8.60	113.74	118.90
1	2A	718	A	N1-C6-N6	8.60	123.76	118.60
1	1A	592	U	N1-C2-O2	-8.60	116.78	122.80
1	1A	1986	G	N3-C2-N2	8.59	125.92	119.90
1	1A	2780	C	N3-C2-O2	-8.59	115.89	121.90
1	1A	494	G	C5-C6-O6	8.59	133.75	128.60
32	2a	993	G	N3-C4-N9	8.59	131.15	126.00
1	1A	2452	C	C6-N1-C2	8.58	123.73	120.30
1	1A	2430	A	C2-N3-C4	8.58	114.89	110.60
1	2A	35	G	C5-C6-O6	8.57	133.74	128.60
1	1A	1130	A	N1-C6-N6	-8.57	113.46	118.60
1	1A	2587	C	N3-C4-C5	8.57	125.33	121.90
1	1A	1474	C	C2-N1-C1'	-8.56	109.38	118.80
1	2A	1087	G	N3-C4-N9	-8.56	120.86	126.00
1	2A	645	C	C5-C6-N1	8.56	125.28	121.00
1	1A	1259	A	C5-N7-C8	8.56	108.18	103.90
1	2A	1992	G	C6-N1-C2	-8.56	119.97	125.10
32	2a	1370	G	N9-C4-C5	-8.55	101.98	105.40
1	1A	554	A	C5-C6-N6	-8.55	116.86	123.70
1	2A	1265	A	O5'-P-OP2	-8.55	98.00	105.70
1	1A	1821	C	N1-C2-O2	-8.55	113.77	118.90
1	1A	2606	C	C4-C5-C6	8.55	121.67	117.40
1	1A	641	G	N3-C2-N2	8.55	125.88	119.90
13	1R	2	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	1A	2630	G	C5-N7-C8	8.54	108.57	104.30
1	1A	1050	C	C2-N3-C4	-8.53	115.63	119.90
32	2a	791	G	N3-C4-C5	8.53	132.87	128.60
1	1A	34	C	O4'-C1'-N1	8.53	115.02	108.20
1	2A	1097	U	C2-N1-C1'	8.53	127.93	117.70
1	1A	2134	G	N3-C4-C5	-8.53	124.34	128.60
32	2a	299	G	N1-C6-O6	8.53	125.02	119.90
1	1A	720	C	N3-C4-C5	8.52	125.31	121.90
1	1A	2840	G	O5'-P-OP2	-8.52	98.03	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1187	G	N1-C6-O6	-8.52	114.79	119.90
32	2a	1027	C	N1-C2-O2	8.52	124.01	118.90
1	1A	1099	C	C5-C6-N1	8.51	125.26	121.00
1	1A	1024	G	C5-C6-O6	8.51	133.70	128.60
1	1A	1291	G	C5-C6-O6	8.51	133.70	128.60
1	1A	859	C	O5'-P-OP1	-8.50	98.05	105.70
32	1a	355	C	C6-N1-C2	-8.50	116.90	120.30
1	1A	398	A	N1-C6-N6	8.50	123.70	118.60
1	1A	1824	C	C2-N3-C4	-8.50	115.65	119.90
32	1a	158	G	N3-C4-N9	-8.49	120.91	126.00
1	2A	527	C	N1-C2-O2	-8.49	113.81	118.90
1	2A	341	G	O5'-P-OP2	-8.49	98.06	105.70
1	1A	1826	C	N3-C4-C5	8.49	125.30	121.90
1	1A	2234	G	C8-N9-C4	8.48	109.79	106.40
1	2A	1913	A	N1-C2-N3	8.48	133.54	129.30
1	1A	731	G	C5-C6-N1	8.47	115.74	111.50
1	1A	1341	C	N3-C2-O2	-8.47	115.97	121.90
32	2a	709	G	C8-N9-C4	-8.47	103.01	106.40
1	1A	181	C	N1-C2-O2	-8.46	113.82	118.90
1	1A	735	U	N1-C2-N3	8.46	119.98	114.90
32	1a	888	G	O5'-P-OP2	-8.46	98.08	105.70
32	1a	1067	A	P-O3'-C3'	8.46	129.85	119.70
1	1A	1518	A	O5'-P-OP1	-8.46	98.09	105.70
1	1A	2024	G	C5-N7-C8	8.46	108.53	104.30
1	1A	854	U	C2-N3-C4	-8.46	121.93	127.00
1	2A	2319	G	N3-C4-C5	8.45	132.83	128.60
32	2a	266	G	C4-N9-C1'	8.45	137.49	126.50
1	1A	1831	C	N3-C4-C5	-8.45	118.52	121.90
1	1A	809	U	C2-N1-C1'	8.45	127.84	117.70
1	2A	958	U	C6-N1-C2	-8.44	115.93	121.00
1	1A	837	C	O5'-P-OP2	-8.44	98.10	105.70
32	2a	1054	C	C2-N1-C1'	8.44	128.08	118.80
1	2A	1471	A	C8-N9-C4	-8.44	102.42	105.80
32	2a	266	G	P-O3'-C3'	8.43	129.82	119.70
1	1A	902	G	N3-C2-N2	8.43	125.80	119.90
1	1A	952	G	C8-N9-C4	-8.43	103.03	106.40
32	2a	1034	G	C6-N1-C2	-8.43	120.04	125.10
1	1A	591	U	C2-N3-C4	-8.43	121.94	127.00
32	1a	479	C	N3-C4-C5	-8.42	118.53	121.90
2	1B	50	G	N1-C6-O6	-8.42	114.85	119.90
1	2A	214	G	O4'-C1'-N9	8.42	114.94	108.20
1	1A	214	A	O5'-P-OP2	-8.41	98.13	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	841	G	C5-C6-O6	8.41	133.65	128.60
1	1A	2056	U	N3-C4-O4	-8.41	113.51	119.40
1	1A	2063	U	C2-N3-C4	-8.41	121.96	127.00
1	1A	2607	G	N1-C6-O6	-8.40	114.86	119.90
1	2A	1834	U	N3-C2-O2	-8.40	116.32	122.20
1	1A	660	C	C6-N1-C2	-8.39	116.94	120.30
1	1A	39	C	O5'-P-OP2	-8.39	98.15	105.70
1	1A	2277	U	C4-C5-C6	8.39	124.73	119.70
32	2a	656	C	C5-C6-N1	8.39	125.19	121.00
1	1A	1301	U	O5'-P-OP2	-8.38	98.16	105.70
1	1A	1474	C	C6-N1-C2	8.38	123.65	120.30
1	1A	2702	C	N1-C2-O2	-8.38	113.87	118.90
1	1A	793	A	O4'-C1'-N9	8.37	114.90	108.20
1	1A	2639	G	C5-C6-N1	8.37	115.69	111.50
32	1a	874	G	C8-N9-C4	8.37	109.75	106.40
1	1A	2510	C	C5-C4-N4	8.37	126.06	120.20
1	1A	403	C	N3-C2-O2	-8.36	116.05	121.90
32	2a	1030	C	C2-N1-C1'	8.36	128.00	118.80
32	2a	1003	G	C4-N9-C1'	8.36	137.37	126.50
32	1a	781	A	N9-C4-C5	-8.36	102.46	105.80
1	1A	809	U	O5'-P-OP1	-8.35	98.18	105.70
32	2a	1422	G	O5'-P-OP2	-8.35	98.19	105.70
32	1a	914	A	C8-N9-C4	-8.33	102.47	105.80
1	2A	2850	A	C8-N9-C4	-8.33	102.47	105.80
1	1A	2627	U	N3-C2-O2	-8.33	116.37	122.20
1	1A	1859	G	C5-C6-N1	-8.33	107.34	111.50
1	1A	582	G	N7-C8-N9	8.32	117.26	113.10
1	1A	2883	A	O5'-P-OP2	-8.32	98.21	105.70
32	2a	1125	U	C2-N1-C1'	8.32	127.69	117.70
32	1a	204	U	C5-C6-N1	8.32	126.86	122.70
1	1A	405	C	C5-C4-N4	-8.32	114.38	120.20
1	1A	1092	A	O4'-C1'-N9	8.32	114.85	108.20
1	1A	2193	A	N1-C6-N6	8.32	123.59	118.60
1	2A	741	G	C5-C6-O6	8.32	133.59	128.60
1	1A	2320	G	C4-C5-N7	8.31	114.12	110.80
1	1A	2383	G	C5-C6-N1	8.31	115.66	111.50
32	1a	750	G	O5'-P-OP1	-8.31	98.22	105.70
1	1A	499	G	N1-C6-O6	-8.31	114.92	119.90
1	1A	494	G	C4-C5-N7	-8.30	107.48	110.80
1	1A	1282	G	N7-C8-N9	-8.30	108.95	113.10
32	2a	1003	G	N7-C8-N9	8.30	117.25	113.10
1	1A	433	G	O5'-P-OP1	-8.30	98.23	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	251	A	C2-N3-C4	-8.29	106.45	110.60
1	2A	2467	C	N3-C4-C5	-8.29	118.58	121.90
32	2a	375	U	O5'-P-OP1	-8.29	98.24	105.70
1	1A	1559	C	O5'-P-OP1	-8.28	98.25	105.70
1	1A	2277	U	N3-C4-O4	8.28	125.19	119.40
1	2A	1778	U	C5-C6-N1	-8.28	118.56	122.70
1	1A	2700	U	N1-C2-O2	-8.27	117.01	122.80
1	1A	2397	C	O5'-P-OP1	-8.26	98.26	105.70
32	1a	1077	G	O5'-P-OP2	-8.26	98.27	105.70
1	2A	2427	C	O5'-P-OP1	-8.26	98.27	105.70
1	2A	2629	A	O4'-C1'-N9	8.26	114.81	108.20
1	1A	2598	C	N3-C2-O2	8.24	127.67	121.90
1	1A	1056	A	C8-N9-C4	8.24	109.10	105.80
1	1A	1092	A	C8-N9-C4	-8.24	102.50	105.80
1	1A	591	U	C5-C4-O4	-8.24	120.96	125.90
32	1a	1422	G	O5'-P-OP2	-8.23	98.29	105.70
1	1A	495	G	C4-C5-N7	-8.23	107.51	110.80
1	1A	1539	C	N3-C2-O2	-8.23	116.14	121.90
1	1A	2439	C	C5-C6-N1	-8.23	116.89	121.00
1	2A	2596	U	C2-N3-C4	-8.23	122.06	127.00
1	1A	98	U	N3-C2-O2	-8.23	116.44	122.20
1	1A	1862	G	C5-C6-N1	-8.23	107.39	111.50
2	1B	31	C	O5'-P-OP2	-8.23	98.30	105.70
1	1A	991	G	O5'-P-OP2	8.22	120.57	110.70
1	1A	2244	U	C5-C6-N1	-8.22	118.59	122.70
1	2A	992	C	C6-N1-C2	-8.22	117.01	120.30
1	2A	1983	C	N1-C2-O2	-8.22	113.97	118.90
1	1A	422	U	N1-C2-O2	8.22	128.55	122.80
1	1A	2620	G	N1-C6-O6	8.22	124.83	119.90
32	1a	165	C	C6-N1-C2	-8.21	117.01	120.30
1	2A	892	G	O5'-P-OP1	-8.21	98.31	105.70
32	1a	299	G	C5-C6-N1	8.21	115.61	111.50
1	1A	836	A	O5'-P-OP2	8.21	120.55	110.70
1	1A	2331	G	N3-C2-N2	-8.21	114.15	119.90
1	1A	2067	C	C4-C5-C6	8.21	121.50	117.40
1	2A	2319	G	N3-C4-N9	-8.20	121.08	126.00
1	2A	1992	G	C2-N3-C4	8.19	116.00	111.90
1	2A	416	C	O5'-P-OP1	8.19	120.53	110.70
32	2a	750	G	O5'-P-OP1	-8.19	98.33	105.70
1	1A	2111	U	C5-C4-O4	-8.19	120.99	125.90
32	1a	174	C	C6-N1-C2	-8.19	117.03	120.30
1	1A	486	A	N1-C6-N6	-8.18	113.69	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2839	C	C6-N1-C2	-8.18	117.03	120.30
1	1A	1294	G	N3-C2-N2	8.18	125.63	119.90
32	2a	830	G	N1-C6-O6	8.18	124.81	119.90
1	1A	2526	U	O5'-P-OP1	-8.18	98.34	105.70
1	1A	665	C	O5'-P-OP2	-8.18	98.34	105.70
1	1A	1522	G	N3-C2-N2	-8.18	114.18	119.90
32	2a	1027	C	C6-N1-C2	-8.18	117.03	120.30
1	1A	665	C	N3-C2-O2	8.17	127.62	121.90
1	1A	2639	G	C8-N9-C4	8.17	109.67	106.40
1	1A	2372	A	O5'-P-OP2	-8.16	98.35	105.70
32	2a	346	G	C6-N1-C2	-8.16	120.20	125.10
1	2A	1210	A	P-O3'-C3'	8.16	129.49	119.70
32	2a	726	C	O5'-P-OP1	-8.16	98.36	105.70
1	1A	215	G	O4'-C1'-N9	8.15	114.72	108.20
1	1A	592	U	C5-C6-N1	-8.15	118.62	122.70
1	1A	472	G	C6-C5-N7	-8.15	125.51	130.40
32	1a	1276	G	C8-N9-C4	-8.15	103.14	106.40
1	1A	355	A	N1-C6-N6	8.14	123.49	118.60
32	2a	904	C	N3-C4-N4	8.14	123.70	118.00
1	1A	1453	C	C5-C6-N1	-8.13	116.94	121.00
32	2a	299	G	N9-C4-C5	-8.13	102.15	105.40
1	1A	2034	G	N1-C6-O6	-8.12	115.03	119.90
1	1A	2598	C	C5-C4-N4	-8.12	114.51	120.20
1	1A	1716	A	N1-C2-N3	8.12	133.36	129.30
14	1S	3	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	2A	1380	G	O5'-P-OP2	-8.12	98.39	105.70
1	2A	2257	U	O5'-P-OP1	-8.12	98.39	105.70
1	1A	495	G	N3-C2-N2	-8.12	114.22	119.90
1	1A	873	U	C5-C6-N1	-8.12	118.64	122.70
1	1A	1986	G	N1-C2-N2	-8.12	108.90	116.20
1	1A	2193	A	C5-C6-N6	-8.12	117.21	123.70
1	1A	2227	G	C4-N9-C1'	-8.12	115.95	126.50
1	2A	961	C	C6-N1-C2	8.12	123.55	120.30
1	1A	2386	C	C6-N1-C2	8.11	123.55	120.30
1	1A	958	C	C6-N1-C2	-8.11	117.06	120.30
32	2a	115	G	C8-N9-C4	-8.11	103.16	106.40
1	1A	1863	C	C6-N1-C2	-8.11	117.06	120.30
1	2A	248	G	C8-N9-C4	-8.11	103.16	106.40
1	2A	2032	G	C5-N7-C8	8.11	108.36	104.30
1	2A	450	G	N1-C6-O6	-8.11	115.04	119.90
1	2A	1984	G	C8-N9-C4	-8.11	103.16	106.40
32	1a	1512	U	N3-C4-O4	-8.10	113.73	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1233	G	N1-C6-O6	-8.09	115.05	119.90
32	2a	5	U	C5-C6-N1	8.09	126.75	122.70
1	1A	827	G	N1-C2-N3	8.09	128.75	123.90
1	2A	11	G	N7-C8-N9	8.09	117.14	113.10
27	25	58	LEU	CA-CB-CG	8.09	133.90	115.30
32	2a	1158	C	C2-N1-C1'	8.09	127.69	118.80
1	1A	2033	U	C6-N1-C2	-8.08	116.15	121.00
1	1A	189	U	O5'-P-OP2	-8.08	98.43	105.70
1	1A	192	C	C6-N1-C2	8.08	123.53	120.30
1	1A	1606	G	O5'-P-OP2	-8.08	98.43	105.70
1	1A	883	G	C8-N9-C4	-8.07	103.17	106.40
1	1A	1418	U	N3-C4-O4	8.07	125.05	119.40
1	1A	2598	C	C2-N3-C4	-8.07	115.86	119.90
1	1A	2823	A	N1-C6-N6	-8.07	113.76	118.60
1	1A	1701	A	C8-N9-C4	8.07	109.03	105.80
1	1A	1104	G	N9-C4-C5	-8.06	102.17	105.40
1	2A	391	G	C6-N1-C2	-8.06	120.26	125.10
1	1A	2587	C	C2-N3-C4	-8.06	115.87	119.90
32	1a	250	A	C8-N9-C4	-8.06	102.58	105.80
1	1A	2375	C	C6-N1-C2	8.06	123.52	120.30
1	1A	1681	A	N9-C4-C5	8.05	109.02	105.80
1	2A	1881	C	O5'-P-OP1	-8.05	98.45	105.70
1	2A	2008	C	O5'-P-OP2	-8.05	98.45	105.70
1	1A	1411	A	C8-N9-C4	8.05	109.02	105.80
1	1A	1379	C	N3-C4-C5	8.04	125.12	121.90
1	1A	1341	C	C2-N3-C4	-8.04	115.88	119.90
1	1A	2618	C	N1-C2-O2	-8.04	114.08	118.90
32	1a	841	U	C2-N1-C1'	8.04	127.34	117.70
1	2A	2017	U	C5-C6-N1	-8.04	118.68	122.70
1	1A	2442	A	N1-C6-N6	-8.03	113.78	118.60
32	1a	175	C	O5'-P-OP1	-8.03	98.47	105.70
1	2A	912	C	C5-C6-N1	8.03	125.02	121.00
1	2A	1372	U	C5-C4-O4	-8.03	121.08	125.90
1	1A	2171	G	C4-N9-C1'	-8.03	116.06	126.50
1	1A	2596	U	N3-C4-O4	-8.03	113.78	119.40
1	2A	12	U	N3-C2-O2	-8.03	116.58	122.20
1	1A	1758	C	OP1-P-OP2	-8.03	107.56	119.60
1	1A	1270	C	C5-C6-N1	-8.03	116.99	121.00
32	1a	297	G	C2-N3-C4	-8.03	107.89	111.90
1	1A	1155	C	N3-C4-N4	8.02	123.61	118.00
1	1A	2804	C	C6-N1-C2	-8.02	117.09	120.30
1	1A	838	C	C6-N1-C2	8.01	123.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1573	G	N3-C2-N2	-8.01	114.29	119.90
1	2A	2071	A	O5'-P-OP1	-8.01	98.49	105.70
1	1A	2200	C	C6-N1-C2	-8.01	117.10	120.30
32	2a	1026	G	C8-N9-C4	-8.01	103.20	106.40
1	1A	515	G	N3-C2-N2	-8.00	114.30	119.90
1	1A	2082	A	N1-C6-N6	-8.00	113.80	118.60
32	2a	913	A	P-O3'-C3'	8.00	129.30	119.70
1	1A	1065	U	O5'-P-OP2	-8.00	98.50	105.70
1	1A	1232	G	O5'-P-OP1	8.00	120.30	110.70
1	1A	1973	U	C5-C6-N1	-7.99	118.70	122.70
32	2a	625	G	C8-N9-C4	-7.99	103.20	106.40
1	1A	1043	G	OP1-P-OP2	-7.99	107.61	119.60
1	2A	1975	G	O5'-P-OP2	-7.99	98.51	105.70
1	1A	501	U	O5'-P-OP1	-7.99	98.51	105.70
1	2A	11	G	C6-C5-N7	-7.99	125.61	130.40
1	1A	2404	A	O5'-P-OP1	-7.99	98.51	105.70
1	2A	469	G	C5-C6-O6	-7.99	123.81	128.60
1	2A	2611	U	O5'-P-OP1	-7.99	98.51	105.70
1	1A	1418	U	C5-C4-O4	-7.97	121.11	125.90
2	2B	54	G	N3-C2-N2	-7.97	114.32	119.90
1	2A	1764	G	N1-C6-O6	-7.97	115.12	119.90
1	1A	752	A	C5-C6-N6	-7.97	117.32	123.70
1	1A	2084	A	O5'-P-OP1	-7.97	98.53	105.70
1	1A	1330	A	O5'-P-OP2	-7.97	98.53	105.70
1	1A	2257	U	C5-C4-O4	-7.97	121.12	125.90
2	2B	59	A	C6-N1-C2	-7.97	113.82	118.60
1	2A	1900	A	O5'-P-OP1	-7.96	98.53	105.70
1	1A	2638	C	C2-N3-C4	-7.96	115.92	119.90
1	1A	1121	C	N1-C2-O2	7.96	123.67	118.90
1	2A	976	C	N1-C2-O2	7.96	123.67	118.90
1	1A	1472	G	N1-C6-O6	7.96	124.67	119.90
1	1A	1377	A	N9-C4-C5	7.96	108.98	105.80
1	1A	2091	G	C5-C6-N1	7.95	115.48	111.50
1	1A	2030	C	C2-N3-C4	-7.95	115.92	119.90
1	2A	277	C	N1-C2-O2	7.95	123.67	118.90
1	2A	1968	G	N1-C6-O6	7.95	124.67	119.90
32	1a	183	G	C8-N9-C4	-7.95	103.22	106.40
1	2A	1662	C	N3-C4-C5	7.95	125.08	121.90
1	1A	766	C	N3-C4-C5	7.95	125.08	121.90
1	1A	735	U	C4-C5-C6	7.94	124.46	119.70
1	1A	1430	A	C8-N9-C4	-7.94	102.62	105.80
1	2A	447	A	C8-N9-C4	7.93	108.97	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	533	A	C4-C5-C6	7.93	120.97	117.00
1	2A	1079	C	O4'-C1'-N1	7.93	114.54	108.20
1	1A	2595	G	C8-N9-C4	7.93	109.57	106.40
1	2A	1692	U	O5'-P-OP2	-7.93	98.57	105.70
1	1A	466	G	C5-C6-N1	-7.92	107.54	111.50
1	1A	579	G	N9-C4-C5	7.92	108.57	105.40
32	2a	1482	G	C5-C6-O6	7.92	133.35	128.60
1	1A	1426	G	N1-C6-O6	7.92	124.65	119.90
1	1A	52	A	C8-N9-C4	-7.92	102.63	105.80
1	1A	1735	U	OP1-P-OP2	7.91	131.47	119.60
1	1A	2042	A	N1-C2-N3	-7.91	125.34	129.30
1	1A	241	G	N9-C4-C5	7.91	108.56	105.40
1	1A	2006	G	N1-C6-O6	-7.91	115.15	119.90
32	1a	343	U	O4'-C1'-N1	7.91	114.53	108.20
1	1A	233	A	O5'-P-OP2	-7.91	98.58	105.70
1	1A	952	G	N3-C4-N9	-7.91	121.25	126.00
1	2A	2080	G	O5'-P-OP2	-7.91	98.58	105.70
1	1A	1179	U	O5'-P-OP2	-7.91	98.58	105.70
1	1A	1303	C	C4-C5-C6	7.91	121.35	117.40
1	2A	2597	G	O5'-P-OP2	-7.91	98.58	105.70
32	2a	316	G	O5'-P-OP2	-7.91	98.58	105.70
1	1A	553	A	O5'-P-OP1	7.91	120.19	110.70
1	1A	1365	G	C8-N9-C4	-7.91	103.24	106.40
1	1A	2624	C	C6-N1-C2	7.90	123.46	120.30
1	2A	529	A	C4-C5-N7	7.90	114.65	110.70
1	1A	1240	G	N1-C6-O6	-7.90	115.16	119.90
1	2A	11	G	N1-C6-O6	7.90	124.64	119.90
1	2A	2626	C	C6-N1-C2	7.90	123.46	120.30
1	1A	1193	C	O5'-P-OP2	-7.90	98.59	105.70
1	1A	1681	A	C8-N9-C4	-7.89	102.64	105.80
32	1a	186	C	C6-N1-C2	-7.89	117.14	120.30
32	1a	533	A	N3-C4-N9	7.89	133.71	127.40
1	2A	1758	G	O5'-P-OP1	-7.89	98.60	105.70
1	1A	2158	C	N1-C2-O2	7.89	123.63	118.90
1	1A	1719	C	C6-N1-C2	-7.89	117.14	120.30
32	1a	560	U	C6-N1-C2	-7.89	116.27	121.00
32	2a	266	G	N7-C8-N9	7.89	117.04	113.10
1	1A	847	A	N1-C6-N6	-7.89	113.87	118.60
1	1A	1833	A	O5'-P-OP1	-7.89	98.60	105.70
1	2A	1936	A	O4'-C1'-N9	7.89	114.51	108.20
1	1A	1826	C	C5-C6-N1	-7.89	117.06	121.00
1	2A	2269	A	O5'-P-OP1	-7.89	98.60	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	857	C	O5'-P-OP2	-7.88	98.60	105.70
1	1A	569	G	C8-N9-C4	-7.88	103.25	106.40
2	1B	33	G	O5'-P-OP2	-7.88	98.61	105.70
1	1A	2576	A	N1-C6-N6	7.87	123.32	118.60
32	1a	174	C	C2-N1-C1'	7.87	127.46	118.80
1	2A	1790	C	C6-N1-C2	7.87	123.45	120.30
1	1A	742	G	N1-C6-O6	-7.87	115.18	119.90
1	1A	835	A	C5-N7-C8	7.87	107.83	103.90
1	1A	2638	C	C5-C4-N4	-7.87	114.69	120.20
1	2A	1664	A	O5'-P-OP2	-7.87	98.62	105.70
1	2A	1791	A	C8-N9-C4	-7.87	102.65	105.80
32	1a	576	G	N3-C4-N9	7.86	130.72	126.00
1	2A	1251	C	N3-C4-N4	7.86	123.50	118.00
1	1A	2257	U	C6-N1-C2	7.86	125.72	121.00
1	1A	1012	C	N3-C4-C5	7.86	125.04	121.90
1	1A	1264	G	C2-N3-C4	-7.86	107.97	111.90
32	1a	1513	A	C2-N3-C4	7.86	114.53	110.60
1	1A	932	C	C5-C6-N1	7.86	124.93	121.00
1	1A	918	U	N3-C4-O4	7.86	124.90	119.40
32	1a	670	G	N1-C6-O6	-7.86	115.19	119.90
1	1A	891	C	C6-N1-C2	7.86	123.44	120.30
1	1A	2014	G	C5-N7-C8	7.85	108.23	104.30
1	1A	1800	G	O5'-P-OP2	-7.85	98.63	105.70
1	1A	2572	C	C2-N3-C4	-7.85	115.97	119.90
19	2X	57	LEU	CA-CB-CG	7.85	133.36	115.30
1	1A	1177	G	N1-C6-O6	-7.85	115.19	119.90
1	2A	72	U	O5'-P-OP1	-7.84	98.64	105.70
1	1A	369	A	C5-C6-N6	-7.84	117.43	123.70
1	1A	1364	C	O5'-P-OP2	7.84	120.11	110.70
1	1A	35	G	N1-C6-O6	-7.83	115.20	119.90
1	1A	1486	G	O5'-P-OP2	-7.83	98.65	105.70
1	2A	601	C	C6-N1-C2	-7.83	117.17	120.30
1	1A	751	G	O4'-C1'-N9	7.83	114.46	108.20
1	1A	892	G	O4'-C1'-N9	7.82	114.46	108.20
1	2A	1771	C	N3-C4-C5	7.82	125.03	121.90
32	1a	156	G	C8-N9-C4	-7.82	103.27	106.40
1	2A	1298	C	O5'-P-OP2	-7.82	98.66	105.70
1	1A	618	C	O5'-P-OP2	-7.82	98.67	105.70
1	2A	1630	G	N9-C4-C5	7.82	108.53	105.40
1	1A	101	A	N1-C6-N6	7.82	123.29	118.60
1	1A	271	U	C5-C4-O4	7.81	130.59	125.90
1	1A	1175	A	OP1-P-OP2	7.81	131.32	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	316	C	O5'-P-OP1	-7.81	98.67	105.70
1	1A	1916	C	C6-N1-C2	-7.81	117.18	120.30
1	1A	2624	C	OP1-P-OP2	7.81	131.31	119.60
1	1A	813	C	C4-C5-C6	7.80	121.30	117.40
1	2A	744	G	O5'-P-OP2	-7.80	98.67	105.70
8	1I	38	LEU	CA-CB-CG	7.80	133.25	115.30
1	2A	633	A	O5'-P-OP1	-7.80	98.68	105.70
1	2A	2032	G	N7-C8-N9	-7.80	109.20	113.10
32	2a	1432	G	N1-C6-O6	-7.80	115.22	119.90
1	1A	191	U	C2-N3-C4	-7.80	122.32	127.00
1	2A	956	G	N1-C6-O6	7.80	124.58	119.90
32	2a	1125	U	N3-C4-O4	-7.80	113.94	119.40
1	1A	184	A	P-O3'-C3'	7.79	129.05	119.70
1	2A	463	G	C5-C6-O6	7.79	133.28	128.60
1	1A	2639	G	N9-C4-C5	-7.79	102.28	105.40
1	1A	2738	A	C2-N3-C4	-7.79	106.71	110.60
1	1A	1213	U	O5'-P-OP2	-7.79	98.69	105.70
1	1A	2335	G	C5-N7-C8	-7.79	100.41	104.30
1	1A	2610	A	C8-N9-C4	7.79	108.91	105.80
1	1A	1262	C	N1-C2-O2	-7.78	114.23	118.90
1	1A	1317	G	OP1-P-OP2	-7.78	107.93	119.60
1	1A	2403	G	O5'-P-OP2	-7.78	98.70	105.70
1	1A	2804	C	N3-C4-C5	-7.78	118.79	121.90
1	2A	2689	U	P-O3'-C3'	7.78	129.03	119.70
1	2A	906	G	C8-N9-C4	-7.78	103.29	106.40
32	1a	1003	G	N3-C4-C5	-7.77	124.71	128.60
1	1A	556	C	C2-N3-C4	-7.77	116.01	119.90
1	2A	1848	A	C8-N9-C4	7.77	108.91	105.80
1	1A	2220	A	O4'-C1'-N9	7.77	114.42	108.20
1	2A	794	G	O5'-P-OP2	-7.77	98.71	105.70
1	1A	2551	C	C5-C6-N1	-7.76	117.12	121.00
1	2A	568	U	C5-C4-O4	-7.76	121.24	125.90
1	1A	1036	A	N1-C2-N3	-7.76	125.42	129.30
32	1a	57	G	C8-N9-C4	-7.76	103.30	106.40
1	2A	780	G	C5-C6-O6	-7.76	123.94	128.60
1	1A	2256	U	C2-N3-C4	-7.76	122.34	127.00
32	1a	1158	C	C4-C5-C6	7.76	121.28	117.40
1	1A	1958	A	C5-N7-C8	-7.75	100.02	103.90
1	1A	779	C	C6-N1-C2	-7.75	117.20	120.30
1	1A	1959	A	C5-C6-N6	7.75	129.90	123.70
32	2a	1335	C	N1-C2-O2	7.75	123.55	118.90
32	2a	346	G	N3-C4-C5	-7.75	124.72	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	189(D)	C	C2-N1-C1'	7.75	127.33	118.80
32	1a	354	G	O5'-P-OP2	-7.75	98.73	105.70
1	1A	702	A	N7-C8-N9	7.74	117.67	113.80
1	2A	906	G	N3-C4-N9	-7.74	121.36	126.00
1	2A	2063	C	O5'-P-OP2	-7.74	98.74	105.70
32	2a	834	C	O5'-P-OP2	-7.74	98.74	105.70
32	1a	460	G	N7-C8-N9	7.73	116.97	113.10
1	2A	153	C	O5'-P-OP2	-7.73	98.74	105.70
1	2A	1721	G	N3-C4-N9	7.73	130.64	126.00
1	1A	2658	C	N3-C4-N4	-7.73	112.59	118.00
1	1A	1661	C	N3-C2-O2	-7.73	116.49	121.90
32	2a	1495	U	C2-N1-C1'	7.73	126.98	117.70
1	1A	415	G	C8-N9-C4	7.73	109.49	106.40
1	1A	1232	G	O5'-P-OP2	-7.73	98.75	105.70
1	1A	1966	U	C2-N3-C4	-7.73	122.36	127.00
1	1A	2137	G	C8-N9-C4	-7.73	103.31	106.40
1	1A	2689	G	N1-C6-O6	-7.73	115.26	119.90
1	1A	2537	G	O5'-P-OP2	-7.73	98.75	105.70
32	2a	142	G	C8-N9-C4	-7.72	103.31	106.40
1	1A	413	G	C8-N9-C4	-7.72	103.31	106.40
1	1A	1007	G	C8-N9-C4	-7.72	103.31	106.40
1	1A	2188	G	N3-C4-N9	-7.72	121.37	126.00
1	1A	2194	U	N3-C2-O2	-7.72	116.80	122.20
1	2A	979	G	O5'-P-OP1	-7.72	98.75	105.70
32	2a	142	G	N3-C4-C5	-7.72	124.74	128.60
1	1A	2767	U	N1-C2-O2	7.72	128.20	122.80
1	1A	1831	C	C6-N1-C2	-7.72	117.21	120.30
1	1A	718	C	C5-C4-N4	7.71	125.60	120.20
1	1A	1411	A	N9-C4-C5	-7.71	102.71	105.80
1	1A	1668	G	O5'-P-OP2	-7.71	98.76	105.70
32	2a	458	C	C6-N1-C2	-7.71	117.22	120.30
1	1A	2453	C	N1-C2-N3	7.71	124.60	119.20
1	1A	2510	C	N3-C4-N4	-7.71	112.60	118.00
1	1A	2517	G	C5-C6-N1	-7.71	107.64	111.50
1	1A	2624	C	O5'-P-OP1	-7.71	98.76	105.70
1	1A	1811	A	C8-N9-C4	-7.71	102.72	105.80
1	2A	2362	G	C4-C5-N7	7.71	113.88	110.80
1	1A	1377	A	OP1-P-O3'	-7.70	88.26	105.20
1	1A	1702	A	N1-C6-N6	-7.70	113.98	118.60
1	1A	2277	U	OP1-P-OP2	-7.70	108.05	119.60
1	1A	2292	G	N1-C6-O6	-7.70	115.28	119.90
32	1a	635	G	O5'-P-OP2	7.70	119.94	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1689	A	N1-C6-N6	7.70	123.22	118.60
1	2A	2041	U	C5-C4-O4	-7.70	121.28	125.90
1	2A	2805	G	N3-C4-N9	7.70	130.62	126.00
1	1A	591	U	N3-C4-C5	7.70	119.22	114.60
1	1A	2752	U	C5-C6-N1	-7.70	118.85	122.70
32	2a	472	A	N7-C8-N9	7.70	117.65	113.80
1	1A	191	U	N3-C4-C5	7.69	119.22	114.60
1	1A	271	U	C6-N1-C1'	7.69	131.97	121.20
1	1A	122	G	N3-C2-N2	7.69	125.28	119.90
1	2A	9	U	C5-C6-N1	7.69	126.55	122.70
1	1A	1000	C	N3-C4-N4	-7.69	112.62	118.00
32	1a	795	C	N1-C2-O2	-7.69	114.29	118.90
1	1A	519	G	N7-C8-N9	7.68	116.94	113.10
1	1A	2505	U	OP2-P-O3'	7.68	122.11	105.20
1	1A	2262	G	OP1-P-OP2	7.68	131.12	119.60
1	1A	405	C	C2-N3-C4	-7.68	116.06	119.90
1	2A	1774	C	C5-C6-N1	7.68	124.84	121.00
1	1A	2630	G	C5-C6-O6	7.68	133.21	128.60
1	1A	725	C	C2-N3-C4	-7.67	116.06	119.90
1	2A	383	U	N1-C2-O2	7.67	128.17	122.80
1	2A	988	A	N1-C6-N6	7.67	123.20	118.60
1	2A	2362	G	C5-C6-O6	-7.67	124.00	128.60
1	1A	1497	G	O5'-P-OP2	-7.67	98.79	105.70
1	1A	1571	G	OP1-P-OP2	7.67	131.11	119.60
1	1A	195	U	C2-N3-C4	-7.67	122.40	127.00
32	2a	686	U	N1-C2-N3	7.67	119.50	114.90
32	2a	908	A	O5'-P-OP2	-7.67	98.80	105.70
1	1A	223	C	N3-C2-O2	-7.67	116.53	121.90
32	1a	615	C	C6-N1-C2	-7.67	117.23	120.30
32	2a	1003	G	N3-C4-N9	7.67	130.60	126.00
1	1A	1155	C	C2-N1-C1'	7.66	127.23	118.80
1	1A	2278	A	O5'-P-OP1	-7.66	98.80	105.70
32	2a	993	G	N3-C4-C5	-7.66	124.77	128.60
1	1A	1766	G	N7-C8-N9	7.66	116.93	113.10
1	1A	354	A	N1-C2-N3	7.66	133.13	129.30
1	1A	733	G	N9-C4-C5	-7.66	102.34	105.40
1	2A	1836	C	O5'-P-OP1	7.66	119.89	110.70
1	2A	2177	C	C6-N1-C2	-7.65	117.24	120.30
1	1A	832	G	C5-C6-O6	7.65	133.19	128.60
1	1A	1052	C	C4-C5-C6	7.65	121.22	117.40
1	2A	1639	U	O5'-P-OP1	7.65	119.88	110.70
1	1A	957	A	OP1-P-OP2	7.64	131.07	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	474	U	C2-N3-C4	-7.64	122.41	127.00
1	1A	150	C	N3-C4-N4	-7.64	112.65	118.00
1	1A	447	C	C6-N1-C2	7.64	123.36	120.30
1	1A	10	G	N1-C6-O6	-7.64	115.32	119.90
1	1A	1099	C	N3-C4-C5	-7.64	118.84	121.90
1	1A	1147	U	N1-C2-O2	7.64	128.15	122.80
32	2a	16	A	N1-C6-N6	-7.64	114.02	118.60
1	1A	1199	C	N1-C2-O2	-7.63	114.32	118.90
1	1A	1630	A	O5'-P-OP2	-7.63	98.83	105.70
1	2A	2691	C	O5'-P-OP1	-7.63	98.83	105.70
32	2a	404	U	C2-N1-C1'	7.63	126.86	117.70
1	2A	2578	G	O5'-P-OP1	-7.63	98.83	105.70
1	2A	2827	C	C5-C4-N4	-7.63	114.86	120.20
1	1A	752	A	C4-C5-N7	7.63	114.52	110.70
1	1A	782	A	N9-C4-C5	7.63	108.85	105.80
1	1A	2284	U	N1-C2-N3	7.63	119.48	114.90
1	2A	1008	C	N1-C2-O2	7.63	123.48	118.90
1	2A	2399	G	N1-C6-O6	-7.63	115.32	119.90
1	1A	1319	U	C5-C4-O4	7.62	130.47	125.90
1	1A	409	G	C5-C6-O6	7.62	133.17	128.60
13	1R	2	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	1A	429	A	O5'-P-OP1	7.62	119.84	110.70
1	1A	2735	G	N7-C8-N9	-7.62	109.29	113.10
1	2A	2585	U	C5-C6-N1	-7.62	118.89	122.70
32	2a	791	G	N3-C4-N9	-7.62	121.43	126.00
1	2A	1082	U	C2-N1-C1'	7.62	126.84	117.70
1	1A	918	U	N3-C2-O2	7.62	127.53	122.20
1	1A	1453	C	C2-N3-C4	-7.61	116.09	119.90
1	2A	2896	C	C5-C6-N1	7.61	124.81	121.00
1	2A	1721	G	N3-C2-N2	7.61	125.23	119.90
1	1A	507	G	O5'-P-OP2	-7.61	98.85	105.70
1	1A	575	G	N1-C2-N2	-7.61	109.35	116.20
1	1A	1455	C	OP2-P-O3'	7.61	121.94	105.20
1	1A	2331	G	C4-C5-N7	7.61	113.84	110.80
1	1A	2597	U	C5-C4-O4	7.61	130.47	125.90
1	2A	2513	G	C8-N9-C4	-7.61	103.36	106.40
1	1A	1013	G	C5-C6-O6	7.61	133.16	128.60
1	1A	1128	U	C5-C6-N1	7.61	126.50	122.70
1	1A	2091	G	N1-C6-O6	-7.61	115.33	119.90
2	1B	32	C	N3-C4-C5	7.61	124.94	121.90
1	1A	335	A	OP1-P-OP2	-7.61	108.19	119.60
1	2A	221	A	O5'-P-OP1	-7.60	98.86	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	332	G	C8-N9-C4	7.60	109.44	106.40
1	1A	2448	G	N1-C6-O6	-7.60	115.34	119.90
32	2a	1028	C	C5-C6-N1	7.60	124.80	121.00
1	1A	202	A	OP2-P-O3'	7.60	121.92	105.20
1	1A	793	A	N7-C8-N9	7.60	117.60	113.80
1	1A	847	A	N9-C4-C5	7.60	108.84	105.80
1	1A	1816	A	C5-N7-C8	-7.59	100.10	103.90
1	2A	1617	C	N1-C2-O2	-7.59	114.34	118.90
1	1A	592	U	C2-N3-C4	-7.59	122.45	127.00
1	2A	2893	G	N3-C4-N9	7.59	130.55	126.00
1	1A	780	G	C5-N7-C8	7.58	108.09	104.30
1	1A	2080	A	N1-C2-N3	7.58	133.09	129.30
32	1a	181	G	C8-N9-C4	-7.58	103.37	106.40
32	1a	768	A	N7-C8-N9	-7.58	110.01	113.80
1	2A	1511	C	C6-N1-C2	-7.58	117.27	120.30
1	1A	2390	A	C4-C5-C6	7.58	120.79	117.00
32	2a	245	C	O5'-P-OP1	-7.58	98.88	105.70
1	1A	554	A	C5-C6-N1	7.58	121.49	117.70
1	1A	1807	G	N3-C4-N9	7.58	130.55	126.00
1	1A	2625	U	N3-C2-O2	-7.58	116.89	122.20
1	1A	1261	G	OP1-P-OP2	-7.58	108.24	119.60
1	1A	2591	C	C2-N3-C4	-7.58	116.11	119.90
1	2A	837	C	N1-C2-O2	-7.58	114.36	118.90
1	2A	2685	G	N1-C6-O6	-7.58	115.36	119.90
32	2a	5	U	C6-N1-C2	-7.58	116.45	121.00
1	1A	1822	A	O5'-P-OP2	7.57	119.78	110.70
1	1A	2718	G	C5-N7-C8	7.57	108.08	104.30
32	1a	58	C	O5'-P-OP1	-7.57	98.89	105.70
1	1A	2610	A	OP2-P-O3'	7.57	121.85	105.20
32	2a	530	G	N3-C4-N9	7.57	130.54	126.00
32	2a	1486	G	O5'-P-OP1	7.57	119.78	110.70
32	1a	46	G	O5'-P-OP2	7.57	119.78	110.70
1	1A	2593	G	N3-C2-N2	7.56	125.19	119.90
1	1A	1278	G	C4-C5-N7	-7.56	107.78	110.80
1	1A	2700	U	C4-C5-C6	7.56	124.24	119.70
1	1A	1054	C	N3-C2-O2	-7.56	116.61	121.90
2	1B	41	U	C5-C6-N1	-7.56	118.92	122.70
1	2A	659	C	C6-N1-C2	7.56	123.32	120.30
1	2A	1471	A	N7-C8-N9	7.56	117.58	113.80
1	1A	2354	C	O5'-P-OP2	7.55	119.76	110.70
1	2A	1903	G	N3-C2-N2	-7.55	114.61	119.90
32	2a	1183	A	P-O3'-C3'	7.55	128.76	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1823	G	C5-C6-O6	7.55	133.13	128.60
1	1A	2579	G	C4-C5-N7	-7.54	107.78	110.80
1	1A	494	G	C5-N7-C8	7.54	108.07	104.30
1	1A	2611	G	C5-C6-O6	7.54	133.12	128.60
1	1A	987	G	N1-C6-O6	-7.54	115.38	119.90
1	1A	1386	U	N3-C4-C5	7.54	119.12	114.60
1	2A	701	G	N3-C4-C5	7.54	132.37	128.60
32	2a	880	C	O5'-P-OP2	-7.54	98.92	105.70
1	1A	2636	G	N1-C6-O6	-7.54	115.38	119.90
32	1a	903	G	O5'-P-OP2	-7.53	98.92	105.70
32	2a	904	C	N1-C2-O2	-7.53	114.38	118.90
1	1A	1294	G	N1-C2-N2	-7.53	109.42	116.20
1	1A	738	C	C6-N1-C2	-7.53	117.29	120.30
1	1A	2134	G	C8-N9-C4	-7.53	103.39	106.40
1	1A	2576	A	C5-C6-N6	-7.53	117.68	123.70
1	1A	2657	G	C5-N7-C8	-7.53	100.54	104.30
1	2A	2378	A	N9-C4-C5	-7.53	102.79	105.80
1	1A	2640	C	N3-C4-C5	7.52	124.91	121.90
32	1a	799	G	C5-C6-O6	7.52	133.11	128.60
1	1A	88	G	C8-N9-C4	-7.52	103.39	106.40
1	1A	2111	U	N3-C4-C5	7.52	119.11	114.60
1	1A	2296	C	N3-C4-C5	-7.52	118.89	121.90
1	1A	1076	G	C2-N3-C4	-7.52	108.14	111.90
32	1a	543	C	C6-N1-C2	-7.52	117.29	120.30
1	2A	1145	C	C6-N1-C2	-7.52	117.29	120.30
32	2a	346	G	C2-N3-C4	7.52	115.66	111.90
1	1A	2704	C	C2-N3-C4	-7.51	116.14	119.90
1	1A	777	C	O5'-P-OP1	-7.51	98.94	105.70
1	1A	1359	U	O5'-P-OP2	7.51	119.72	110.70
1	2A	2355	C	O5'-P-OP1	-7.51	98.94	105.70
1	1A	1067	A	C6-N1-C2	-7.51	114.10	118.60
1	1A	1842	G	N1-C6-O6	-7.51	115.40	119.90
1	1A	1700	G	P-O3'-C3'	7.50	128.71	119.70
1	1A	1294	G	C4-C5-N7	7.50	113.80	110.80
1	2A	1066	U	N1-C2-N3	7.50	119.40	114.90
32	2a	343	U	N3-C4-C5	7.50	119.10	114.60
1	1A	810	G	N1-C2-N2	-7.50	109.45	116.20
32	1a	1515	C	O5'-P-OP2	-7.50	98.95	105.70
1	1A	1725	G	N3-C2-N2	-7.50	114.65	119.90
32	1a	1279	A	C8-N9-C4	-7.50	102.80	105.80
1	1A	1875	C	C6-N1-C2	7.50	123.30	120.30
1	2A	2794	C	C5-C6-N1	7.50	124.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2696	U	O5'-P-OP1	-7.49	98.95	105.70
1	1A	82	G	C2-N3-C4	-7.49	108.15	111.90
1	1A	2158	C	N3-C2-O2	-7.49	116.66	121.90
1	1A	1994	A	C5-N7-C8	-7.49	100.15	103.90
1	1A	1365	G	N7-C8-N9	7.49	116.84	113.10
1	1A	2024	G	N7-C8-N9	-7.49	109.36	113.10
32	2a	1378	C	C6-N1-C2	-7.49	117.31	120.30
1	1A	1330	A	OP1-P-OP2	7.49	130.83	119.60
1	1A	2428	C	N3-C4-N4	-7.49	112.76	118.00
1	1A	149	A	O5'-P-OP1	-7.48	98.97	105.70
1	1A	2625	U	N1-C2-O2	7.48	128.04	122.80
1	2A	251	A	N1-C2-N3	7.48	133.04	129.30
1	1A	859	C	N1-C2-O2	-7.48	114.41	118.90
1	1A	2060	G	C5-N7-C8	7.48	108.04	104.30
32	1a	639	G	C8-N9-C4	-7.48	103.41	106.40
1	2A	1046	A	C8-N9-C4	-7.48	102.81	105.80
1	1A	60	G	N3-C2-N2	-7.47	114.67	119.90
1	1A	990	A	O5'-P-OP1	7.47	119.67	110.70
1	2A	527	C	C2-N1-C1'	-7.47	110.58	118.80
1	2A	1253	A	C5-N7-C8	7.47	107.64	103.90
32	1a	299	G	C4-C5-N7	7.47	113.79	110.80
32	1a	804	U	O5'-P-OP1	7.47	119.67	110.70
1	2A	1983	C	N3-C2-O2	7.47	127.13	121.90
1	1A	2010	C	C2-N3-C4	-7.47	116.17	119.90
1	1A	2341	G	C5-C6-O6	-7.47	124.12	128.60
2	1B	1	U	C5-C6-N1	7.47	126.44	122.70
1	1A	1278	G	O5'-P-OP1	-7.46	98.98	105.70
32	1a	738	C	C6-N1-C2	-7.46	117.31	120.30
1	1A	1420	G	O5'-P-OP2	7.46	119.66	110.70
1	2A	1275	A	C8-N9-C4	7.46	108.78	105.80
32	2a	902	G	C5-N7-C8	7.46	108.03	104.30
1	1A	2618	C	C4-C5-C6	7.46	121.13	117.40
1	1A	2649	U	N3-C2-O2	-7.46	116.98	122.20
32	1a	863	U	C2-N1-C1'	-7.46	108.75	117.70
1	1A	315	C	O5'-P-OP1	-7.46	98.99	105.70
32	1a	914	A	O5'-P-OP1	-7.46	98.99	105.70
32	1a	1442	G	C2-N3-C4	7.46	115.63	111.90
1	1A	1965	U	C2-N3-C4	-7.45	122.53	127.00
1	1A	582	G	C8-N9-C4	-7.45	103.42	106.40
1	1A	2038	U	N3-C4-O4	-7.44	114.19	119.40
1	2A	697	C	N3-C4-C5	-7.44	118.92	121.90
1	2A	2185	C	N1-C2-O2	7.44	123.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1109	G	N1-C2-N3	-7.44	119.44	123.90
32	1a	1176	A	C8-N9-C4	-7.44	102.83	105.80
1	2A	572	A	C8-N9-C4	-7.44	102.83	105.80
1	1A	322	G	O5'-P-OP1	7.43	119.62	110.70
1	1A	2511	C	C2-N3-C4	7.43	123.62	119.90
32	1a	754	C	N1-C2-O2	7.43	123.36	118.90
32	1a	1522	U	OP1-P-OP2	7.43	130.75	119.60
2	1B	79	C	N3-C2-O2	-7.43	116.70	121.90
1	2A	990	A	O5'-P-OP2	-7.43	99.01	105.70
1	1A	826	U	N3-C4-O4	7.43	124.60	119.40
1	1A	1336	C	C6-N1-C2	-7.43	117.33	120.30
1	1A	1427	G	N1-C6-O6	-7.43	115.44	119.90
1	2A	35	G	N1-C6-O6	-7.43	115.44	119.90
1	1A	220	C	C4-C5-C6	7.43	121.11	117.40
1	1A	1855	G	O5'-P-OP2	-7.43	99.02	105.70
1	1A	2597	U	C5-C6-N1	-7.43	118.99	122.70
32	1a	174	C	N1-C2-O2	7.43	123.36	118.90
1	2A	1309	G	O5'-P-OP1	7.43	119.61	110.70
32	2a	1219	U	C5-C6-N1	7.43	126.41	122.70
1	1A	649	C	C2-N3-C4	-7.42	116.19	119.90
1	1A	702	A	N3-C4-N9	-7.42	121.46	127.40
1	1A	1992	A	O5'-P-OP1	-7.42	99.02	105.70
1	1A	2826	C	O5'-P-OP2	-7.42	99.02	105.70
1	1A	2673	G	N1-C6-O6	-7.42	115.45	119.90
32	1a	1486	G	N1-C6-O6	7.42	124.35	119.90
1	2A	271(K)	U	C6-N1-C2	-7.42	116.55	121.00
32	2a	493	G	O5'-P-OP1	-7.42	99.02	105.70
1	1A	2038	U	C5-C4-O4	7.42	130.35	125.90
1	2A	885	C	C5-C6-N1	7.42	124.71	121.00
32	2a	340	U	O5'-P-OP2	-7.42	99.02	105.70
32	1a	191	G	C8-N9-C4	-7.42	103.43	106.40
1	2A	1074	G	O5'-P-OP2	-7.42	99.02	105.70
1	1A	260	A	C8-N9-C4	7.42	108.77	105.80
1	1A	878	G	C2-N3-C4	-7.42	108.19	111.90
1	1A	1783	C	N1-C2-O2	-7.41	114.45	118.90
32	1a	1021	G	C2-N3-C4	7.41	115.61	111.90
1	2A	2451	A	C5-N7-C8	-7.41	100.19	103.90
32	2a	896	C	C6-N1-C2	7.41	123.26	120.30
1	2A	1051	G	N1-C6-O6	7.41	124.34	119.90
2	1B	50	G	O5'-P-OP2	-7.41	99.03	105.70
32	1a	897	C	O5'-P-OP2	-7.41	99.03	105.70
1	1A	2460	A	C5-C6-N1	7.41	121.40	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2550	C	N3-C4-C5	7.41	124.86	121.90
1	1A	2788	A	C8-N9-C4	7.40	108.76	105.80
32	1a	189(D)	C	N1-C2-O2	7.40	123.34	118.90
1	1A	641	G	C5-C6-O6	7.40	133.04	128.60
1	1A	1102	G	N9-C4-C5	-7.40	102.44	105.40
1	1A	2535	G	C5-C6-O6	7.40	133.04	128.60
32	1a	326	G	C4-C5-N7	-7.40	107.84	110.80
1	1A	1371	G	N9-C4-C5	7.40	108.36	105.40
1	1A	2194	U	C6-N1-C2	-7.40	116.56	121.00
1	1A	2272	C	C4-C5-C6	7.40	121.10	117.40
1	2A	673	C	N1-C2-O2	-7.40	114.46	118.90
1	1A	2598	C	N3-C4-N4	7.40	123.18	118.00
32	1a	996	A	C8-N9-C4	-7.40	102.84	105.80
1	1A	125	A	C2-N3-C4	7.39	114.30	110.60
1	1A	274	U	C5-C4-O4	-7.39	121.46	125.90
1	1A	451	G	C5-C6-N1	7.39	115.20	111.50
1	1A	1746	G	O5'-P-OP2	-7.39	99.05	105.70
1	1A	903	C	C5-C6-N1	7.39	124.69	121.00
32	2a	5	U	C2-N1-C1'	7.39	126.57	117.70
32	1a	577	G	OP2-P-O3'	7.39	121.45	105.20
1	2A	791	C	C2-N3-C4	-7.39	116.21	119.90
1	1A	2294	G	N3-C2-N2	7.38	125.07	119.90
32	1a	1211	U	C5-C6-N1	-7.38	119.01	122.70
1	1A	1210	G	C4-C5-N7	-7.38	107.85	110.80
32	1a	605	U	C5-C4-O4	7.38	130.33	125.90
1	1A	486	A	N9-C4-C5	7.38	108.75	105.80
1	1A	985	G	C5-N7-C8	7.38	107.99	104.30
1	1A	2780	C	C6-N1-C2	-7.38	117.35	120.30
1	2A	2699	C	C5-C6-N1	-7.38	117.31	121.00
1	1A	1341	C	N3-C4-C5	7.37	124.85	121.90
1	1A	1518	A	C8-N9-C4	-7.37	102.85	105.80
32	1a	172	A	C8-N9-C4	-7.37	102.85	105.80
1	1A	2063	U	N1-C2-N3	7.37	119.32	114.90
1	2A	2894	G	N3-C4-N9	-7.37	121.58	126.00
32	2a	65	U	P-O3'-C3'	7.37	128.54	119.70
1	1A	2832	G	C5-C6-O6	-7.37	124.18	128.60
1	2A	1271	G	C8-N9-C4	7.37	109.35	106.40
1	1A	2460	A	N7-C8-N9	-7.37	110.12	113.80
1	2A	1647	G	C5-C6-O6	-7.37	124.18	128.60
1	1A	881	C	N1-C2-O2	-7.37	114.48	118.90
1	1A	2548	G	C2-N3-C4	-7.37	108.22	111.90
32	1a	557	G	N3-C4-N9	7.37	130.42	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	574	A	N1-C6-N6	7.37	123.02	118.60
1	1A	2818	U	N3-C2-O2	7.36	127.36	122.20
32	2a	990	C	N1-C2-O2	7.36	123.32	118.90
1	2A	445	C	N1-C2-O2	-7.36	114.48	118.90
1	2A	2454	G	C5-C6-O6	7.36	133.02	128.60
1	1A	2188	G	C4-N9-C1'	-7.36	116.93	126.50
1	1A	2858	G	N3-C2-N2	-7.36	114.75	119.90
32	2a	428	G	O5'-P-OP2	-7.36	99.08	105.70
1	1A	492	A	N1-C6-N6	-7.36	114.19	118.60
1	1A	718	C	N3-C4-N4	-7.36	112.85	118.00
1	1A	751	G	N3-C2-N2	-7.36	114.75	119.90
1	1A	1255	A	P-O3'-C3'	7.36	128.53	119.70
32	1a	13	U	C5-C6-N1	-7.35	119.02	122.70
1	2A	2220	G	N3-C2-N2	-7.35	114.75	119.90
1	2A	785	G	O5'-P-OP2	-7.35	99.08	105.70
1	1A	2788	A	N7-C8-N9	-7.35	110.12	113.80
1	1A	1361	C	C2-N3-C4	-7.35	116.23	119.90
32	2a	909	A	N1-C6-N6	7.35	123.01	118.60
1	1A	648	G	N1-C6-O6	-7.34	115.49	119.90
1	1A	1013	G	N1-C6-O6	-7.34	115.49	119.90
1	1A	2487	C	N1-C2-O2	-7.34	114.49	118.90
1	1A	2260	C	N3-C4-C5	7.34	124.84	121.90
1	2A	135	G	OP2-P-O3'	7.34	121.35	105.20
1	2A	740	U	O5'-P-OP2	-7.34	99.09	105.70
1	1A	807	G	C2-N3-C4	-7.34	108.23	111.90
1	1A	975	U	C5-C4-O4	-7.34	121.50	125.90
1	1A	27	G	O4'-C1'-N9	7.34	114.07	108.20
1	1A	2459	G	OP2-P-O3'	7.34	121.34	105.20
1	1A	790	G	C5-C6-O6	7.34	133.00	128.60
32	1a	1505	G	N9-C4-C5	7.34	108.33	105.40
1	2A	1203	G	C4-C5-N7	7.34	113.73	110.80
1	2A	1969	A	OP1-P-O3'	7.34	121.34	105.20
32	2a	1132	C	C6-N1-C2	-7.34	117.36	120.30
1	1A	2890	C	OP1-P-OP2	7.33	130.60	119.60
1	1A	1846	A	N1-C2-N3	7.33	132.97	129.30
32	1a	841	U	C5-C6-N1	7.33	126.37	122.70
2	1B	102	A	C6-N1-C2	-7.33	114.20	118.60
1	1A	1686	U	O5'-P-OP2	-7.33	99.10	105.70
1	2A	1678	G	C8-N9-C4	-7.33	103.47	106.40
1	2A	2388	A	O5'-P-OP1	7.33	119.49	110.70
32	2a	332	G	O5'-P-OP1	-7.33	99.11	105.70
32	1a	1523	G	O5'-P-OP2	-7.33	99.11	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1108	G	N3-C4-N9	7.33	130.40	126.00
1	1A	539	A	OP1-P-OP2	7.32	130.58	119.60
1	1A	2089	G	C8-N9-C4	-7.32	103.47	106.40
32	1a	1495	U	C2-N1-C1'	7.32	126.48	117.70
32	2a	1515	C	O5'-P-OP2	-7.32	99.11	105.70
1	1A	1655	A	C8-N9-C4	7.32	108.73	105.80
1	2A	1963	U	N1-C2-O2	7.31	127.92	122.80
1	1A	2111	U	C2-N3-C4	-7.31	122.61	127.00
1	2A	2157	G	C8-N9-C4	-7.31	103.47	106.40
32	2a	487	A	N7-C8-N9	-7.31	110.14	113.80
32	1a	405	U	O5'-P-OP1	-7.31	99.12	105.70
1	1A	1007	G	C2-N3-C4	7.31	115.55	111.90
32	2a	560	U	C6-N1-C2	-7.31	116.62	121.00
1	1A	2290	A	OP2-P-O3'	7.30	121.27	105.20
1	1A	2595	G	N7-C8-N9	-7.30	109.45	113.10
1	2A	203	C	O5'-P-OP2	-7.30	99.13	105.70
32	1a	483	C	C6-N1-C2	7.30	123.22	120.30
1	1A	1742	G	C4-C5-N7	7.30	113.72	110.80
32	2a	1532	U	C5-C6-N1	7.30	126.35	122.70
32	2a	1478	C	C6-N1-C2	-7.29	117.38	120.30
1	1A	2443	U	N3-C2-O2	-7.29	117.10	122.20
1	2A	1170	G	N1-C6-O6	7.29	124.28	119.90
1	1A	373	G	O5'-P-OP2	-7.29	99.14	105.70
1	1A	2069	U	C2-N3-C4	-7.29	122.63	127.00
1	1A	2106	C	C5-C6-N1	-7.29	117.36	121.00
1	1A	2526	U	OP1-P-OP2	7.29	130.53	119.60
1	2A	1941	C	N1-C2-O2	-7.29	114.53	118.90
1	1A	2588	G	C2-N3-C4	7.29	115.54	111.90
1	1A	2833	A	C8-N9-C4	-7.29	102.89	105.80
32	2a	562	C	C5-C4-N4	-7.29	115.10	120.20
1	1A	1394	G	N1-C6-O6	-7.28	115.53	119.90
1	1A	1720	U	N3-C2-O2	7.28	127.30	122.20
1	1A	217	A	C8-N9-C1'	7.28	140.80	127.70
2	1B	36	C	N1-C2-O2	-7.28	114.53	118.90
1	1A	1453	C	N1-C2-O2	-7.28	114.53	118.90
1	1A	1852	A	C2-N3-C4	7.28	114.24	110.60
1	2A	906	G	C4-C5-N7	-7.28	107.89	110.80
32	2a	797	C	O5'-P-OP2	7.28	119.43	110.70
1	1A	198	C	C2-N3-C4	-7.28	116.26	119.90
1	1A	1093	G	N3-C4-C5	-7.28	124.96	128.60
1	1A	1724	A	C2-N3-C4	-7.28	106.96	110.60
32	1a	825	G	OP2-P-O3'	7.28	121.21	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	913	A	P-O3'-C3'	7.28	128.43	119.70
1	1A	2138	G	C4-N9-C1'	7.27	135.96	126.50
1	1A	2689	G	C5-C6-O6	7.27	132.96	128.60
1	2A	834	C	N3-C2-O2	-7.27	116.81	121.90
1	1A	661	G	N1-C6-O6	7.27	124.26	119.90
1	1A	1437	U	C5-C4-O4	-7.27	121.54	125.90
1	1A	2883	A	OP1-P-OP2	7.27	130.51	119.60
1	2A	1075	C	C6-N1-C2	-7.27	117.39	120.30
1	1A	2517	G	C6-N1-C2	7.27	129.46	125.10
32	2a	1406	U	N1-C2-N3	7.27	119.26	114.90
1	1A	553	A	N3-C4-C5	-7.27	121.71	126.80
1	2A	2207	G	C4-N9-C1'	7.27	135.95	126.50
32	2a	1067	A	P-O3'-C3'	7.27	128.42	119.70
32	1a	784	C	C6-N1-C2	7.26	123.20	120.30
32	1a	1442	G	N3-C4-C5	-7.26	124.97	128.60
8	2I	116	LEU	CA-CB-CG	7.26	132.00	115.30
1	1A	1264	G	O5'-P-OP2	-7.26	99.17	105.70
32	2a	1505	G	O5'-P-OP2	-7.26	99.17	105.70
1	1A	1270	C	C2-N3-C4	-7.26	116.27	119.90
32	1a	560	U	N3-C2-O2	-7.26	117.12	122.20
1	1A	722	A	N1-C6-N6	7.25	122.95	118.60
1	1A	848	G	C8-N9-C4	-7.25	103.50	106.40
1	2A	2427	C	N1-C2-O2	-7.25	114.55	118.90
32	2a	506	G	O5'-P-OP1	-7.25	99.17	105.70
1	2A	912	C	N1-C2-O2	7.25	123.25	118.90
1	1A	98	U	C2-N1-C1'	7.25	126.40	117.70
1	1A	852	G	N3-C2-N2	7.25	124.97	119.90
1	1A	1456	G	N3-C4-C5	7.25	132.22	128.60
1	2A	2385	C	O5'-P-OP1	-7.25	99.18	105.70
1	1A	1618	A	O5'-P-OP2	-7.24	99.18	105.70
1	2A	1838	C	C6-N1-C2	-7.24	117.40	120.30
1	2A	2821	A	C8-N9-C4	7.24	108.70	105.80
32	1a	1217	C	O5'-P-OP2	-7.24	99.18	105.70
32	1a	343	U	C5-C6-N1	-7.24	119.08	122.70
32	1a	817	C	O5'-P-OP1	-7.24	99.18	105.70
1	1A	2033	U	N1-C2-N3	7.24	119.24	114.90
32	2a	1054	C	C6-N1-C1'	-7.24	112.11	120.80
1	1A	1783	C	N3-C2-O2	7.24	126.96	121.90
1	1A	2525	G	C2-N3-C4	-7.24	108.28	111.90
1	2A	856	C	P-O3'-C3'	7.24	128.38	119.70
1	2A	1925	C	N1-C2-O2	-7.24	114.56	118.90
1	1A	2604	G	C5-C6-O6	7.23	132.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	514	G	C5-C6-O6	7.23	132.94	128.60
1	2A	2511	U	N1-C2-O2	-7.23	117.74	122.80
1	1A	243	G	C5-C6-O6	7.23	132.94	128.60
1	1A	1269	G	N1-C6-O6	-7.23	115.56	119.90
1	1A	1807	G	C4-C5-N7	7.23	113.69	110.80
1	2A	247	G	C2-N3-C4	-7.23	108.28	111.90
1	2A	1902	C	O5'-P-OP2	7.23	119.37	110.70
1	2A	2041	U	N1-C2-O2	-7.23	117.74	122.80
1	2A	236	C	C5-C6-N1	-7.22	117.39	121.00
1	2A	2049	G	C5-C6-O6	7.22	132.94	128.60
32	2a	1158	C	N3-C2-O2	-7.22	116.84	121.90
1	1A	702	A	C2-N3-C4	-7.22	106.99	110.60
1	1A	1167	C	N3-C2-O2	-7.22	116.84	121.90
32	1a	841	U	C6-N1-C2	-7.22	116.67	121.00
32	1a	913	A	N9-C4-C5	7.22	108.69	105.80
32	1a	925	G	O5'-P-OP2	-7.22	99.20	105.70
1	2A	807	U	N1-C2-N3	7.22	119.23	114.90
32	2a	398	C	N3-C4-N4	-7.22	112.94	118.00
1	1A	504	A	C8-N9-C4	-7.22	102.91	105.80
1	2A	312	G	C5-C6-O6	-7.22	124.27	128.60
32	2a	1287	A	C5-C6-N6	7.22	129.47	123.70
1	2A	1236	G	O5'-P-OP1	-7.22	99.20	105.70
1	1A	820	U	C5-C6-N1	-7.21	119.09	122.70
1	1A	821	A	C8-N9-C4	-7.21	102.91	105.80
32	1a	889	A	OP1-P-OP2	7.21	130.42	119.60
32	2a	44	G	C2-N3-C4	-7.21	108.29	111.90
1	1A	215	G	N9-C4-C5	7.21	108.28	105.40
32	1a	667	G	O5'-P-OP1	7.21	119.36	110.70
1	1A	45	C	N3-C4-C5	7.21	124.78	121.90
1	1A	1832	G	O5'-P-OP1	-7.21	99.21	105.70
1	2A	353	G	N1-C6-O6	7.21	124.23	119.90
1	2A	474	G	N9-C4-C5	7.21	108.28	105.40
1	1A	1278	G	O5'-P-OP2	7.21	119.35	110.70
1	2A	792	G	O4'-C1'-N9	-7.21	102.43	108.20
1	2A	1046	A	C2-N3-C4	7.21	114.20	110.60
1	2A	1848	A	N7-C8-N9	-7.21	110.20	113.80
1	2A	2300	G	C8-N9-C4	-7.21	103.52	106.40
1	1A	50	G	O5'-P-OP2	-7.21	99.21	105.70
1	1A	725	C	C5-C6-N1	-7.21	117.40	121.00
1	1A	2023	A	N9-C4-C5	7.21	108.68	105.80
32	2a	485	G	N3-C4-C5	-7.21	125.00	128.60
1	1A	399	G	O4'-C1'-N9	7.20	113.96	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	444	C	C6-N1-C2	7.20	123.18	120.30
1	1A	903	C	N3-C4-C5	-7.20	119.02	121.90
1	2A	2505	G	C5-C6-O6	7.20	132.92	128.60
1	1A	1707	C	N3-C2-O2	-7.20	116.86	121.90
32	1a	888	G	C4-C5-N7	7.20	113.68	110.80
1	2A	608	A	C8-N9-C4	-7.20	102.92	105.80
1	1A	2516	U	N3-C4-C5	7.20	118.92	114.60
1	2A	2157	G	N7-C8-N9	7.20	116.70	113.10
1	1A	2240	G	C8-N9-C4	-7.19	103.52	106.40
1	2A	1984	G	N7-C8-N9	7.19	116.70	113.10
1	1A	330	U	N3-C4-C5	-7.19	110.28	114.60
1	1A	1853	G	N3-C2-N2	7.19	124.94	119.90
1	2A	1992	G	C5-C6-N1	7.19	115.09	111.50
1	2A	2378	A	C6-C5-N7	-7.19	127.27	132.30
1	1A	1181	G	N9-C4-C5	-7.19	102.53	105.40
1	1A	1396	C	N3-C4-C5	7.19	124.78	121.90
1	1A	2724	U	C5-C4-O4	-7.19	121.59	125.90
1	1A	472	G	C5-N7-C8	-7.19	100.71	104.30
1	2A	1979	C	C6-N1-C2	-7.19	117.42	120.30
1	1A	1035	G	C2-N3-C4	7.19	115.49	111.90
1	1A	1420	G	OP1-P-OP2	-7.18	108.83	119.60
1	2A	2138	C	C5-C6-N1	7.18	124.59	121.00
1	1A	2467	G	N1-C2-N2	-7.18	109.74	116.20
32	1a	57	G	O5'-P-OP1	-7.18	99.24	105.70
1	2A	668	G	O5'-P-OP1	-7.18	99.24	105.70
1	1A	832	G	N1-C6-O6	-7.18	115.59	119.90
1	1A	217	A	C4-C5-C6	-7.18	113.41	117.00
1	1A	666	C	C6-N1-C2	-7.18	117.43	120.30
1	1A	1917	C	C6-N1-C2	-7.18	117.43	120.30
1	1A	2453	C	C5-C6-N1	-7.18	117.41	121.00
32	1a	1067	A	C8-N9-C4	-7.18	102.93	105.80
1	2A	741	G	N9-C4-C5	7.18	108.27	105.40
32	2a	1163	C	C5-C6-N1	7.18	124.59	121.00
1	1A	184	A	C5-C6-N1	-7.17	114.11	117.70
1	1A	192	C	N3-C4-N4	-7.17	112.98	118.00
1	1A	677	C	N3-C4-C5	7.17	124.77	121.90
1	2A	598	G	N1-C6-O6	-7.17	115.59	119.90
1	1A	127	C	N1-C2-O2	-7.17	114.60	118.90
1	1A	2637	G	N1-C6-O6	-7.17	115.60	119.90
1	1A	2183	C	C6-N1-C2	-7.17	117.43	120.30
2	1B	28	C	O5'-P-OP2	-7.17	99.25	105.70
32	1a	183	G	N7-C8-N9	7.17	116.69	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1184	G	C5-C6-O6	-7.17	124.30	128.60
1	1A	1718	U	N3-C4-C5	7.17	118.90	114.60
10	1O	8	LEU	CA-CB-CG	7.17	131.79	115.30
1	2A	1783	A	O4'-C1'-N9	-7.17	102.47	108.20
1	1A	82	G	C6-C5-N7	-7.17	126.10	130.40
1	1A	923	C	O5'-P-OP1	-7.16	99.25	105.70
32	1a	763	G	O5'-P-OP2	-7.16	99.25	105.70
32	1a	1030	C	C5-C6-N1	7.16	124.58	121.00
32	1a	781	A	N1-C2-N3	-7.16	125.72	129.30
32	1a	1054	C	N3-C2-O2	-7.16	116.89	121.90
32	2a	912	C	C6-N1-C2	7.16	123.17	120.30
1	1A	2610	A	C5-N7-C8	7.16	107.48	103.90
32	2a	15	G	C8-N9-C4	-7.16	103.54	106.40
1	1A	716	G	N3-C4-C5	7.16	132.18	128.60
1	1A	2834	C	C2-N3-C4	7.16	123.48	119.90
32	2a	983	A	O5'-P-OP1	-7.16	99.26	105.70
32	2a	1499	A	C8-N9-C4	7.16	108.66	105.80
1	2A	1992	G	C2'-C3'-O3'	7.16	125.25	109.50
32	2a	218	C	N3-C4-C5	-7.16	119.04	121.90
1	1A	500	G	N1-C2-N2	-7.16	109.76	116.20
1	1A	2194	U	N3-C4-O4	-7.16	114.39	119.40
1	2A	1890	A	C8-N9-C4	7.16	108.66	105.80
32	2a	1027	C	N3-C2-O2	-7.16	116.89	121.90
1	1A	1210	G	C5-N7-C8	7.15	107.88	104.30
1	1A	126	C	N1-C2-O2	-7.15	114.61	118.90
1	1A	1804	A	N1-C6-N6	7.15	122.89	118.60
1	1A	905	U	O5'-P-OP2	-7.15	99.26	105.70
1	1A	2004	C	C5-C4-N4	7.15	125.20	120.20
1	2A	1992	G	P-O3'-C3'	7.15	128.28	119.70
1	1A	545	G	OP2-P-O3'	7.15	120.93	105.20
1	1A	2639	G	C6-N1-C2	-7.15	120.81	125.10
1	2A	482	A	O5'-P-OP2	-7.15	99.27	105.70
1	1A	1811	A	N7-C8-N9	7.14	117.37	113.80
1	1A	1827	U	C5-C6-N1	-7.14	119.13	122.70
1	1A	2173	G	N9-C1'-C2'	-7.14	104.14	112.00
32	2a	261	U	N1-C2-N3	7.14	119.19	114.90
1	1A	108	G	N1-C6-O6	-7.14	115.61	119.90
1	1A	2485	U	C2-N1-C1'	7.14	126.27	117.70
1	1A	2276	C	OP2-P-O3'	7.14	120.91	105.20
1	2A	507	A	C4-C5-C6	-7.14	113.43	117.00
1	2A	1008	C	N3-C2-O2	-7.14	116.90	121.90
1	1A	428	A	C8-N9-C4	-7.14	102.95	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2188	G	N3-C4-C5	7.14	132.17	128.60
27	15	58	LEU	CA-CB-CG	7.14	131.71	115.30
32	2a	299	G	C8-N9-C4	7.14	109.25	106.40
1	1A	1683	C	N1-C2-O2	7.13	123.18	118.90
1	1A	478	G	C5-C6-N1	7.13	115.07	111.50
1	1A	2833	A	N9-C4-C5	7.13	108.65	105.80
1	1A	1842	G	N9-C4-C5	7.13	108.25	105.40
1	1A	2201	C	C6-N1-C2	-7.13	117.45	120.30
1	1A	1428	G	N1-C6-O6	7.13	124.18	119.90
1	2A	988	A	C5-N7-C8	-7.13	100.34	103.90
1	1A	1130	A	C5-C6-N6	7.12	129.40	123.70
32	1a	158	G	N3-C2-N2	-7.12	114.91	119.90
32	1a	888	G	N3-C2-N2	7.12	124.89	119.90
32	2a	23	C	O5'-P-OP2	7.12	119.25	110.70
1	1A	436	C	C6-N1-C2	7.12	123.15	120.30
1	2A	1240	U	N3-C4-O4	7.12	124.39	119.40
1	2A	1605	C	C4-C5-C6	7.12	120.96	117.40
1	2A	1416	G	O4'-C1'-N9	7.12	113.90	108.20
1	1A	196	A	N1-C6-N6	7.12	122.87	118.60
1	1A	660	C	N3-C2-O2	-7.12	116.92	121.90
1	1A	194	G	N3-C2-N2	7.12	124.88	119.90
1	1A	883	G	N7-C8-N9	7.12	116.66	113.10
1	1A	1549	U	N1-C2-O2	-7.12	117.82	122.80
1	2A	90	U	C5-C4-O4	7.11	130.17	125.90
1	2A	193	U	N1-C2-O2	-7.11	117.82	122.80
32	2a	1507	A	C8-N9-C4	7.11	108.64	105.80
1	1A	2778	A	C4-C5-C6	7.11	120.56	117.00
2	1B	114	C	N3-C4-C5	7.11	124.75	121.90
1	1A	554	A	O4'-C1'-N9	7.11	113.89	108.20
1	2A	1202	C	O5'-P-OP2	-7.11	99.30	105.70
1	2A	2596	U	N1-C2-O2	-7.11	117.83	122.80
1	1A	1294	G	C8-N9-C4	7.11	109.24	106.40
1	1A	2443	U	C2-N3-C4	-7.11	122.74	127.00
1	1A	283	G	N9-C4-C5	7.10	108.24	105.40
1	2A	2454	G	N1-C6-O6	-7.10	115.64	119.90
1	1A	1207	C	N1-C2-O2	-7.10	114.64	118.90
1	1A	2320	G	C5-N7-C8	-7.10	100.75	104.30
1	1A	2395	G	C5-C6-O6	7.10	132.86	128.60
32	1a	724	G	OP1-P-O3'	7.10	120.82	105.20
1	1A	2593	G	N9-C4-C5	-7.10	102.56	105.40
1	2A	683	C	O5'-P-OP1	-7.10	99.31	105.70
1	2A	912	C	N3-C2-O2	-7.10	116.93	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2250	G	OP1-P-OP2	7.10	130.25	119.60
32	2a	144	G	C8-N9-C4	-7.10	103.56	106.40
1	1A	188	A	N9-C4-C5	7.10	108.64	105.80
1	1A	543	G	N1-C6-O6	-7.10	115.64	119.90
1	1A	583	C	C5-C6-N1	-7.10	117.45	121.00
1	1A	760	G	N9-C4-C5	-7.10	102.56	105.40
1	1A	2387	G	C5-C6-O6	-7.10	124.34	128.60
1	1A	1360	C	O5'-P-OP1	-7.10	99.31	105.70
32	1a	1495	U	N3-C2-O2	-7.10	117.23	122.20
32	2a	902	G	N1-C6-O6	-7.09	115.64	119.90
1	1A	1627	A	N1-C6-N6	7.09	122.86	118.60
1	1A	2244	U	O5'-P-OP2	-7.09	99.32	105.70
1	1A	2301	G	N1-C6-O6	7.09	124.15	119.90
1	1A	874	U	N3-C4-O4	-7.09	114.44	119.40
1	1A	198	C	N3-C4-C5	7.09	124.73	121.90
1	1A	800	C	N3-C4-N4	-7.09	113.04	118.00
32	1a	1286	A	N1-C6-N6	-7.09	114.35	118.60
1	1A	1810	U	O4'-C1'-N1	7.08	113.87	108.20
1	1A	271	U	C2-N1-C1'	-7.08	109.20	117.70
1	1A	1006	C	C2-N3-C4	-7.08	116.36	119.90
1	1A	1240	G	N9-C4-C5	7.08	108.23	105.40
1	1A	1821	C	N3-C2-O2	7.08	126.86	121.90
1	2A	1690	A	C5-C6-N6	-7.08	118.03	123.70
1	2A	2356	C	N1-C2-O2	-7.08	114.65	118.90
1	1A	1069	U	OP1-P-OP2	7.08	130.22	119.60
1	1A	1431	G	O4'-C1'-N9	7.08	113.86	108.20
1	1A	2590	G	C5-C6-O6	7.07	132.84	128.60
32	1a	1528	U	O5'-P-OP2	-7.07	99.33	105.70
1	1A	999	G	C5-C6-O6	7.07	132.84	128.60
1	1A	217	A	C5-C6-N1	7.07	121.23	117.70
1	1A	735	U	N3-C2-O2	-7.07	117.25	122.20
1	1A	1054	C	C5-C6-N1	7.07	124.53	121.00
1	1A	1851	U	N3-C2-O2	-7.07	117.25	122.20
1	1A	35	G	C5-N7-C8	7.07	107.83	104.30
1	1A	2718	G	N7-C8-N9	-7.07	109.57	113.10
1	2A	1128	A	C8-N9-C4	7.07	108.63	105.80
1	2A	1079	C	C6-N1-C2	-7.06	117.47	120.30
1	2A	2499	C	N1-C2-O2	-7.06	114.66	118.90
1	2A	2848	G	O4'-C1'-N9	7.06	113.85	108.20
1	1A	1072	U	N1-C2-O2	7.06	127.74	122.80
1	1A	1257	G	O4'-C1'-N9	7.06	113.85	108.20
1	1A	1035	G	N1-C6-O6	-7.06	115.66	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	71	U	O5'-P-OP1	-7.06	99.35	105.70
1	1A	436	C	N3-C4-C5	7.06	124.72	121.90
1	2A	1639	U	C5-C6-N1	-7.06	119.17	122.70
1	1A	2858	G	C6-C5-N7	7.06	134.63	130.40
32	1a	310	G	O5'-P-OP2	7.06	119.17	110.70
1	1A	352	U	N3-C2-O2	-7.06	117.26	122.20
1	2A	975	C	O5'-P-OP1	-7.06	99.35	105.70
32	2a	719	C	N1-C2-O2	-7.06	114.67	118.90
1	1A	166	G	C5-C6-O6	7.05	132.83	128.60
1	1A	183	G	N1-C6-O6	-7.05	115.67	119.90
1	1A	322	G	C5-N7-C8	7.05	107.83	104.30
1	1A	859	C	N3-C4-C5	7.05	124.72	121.90
1	1A	1046	A	O5'-P-OP1	-7.05	99.35	105.70
32	1a	441	A	O5'-P-OP2	-7.05	99.35	105.70
1	2A	2447	G	C6-N1-C2	-7.05	120.87	125.10
32	2a	1125	U	N3-C2-O2	-7.05	117.26	122.20
1	1A	2023	A	C2-N3-C4	7.05	114.13	110.60
2	1B	32	C	C6-N1-C2	7.05	123.12	120.30
1	2A	2834	G	N1-C6-O6	-7.05	115.67	119.90
1	1A	194	G	N7-C8-N9	-7.05	109.58	113.10
32	2a	1030	C	N1-C2-O2	7.05	123.13	118.90
1	1A	1723	A	N1-C2-N3	-7.05	125.78	129.30
2	1B	77	U	C5-C4-O4	-7.05	121.67	125.90
1	2A	154	G	N7-C8-N9	-7.05	109.58	113.10
32	1a	254	G	O5'-P-OP1	-7.05	99.36	105.70
1	2A	1914	C	C5-C6-N1	7.04	124.52	121.00
1	1A	2421	G	O5'-P-OP2	-7.04	99.36	105.70
1	1A	1723	A	C5-N7-C8	7.04	107.42	103.90
1	1A	1124	U	O4'-C1'-N1	7.04	113.83	108.20
1	2A	1666	G	C5-C6-O6	7.04	132.82	128.60
1	2A	1087	G	C6-C5-N7	7.04	134.62	130.40
1	1A	1652	G	OP1-P-O3'	7.04	120.68	105.20
1	1A	1824	C	N3-C4-C5	7.04	124.71	121.90
1	1A	2451	A	N9-C4-C5	-7.04	102.99	105.80
1	1A	2723	A	O5'-P-OP2	-7.04	99.37	105.70
1	1A	2838	C	C6-N1-C2	-7.04	117.49	120.30
32	2a	27	G	C4-C5-N7	7.04	113.61	110.80
1	1A	1007	G	N3-C4-C5	-7.03	125.08	128.60
1	1A	1210	G	N1-C6-O6	-7.03	115.68	119.90
1	2A	562	U	N3-C2-O2	-7.03	117.28	122.20
32	2a	498	U	C5-C4-O4	7.03	130.12	125.90
1	1A	2449	U	C2-N3-C4	-7.03	122.78	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	855	G	N7-C8-N9	-7.03	109.58	113.10
1	1A	1823	G	C5-N7-C8	7.03	107.81	104.30
32	2a	1475	G	C8-N9-C4	-7.03	103.59	106.40
1	1A	1522	G	N1-C2-N2	7.02	122.52	116.20
1	1A	2622	C	C5-C4-N4	-7.02	115.28	120.20
32	1a	1522	U	O5'-P-OP1	-7.02	99.38	105.70
32	1a	569	C	N3-C4-C5	7.02	124.71	121.90
1	1A	654	G	C4-C5-N7	-7.02	107.99	110.80
1	1A	1117	G	C8-N9-C4	-7.02	103.59	106.40
1	1A	2030	C	N3-C2-O2	-7.02	116.99	121.90
1	1A	2527	C	N3-C4-C5	7.02	124.71	121.90
32	1a	1228	C	C6-N1-C2	-7.02	117.49	120.30
1	2A	2046	G	C8-N9-C4	7.02	109.21	106.40
1	2A	2140	C	C5-C6-N1	7.02	124.51	121.00
1	2A	2427	C	N3-C2-O2	7.02	126.81	121.90
32	2a	1531	A	N1-C6-N6	7.02	122.81	118.60
1	1A	607	C	OP1-P-O3'	7.02	120.64	105.20
1	1A	842	C	C5-C4-N4	7.02	125.11	120.20
1	1A	716	G	C4-C5-C6	-7.02	114.59	118.80
1	2A	2896	C	C2-N1-C1'	7.02	126.52	118.80
1	1A	1658	C	C6-N1-C2	7.01	123.11	120.30
1	1A	1692	G	C5-N7-C8	7.01	107.81	104.30
1	1A	2134	G	C5-C6-N1	7.01	115.01	111.50
1	1A	1259	A	N7-C8-N9	-7.01	110.30	113.80
32	2a	945	G	C5-C6-O6	-7.01	124.39	128.60
1	1A	838	C	C5-C6-N1	-7.01	117.50	121.00
1	1A	2060	G	C4-C5-N7	-7.01	108.00	110.80
1	2A	2679	A	N1-C6-N6	-7.01	114.39	118.60
32	2a	1452	C	C6-N1-C2	-7.01	117.50	120.30
1	2A	363(C)	G	C8-N9-C4	7.01	109.20	106.40
2	2B	59	A	C5-C6-N1	7.01	121.20	117.70
1	1A	2586	G	N3-C2-N2	7.00	124.80	119.90
1	1A	2902	G	C4-C5-N7	7.00	113.60	110.80
1	2A	213	A	C4-C5-C6	-7.00	113.50	117.00
1	1A	2511	C	N3-C2-O2	7.00	126.80	121.90
32	1a	68	G	C8-N9-C4	7.00	109.20	106.40
32	1a	613	C	C6-N1-C2	-7.00	117.50	120.30
1	2A	1983	C	C5-C4-N4	-7.00	115.30	120.20
1	1A	619	G	C8-N9-C4	7.00	109.20	106.40
1	1A	1539	C	C4-C5-C6	7.00	120.90	117.40
1	1A	1959	A	O4'-C1'-N9	7.00	113.80	108.20
1	1A	1982	A	N1-C2-N3	-7.00	125.80	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2611	G	N9-C4-C5	7.00	108.20	105.40
1	1A	2031	G	N3-C2-N2	-6.99	115.00	119.90
1	1A	2050	U	N3-C4-O4	-6.99	114.50	119.40
32	1a	187	C	C6-N1-C2	-6.99	117.50	120.30
32	1a	175	C	C6-N1-C2	-6.99	117.50	120.30
1	1A	1151	U	N3-C2-O2	6.99	127.09	122.20
32	2a	898	G	C8-N9-C4	6.99	109.20	106.40
1	1A	1094	A	C8-N9-C4	-6.99	103.00	105.80
1	1A	1593	C	O5'-P-OP2	6.99	119.08	110.70
32	1a	189(L)	G	N3-C4-N9	6.99	130.19	126.00
1	2A	744	G	N1-C6-O6	-6.99	115.71	119.90
1	2A	2037	G	C5-C6-O6	6.99	132.79	128.60
2	2B	65	C	O5'-P-OP2	6.99	119.09	110.70
2	2B	115	G	N3-C4-C5	6.99	132.09	128.60
1	1A	2463	A	C5-N7-C8	-6.99	100.41	103.90
1	2A	1073	A	N9-C1'-C2'	-6.99	104.32	112.00
1	2A	2041	U	N3-C4-O4	6.99	124.29	119.40
1	1A	2858	G	C5-N7-C8	6.98	107.79	104.30
1	2A	2144	U	N3-C2-O2	-6.98	117.31	122.20
1	1A	1307	C	C2-N3-C4	-6.98	116.41	119.90
1	1A	1382	A	N9-C4-C5	6.98	108.59	105.80
1	1A	1729	G	C5-C6-N1	6.98	114.99	111.50
1	1A	2330	G	N9-C1'-C2'	-6.98	104.32	112.00
1	2A	1652	A	C2-N3-C4	-6.98	107.11	110.60
32	2a	728	A	O5'-P-OP2	-6.98	99.42	105.70
32	1a	191	G	N9-C4-C5	6.98	108.19	105.40
1	2A	2237	G	N1-C6-O6	-6.98	115.71	119.90
1	1A	292	G	C2-N3-C4	-6.98	108.41	111.90
1	1A	555	G	O5'-P-OP1	-6.98	99.42	105.70
1	1A	2234	G	C2-N3-C4	-6.98	108.41	111.90
1	2A	913	U	O5'-P-OP2	-6.98	99.42	105.70
1	1A	1657	C	N3-C2-O2	-6.98	117.02	121.90
1	1A	1658	C	C5-C6-N1	-6.97	117.51	121.00
1	1A	2279	A	O5'-P-OP1	-6.97	99.42	105.70
1	1A	543	G	OP1-P-OP2	6.97	130.06	119.60
1	1A	985	G	C4-C5-N7	-6.97	108.01	110.80
1	1A	1294	G	C2-N3-C4	-6.97	108.41	111.90
1	2A	1655	A	C8-N9-C4	6.97	108.59	105.80
1	2A	2010	G	N1-C6-O6	6.97	124.08	119.90
1	1A	1407	G	N1-C6-O6	-6.97	115.72	119.90
32	1a	752	G	C8-N9-C4	6.97	109.19	106.40
32	1a	854	G	O5'-P-OP1	-6.97	99.43	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2133	G	N1-C6-O6	6.97	124.08	119.90
1	1A	1456	G	OP2-P-O3'	6.97	120.53	105.20
1	1A	2227	G	C8-N9-C1'	6.97	136.06	127.00
32	2a	615	C	C6-N1-C2	-6.97	117.51	120.30
1	1A	406	G	C8-N9-C4	6.96	109.19	106.40
1	2A	180	G	O5'-P-OP1	-6.96	99.43	105.70
1	1A	1700	G	O4'-C1'-N9	-6.96	102.63	108.20
1	2A	2318	G	C8-N9-C4	-6.96	103.61	106.40
1	1A	2579	G	C5-N7-C8	6.96	107.78	104.30
32	1a	1530	G	C8-N9-C4	6.96	109.18	106.40
2	2B	47	C	O5'-P-OP1	-6.96	99.44	105.70
1	1A	2266	C	N1-C2-O2	-6.96	114.72	118.90
32	1a	557	G	N3-C4-C5	-6.96	125.12	128.60
1	1A	225	C	C5-C6-N1	-6.96	117.52	121.00
1	2A	614	U	N1-C2-N3	6.96	119.07	114.90
1	1A	1859	G	C6-N1-C2	6.95	129.27	125.10
1	2A	271	A	O5'-P-OP2	-6.95	99.44	105.70
32	2a	289	G	O5'-P-OP2	6.95	119.04	110.70
1	1A	119	G	C8-N9-C4	6.95	109.18	106.40
1	1A	193	A	C2-N3-C4	6.95	114.08	110.60
1	2A	2070	G	N1-C6-O6	-6.95	115.73	119.90
32	2a	782	A	O5'-P-OP1	-6.95	99.44	105.70
1	1A	958	C	N3-C2-O2	-6.95	117.04	121.90
32	1a	676	A	C2-N3-C4	-6.95	107.13	110.60
32	2a	372	C	N1-C2-N3	-6.95	114.34	119.20
1	1A	1796	C	O5'-P-OP2	-6.95	99.45	105.70
1	1A	2638	C	N1-C2-O2	-6.95	114.73	118.90
32	1a	1003	G	N3-C4-N9	6.95	130.17	126.00
1	1A	619	G	N7-C8-N9	-6.95	109.63	113.10
1	1A	1451	U	N3-C4-O4	-6.95	114.54	119.40
2	1B	62	C	OP1-P-OP2	6.95	130.02	119.60
1	2A	906	G	N1-C6-O6	-6.95	115.73	119.90
1	1A	598	A	O5'-P-OP2	6.94	119.03	110.70
1	1A	316	C	C6-N1-C2	6.94	123.08	120.30
1	1A	1093	G	N3-C4-N9	6.94	130.16	126.00
1	1A	2560	G	C4-C5-N7	-6.94	108.02	110.80
1	2A	2577	A	C5-C6-N1	-6.94	114.23	117.70
1	1A	503	A	O5'-P-OP2	-6.94	99.45	105.70
1	1A	260	A	N7-C8-N9	-6.94	110.33	113.80
1	1A	295	C	N1-C2-O2	6.94	123.06	118.90
1	1A	1821	C	N3-C4-N4	6.94	122.86	118.00
1	1A	295	C	O5'-P-OP1	6.93	119.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	798	A	O5'-P-OP1	-6.93	99.46	105.70
32	1a	1504	G	N1-C6-O6	6.93	124.06	119.90
1	1A	826	U	C4-C5-C6	6.93	123.86	119.70
1	1A	2566	U	C5-C4-O4	-6.93	121.74	125.90
1	2A	2599	G	C5-C6-O6	6.93	132.76	128.60
32	1a	172	A	N7-C8-N9	6.93	117.27	113.80
1	2A	859	G	O4'-C1'-N9	-6.93	102.66	108.20
32	1a	1097	C	C6-N1-C2	-6.93	117.53	120.30
1	1A	2529	C	O4'-C1'-N1	6.93	113.74	108.20
1	2A	2611	U	N1-C2-O2	-6.93	117.95	122.80
1	2A	1933	G	C4-C5-N7	-6.92	108.03	110.80
1	2A	2399	G	C5-C6-O6	6.92	132.75	128.60
1	1A	1817	A	O5'-P-OP2	-6.92	99.47	105.70
1	1A	1829	U	N3-C4-C5	6.92	118.75	114.60
32	1a	188	C	N3-C2-O2	-6.92	117.06	121.90
1	2A	1092	C	N3-C2-O2	-6.92	117.06	121.90
32	2a	500	G	N1-C6-O6	6.92	124.05	119.90
1	1A	2577	A	C5-C6-N1	6.92	121.16	117.70
1	2A	2197	U	N3-C2-O2	-6.92	117.36	122.20
32	2a	368	U	O5'-P-OP1	-6.92	99.48	105.70
1	1A	1679	A	C5-N7-C8	6.91	107.36	103.90
1	2A	2511	U	N1-C2-N3	6.91	119.05	114.90
1	1A	474	U	C5-C6-N1	-6.91	119.25	122.70
1	1A	827	G	C5-N7-C8	6.91	107.75	104.30
1	2A	2164	C	C6-N1-C2	-6.91	117.54	120.30
1	1A	2006	G	C6-N1-C2	6.91	129.24	125.10
1	2A	1792	G	O5'-P-OP1	-6.91	99.48	105.70
32	1a	233	C	C6-N1-C2	-6.91	117.54	120.30
32	1a	913	A	C8-N9-C4	-6.91	103.04	105.80
1	2A	713	G	C2-N3-C4	-6.91	108.45	111.90
32	2a	1436	U	N1-C2-N3	6.91	119.04	114.90
32	2a	1493	A	C8-N9-C4	6.91	108.56	105.80
1	2A	83	G	O5'-P-OP2	-6.90	99.49	105.70
1	2A	2378	A	C4-C5-C6	6.90	120.45	117.00
1	1A	514	G	N1-C6-O6	-6.90	115.76	119.90
1	2A	2324	C	C6-N1-C2	6.90	123.06	120.30
32	2a	816	A	O5'-P-OP1	6.90	118.98	110.70
1	1A	842	C	N3-C2-O2	-6.90	117.07	121.90
1	1A	854	U	N1-C2-N3	6.89	119.04	114.90
1	1A	2171	G	C8-N9-C4	6.89	109.16	106.40
1	1A	1130	A	C6-C5-N7	6.89	137.12	132.30
1	1A	2234	G	C5-C6-N1	-6.89	108.05	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2246	G	N1-C6-O6	-6.89	115.77	119.90
1	1A	2633	A	OP1-P-OP2	6.89	129.94	119.60
32	2a	1027	C	C5-C6-N1	6.89	124.45	121.00
1	1A	2164	C	C5-C6-N1	6.89	124.44	121.00
1	1A	1451	U	C5-C6-N1	-6.89	119.25	122.70
1	1A	1665	G	N9-C4-C5	-6.89	102.64	105.40
32	1a	284	G	O5'-P-OP2	-6.89	99.50	105.70
1	1A	474	U	N3-C2-O2	-6.89	117.38	122.20
1	1A	1842	G	C5-C6-O6	6.89	132.73	128.60
1	1A	1843	A	O5'-P-OP1	-6.89	99.50	105.70
1	1A	1450	C	OP1-P-OP2	6.88	129.93	119.60
1	2A	1075	C	C5-C6-N1	6.88	124.44	121.00
1	2A	2378	A	C5-C6-N6	-6.88	118.19	123.70
1	1A	600	G	C5-N7-C8	6.88	107.74	104.30
1	1A	1028	C	N1-C2-O2	-6.88	114.77	118.90
1	1A	2082	A	N1-C2-N3	-6.88	125.86	129.30
1	1A	2003	A	C5-C6-N1	6.88	121.14	117.70
1	1A	243	G	N1-C6-O6	-6.88	115.78	119.90
1	1A	1991	A	OP1-P-O3'	6.88	120.33	105.20
1	2A	447	A	N7-C8-N9	-6.88	110.36	113.80
1	1A	1029	A	OP2-P-O3'	6.87	120.32	105.20
1	1A	1092	A	OP2-P-O3'	6.87	120.32	105.20
1	1A	149	A	N1-C2-N3	6.87	132.74	129.30
1	1A	2100	C	N3-C4-C5	6.87	124.65	121.90
1	1A	2580	C	C5-C4-N4	-6.87	115.39	120.20
1	2A	1071	G	C4-C5-C6	6.87	122.92	118.80
32	2a	904	C	C5-C4-N4	-6.87	115.39	120.20
1	2A	214	G	O5'-P-OP2	-6.87	99.52	105.70
1	1A	2632	C	N3-C4-N4	-6.87	113.19	118.00
32	1a	512	U	O5'-P-OP2	-6.87	99.52	105.70
1	2A	2867	G	C8-N9-C4	6.87	109.15	106.40
32	2a	442	C	C6-N1-C2	-6.86	117.56	120.30
1	1A	1304	C	C5-C6-N1	-6.86	117.57	121.00
32	1a	356	A	C2-N3-C4	6.86	114.03	110.60
32	1a	841	U	N3-C2-O2	-6.86	117.40	122.20
1	1A	2043	C	O5'-P-OP2	-6.86	99.53	105.70
16	1U	55	ARG	NE-CZ-NH1	-6.86	116.87	120.30
32	1a	1495	U	C2-N3-C4	6.86	131.11	127.00
1	2A	535	C	N1-C2-O2	-6.86	114.78	118.90
32	2a	346	G	C5-C6-N1	6.86	114.93	111.50
1	1A	2902	G	N3-C4-C5	6.86	132.03	128.60
32	1a	1184	G	N9-C4-C5	-6.86	102.66	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1119	C	C6-N1-C2	-6.86	117.56	120.30
1	1A	848	G	OP2-P-O3'	6.85	120.28	105.20
1	1A	2083	G	C8-N9-C4	-6.85	103.66	106.40
1	1A	2420	U	N3-C2-O2	-6.85	117.41	122.20
1	1A	2551	C	C2-N1-C1'	-6.85	111.27	118.80
1	2A	1769	G	C5-C6-O6	-6.85	124.49	128.60
32	2a	1026	G	N7-C8-N9	6.85	116.53	113.10
1	1A	235	C	O5'-P-OP1	-6.85	99.54	105.70
1	1A	2100	C	N1-C2-N3	6.85	123.99	119.20
32	1a	474	G	O5'-P-OP2	-6.85	99.54	105.70
1	1A	116	A	N9-C4-C5	6.84	108.54	105.80
1	1A	2449	U	N1-C2-N3	6.84	119.01	114.90
1	1A	856	G	C5-C6-N1	6.84	114.92	111.50
1	2A	739	G	O5'-P-OP1	-6.84	99.54	105.70
1	2A	2426	A	N1-C6-N6	6.84	122.70	118.60
1	1A	556	C	N3-C4-C5	6.84	124.64	121.90
1	1A	582	G	C5-N7-C8	-6.84	100.88	104.30
1	1A	1186	U	C6-N1-C2	-6.84	116.90	121.00
1	2A	1283	G	O5'-P-OP2	-6.84	99.55	105.70
1	2A	1399	C	OP2-P-O3'	6.84	120.24	105.20
1	1A	2453	C	N3-C2-O2	-6.83	117.12	121.90
1	2A	1890	A	N7-C8-N9	-6.83	110.38	113.80
1	1A	215	G	N3-C2-N2	-6.83	115.12	119.90
1	1A	2467	G	N1-C6-O6	-6.83	115.80	119.90
1	1A	23	G	N9-C4-C5	6.83	108.13	105.40
1	2A	189	G	C4-C5-N7	-6.83	108.07	110.80
1	1A	1043	G	N1-C6-O6	-6.83	115.80	119.90
1	1A	1812	C	C6-N1-C2	6.83	123.03	120.30
1	1A	1850	A	C5-C6-N1	-6.83	114.29	117.70
1	2A	2138	C	C6-N1-C2	-6.83	117.57	120.30
1	1A	1742	G	C6-C5-N7	-6.83	126.30	130.40
1	2A	2440	C	O5'-P-OP2	-6.83	99.56	105.70
1	2A	2010	G	N3-C2-N2	-6.83	115.12	119.90
1	2A	2186	G	N3-C2-N2	-6.83	115.12	119.90
5	1F	54	ARG	NE-CZ-NH2	-6.82	116.89	120.30
32	1a	819	A	N9-C4-C5	-6.82	103.07	105.80
32	1a	299	G	C5-C6-O6	-6.82	124.51	128.60
32	1a	858	G	C8-N9-C4	-6.82	103.67	106.40
1	1A	654	G	C5-N7-C8	6.82	107.71	104.30
1	1A	961	C	N1-C2-O2	6.82	122.99	118.90
1	1A	1324	A	OP1-P-OP2	-6.82	109.37	119.60
1	2A	421	U	OP2-P-O3'	-6.82	90.20	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2645	G	N3-C4-N9	-6.82	121.91	126.00
1	1A	573	G	N9-C4-C5	6.82	108.13	105.40
1	1A	815	G	N9-C4-C5	6.82	108.13	105.40
1	1A	2312	G	O5'-P-OP2	6.82	118.88	110.70
1	2A	2610	C	O5'-P-OP1	-6.82	99.56	105.70
1	1A	326	C	C6-N1-C2	-6.82	117.57	120.30
1	1A	1278	G	N9-C4-C5	6.81	108.13	105.40
1	1A	1298	G	N3-C4-C5	6.81	132.01	128.60
1	1A	1802	C	C5-C6-N1	-6.81	117.59	121.00
2	1B	108	U	O5'-P-OP1	6.81	118.88	110.70
1	1A	2427	G	OP1-P-OP2	-6.81	109.38	119.60
1	1A	1222	A	O5'-P-OP1	-6.81	99.57	105.70
1	1A	1245	C	N3-C4-C5	6.81	124.62	121.90
1	1A	2265	G	N3-C2-N2	-6.81	115.14	119.90
1	1A	2743	C	OP2-P-O3'	6.81	120.18	105.20
32	1a	576	G	N3-C4-C5	-6.81	125.20	128.60
1	2A	1118	C	C6-N1-C2	-6.81	117.58	120.30
1	2A	1261	C	O5'-P-OP1	-6.81	99.57	105.70
2	1B	13	A	N7-C8-N9	-6.81	110.40	113.80
1	1A	192	C	N1-C2-O2	6.80	122.98	118.90
32	1a	186	C	C5-C6-N1	6.80	124.40	121.00
1	1A	2020	G	C5-C6-O6	6.80	132.68	128.60
1	1A	891	C	C4-C5-C6	6.80	120.80	117.40
1	1A	2227	G	O4'-C1'-N9	6.80	113.64	108.20
1	2A	1062	G	C8-N9-C4	-6.80	103.68	106.40
1	1A	1067	A	O5'-P-OP1	-6.80	99.58	105.70
1	1A	1863	C	N3-C2-O2	-6.80	117.14	121.90
1	1A	1725	G	C5-C6-O6	-6.80	124.52	128.60
1	1A	1853	G	N7-C8-N9	-6.80	109.70	113.10
1	1A	2364	A	O5'-P-OP1	-6.80	99.58	105.70
32	1a	552	U	O5'-P-OP2	-6.80	99.58	105.70
32	2a	441	A	OP2-P-O3'	6.80	120.15	105.20
32	2a	1460	A	O5'-P-OP1	6.80	118.86	110.70
1	1A	2784	C	C2-N3-C4	-6.79	116.50	119.90
1	1A	2001	C	N3-C4-C5	6.79	124.62	121.90
1	1A	2881	C	C5-C4-N4	-6.79	115.44	120.20
1	1A	418	G	N7-C8-N9	-6.79	109.70	113.10
1	1A	1814	A	N1-C2-N3	-6.79	125.90	129.30
32	1a	1499	A	O5'-P-OP1	6.79	118.85	110.70
1	1A	476	G	C8-N9-C4	6.79	109.11	106.40
32	1a	397	A	OP2-P-O3'	6.79	120.14	105.20
1	1A	727	G	C8-N9-C4	-6.79	103.69	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1693	C	N1-C2-O2	-6.79	114.83	118.90
1	2A	1793	C	N3-C4-N4	-6.79	113.25	118.00
1	1A	171	A	O5'-P-OP1	-6.79	99.59	105.70
1	2A	718	A	C6-C5-N7	-6.79	127.55	132.30
1	2A	1281	G	O5'-P-OP1	-6.79	99.59	105.70
1	2A	1312	U	C5-C4-O4	6.79	129.97	125.90
32	2a	1527	C	O5'-P-OP2	-6.79	99.59	105.70
1	1A	1803	G	C5-N7-C8	6.78	107.69	104.30
1	1A	2286	A	C5-C6-N1	-6.78	114.31	117.70
1	2A	1966	A	N1-C6-N6	-6.78	114.53	118.60
1	1A	739	C	C4-C5-C6	-6.78	114.01	117.40
1	2A	2433	A	C5-C6-N1	6.78	121.09	117.70
1	1A	2835	C	C5-C6-N1	-6.78	117.61	121.00
32	2a	1149	C	C5-C6-N1	6.78	124.39	121.00
1	1A	1028	C	N3-C2-O2	6.78	126.64	121.90
1	1A	1637	G	N1-C6-O6	-6.78	115.83	119.90
1	1A	1995	G	C4-C5-N7	-6.78	108.09	110.80
1	1A	1178	A	OP2-P-O3'	6.77	120.10	105.20
1	1A	1135	G	N3-C4-C5	-6.77	125.21	128.60
1	1A	1470	G	C2-N3-C4	-6.77	108.51	111.90
1	1A	1786	A	C8-N9-C4	-6.77	103.09	105.80
1	1A	2256	U	C5-C6-N1	-6.77	119.31	122.70
32	1a	1417	G	C5-C6-N1	6.77	114.89	111.50
1	1A	557	A	N1-C6-N6	-6.77	114.54	118.60
1	1A	906	G	N7-C8-N9	-6.77	109.72	113.10
1	1A	1155	C	C5-C6-N1	6.77	124.39	121.00
1	1A	1243	U	N1-C2-N3	6.77	118.96	114.90
1	1A	2376	C	C6-N1-C2	6.77	123.01	120.30
32	1a	657	G	O5'-P-OP2	-6.77	99.61	105.70
1	1A	271	U	O4'-C1'-N1	6.77	113.61	108.20
32	1a	536	C	O5'-P-OP2	-6.77	99.61	105.70
1	1A	1314	A	C5-C6-N1	-6.76	114.32	117.70
2	1B	91	C	N3-C4-C5	6.76	124.61	121.90
1	2A	2447	G	C5-C6-O6	-6.76	124.54	128.60
1	1A	1813	C	C5-C6-N1	-6.76	117.62	121.00
1	2A	2848	G	C4-C5-N7	-6.76	108.09	110.80
1	1A	130	G	C5-N7-C8	6.76	107.68	104.30
1	1A	415	G	N9-C4-C5	-6.76	102.70	105.40
1	1A	1959	A	N9-C4-C5	6.76	108.50	105.80
2	1B	23	G	O5'-P-OP1	-6.76	99.61	105.70
32	2a	1062	U	N1-C2-O2	6.76	127.53	122.80
1	1A	1543	U	C2-N3-C4	-6.76	122.94	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1V	82	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	1A	729	G	O5'-P-OP1	-6.76	99.62	105.70
1	1A	2269	U	N3-C2-O2	-6.76	117.47	122.20
1	2A	1935	G	C5-C6-N1	6.76	114.88	111.50
2	2B	101	G	C5-C6-O6	-6.76	124.55	128.60
32	2a	1149	C	C6-N1-C2	-6.76	117.60	120.30
1	1A	444	C	C6-N1-C2	-6.75	117.60	120.30
1	2A	2827	C	N1-C2-O2	-6.75	114.85	118.90
1	1A	1221	G	C4-N9-C1'	-6.75	117.72	126.50
1	2A	290	G	O5'-P-OP1	-6.75	99.62	105.70
1	2A	882	G	C8-N9-C1'	6.75	135.78	127.00
1	1A	827	G	C4-C5-N7	-6.75	108.10	110.80
1	2A	834	C	C6-N1-C2	-6.75	117.60	120.30
1	1A	438	G	O5'-P-OP1	6.75	118.80	110.70
1	1A	849	A	C2-N3-C4	6.75	113.97	110.60
1	2A	1630	G	C8-N9-C4	-6.75	103.70	106.40
1	1A	2188	G	C8-N9-C1'	6.75	135.77	127.00
44	2l	87	GLY	N-CA-C	6.75	129.96	113.10
1	1A	2463	A	C5-C6-N1	6.74	121.07	117.70
32	1a	854	G	O5'-P-OP2	6.74	118.79	110.70
2	1B	52	A	C8-N9-C4	6.74	108.50	105.80
1	2A	238	C	N3-C4-C5	-6.74	119.20	121.90
1	2A	1710	C	O5'-P-OP1	6.74	118.79	110.70
32	2a	1125	U	O4'-C1'-N1	6.74	113.59	108.20
1	1A	561	A	O5'-P-OP2	-6.74	99.64	105.70
1	1A	2440	G	N3-C4-C5	-6.74	125.23	128.60
32	2a	848	C	C5-C6-N1	6.74	124.37	121.00
1	2A	1075	C	N1-C2-O2	6.74	122.94	118.90
1	1A	2439	C	O5'-P-OP1	-6.74	99.64	105.70
1	2A	743	G	C5-C6-O6	6.74	132.64	128.60
1	2A	1321	A	C8-N9-C4	6.74	108.49	105.80
1	2A	1618	A	C8-N9-C4	-6.74	103.11	105.80
1	2A	1681	G	N3-C4-C5	6.74	131.97	128.60
13	2R	67	LEU	CA-CB-CG	6.74	130.79	115.30
1	1A	2019	G	O5'-P-OP1	6.73	118.78	110.70
1	1A	1038	C	N3-C4-C5	6.73	124.59	121.90
1	1A	1986	G	C2-N3-C4	-6.73	108.53	111.90
32	1a	181	G	O4'-C1'-N9	6.73	113.58	108.20
1	2A	912	C	C2-N1-C1'	6.73	126.20	118.80
32	1a	863	U	C5-C4-O4	6.73	129.94	125.90
1	2A	1807	G	C8-N9-C4	6.73	109.09	106.40
1	2A	450	G	C5-C6-N1	6.73	114.86	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	662	G	O5'-P-OP2	6.72	118.77	110.70
1	2A	976	C	N3-C2-O2	-6.72	117.19	121.90
1	1A	1069	U	C2-N3-C4	-6.72	122.97	127.00
1	1A	1846	A	O5'-P-OP1	-6.72	99.65	105.70
1	1A	2320	G	C5-C6-O6	-6.72	124.57	128.60
1	1A	422	U	N3-C2-O2	-6.72	117.50	122.20
1	2A	1929	G	O5'-P-OP2	-6.72	99.65	105.70
1	2A	2893	G	C2-N3-C4	6.72	115.26	111.90
1	1A	23	G	C4-C5-N7	-6.72	108.11	110.80
1	1A	1769	G	C5-C6-O6	6.72	132.63	128.60
32	1a	1176	A	N9-C4-C5	6.72	108.49	105.80
1	1A	999	G	N1-C6-O6	-6.72	115.87	119.90
1	1A	673	G	C2-N3-C4	-6.72	108.54	111.90
1	1A	696	C	C6-N1-C2	-6.72	117.61	120.30
1	1A	1718	U	C5-C6-N1	-6.72	119.34	122.70
1	1A	1988	A	C8-N9-C4	6.72	108.49	105.80
2	1B	1	U	C2-N1-C1'	6.72	125.76	117.70
1	1A	486	A	C8-N9-C4	-6.71	103.11	105.80
1	1A	990	A	O4'-C1'-N9	-6.71	102.83	108.20
1	2A	1635	G	C8-N9-C4	6.71	109.09	106.40
1	1A	107	G	N1-C6-O6	-6.71	115.87	119.90
1	1A	1007	G	N9-C4-C5	6.71	108.08	105.40
1	1A	2083	G	N3-C4-C5	-6.71	125.24	128.60
1	2A	2425	A	C8-N9-C4	-6.71	103.11	105.80
1	1A	841	G	N3-C2-N2	6.71	124.60	119.90
1	2A	1763	G	N9-C4-C5	6.71	108.08	105.40
1	1A	344	A	C8-N9-C4	-6.71	103.12	105.80
1	1A	1181	G	C5-C6-O6	-6.71	124.58	128.60
1	1A	789	G	N7-C8-N9	-6.71	109.75	113.10
1	1A	2357	G	OP1-P-O3'	6.71	119.95	105.20
32	1a	557	G	OP1-P-O3'	6.71	119.96	105.20
1	2A	882	G	N3-C4-N9	-6.71	121.98	126.00
1	2A	1574	C	C4-C5-C6	-6.71	114.05	117.40
1	2A	1778	U	C6-N1-C2	6.71	125.02	121.00
32	2a	230	G	C4-C5-N7	-6.71	108.12	110.80
32	2a	881	G	C8-N9-C4	6.71	109.08	106.40
1	1A	572	A	C8-N9-C4	-6.70	103.12	105.80
1	1A	720	C	O5'-P-OP2	-6.70	99.67	105.70
1	1A	1341	C	N3-C4-N4	-6.70	113.31	118.00
1	1A	1991	A	OP1-P-OP2	-6.70	109.55	119.60
32	2a	1027	C	C2-N1-C1'	6.70	126.17	118.80
1	1A	592	U	N1-C2-N3	6.70	118.92	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1000	C	C5-C4-N4	6.70	124.89	120.20
1	1A	1045	U	O5'-P-OP2	-6.70	99.67	105.70
1	1A	2390	A	N1-C6-N6	6.70	122.62	118.60
2	1B	18	G	C5-C6-O6	-6.70	124.58	128.60
1	1A	1173	A	N1-C2-N3	-6.70	125.95	129.30
32	1a	1530	G	N9-C4-C5	-6.70	102.72	105.40
32	2a	776	G	O5'-P-OP2	-6.70	99.67	105.70
1	1A	1701	A	N7-C8-N9	-6.70	110.45	113.80
1	1A	2361	G	O5'-P-OP1	-6.70	99.67	105.70
1	2A	2612	C	O5'-P-OP2	-6.70	99.67	105.70
32	2a	550	G	O5'-P-OP1	-6.70	99.67	105.70
32	2a	1019	C	C6-N1-C2	-6.70	117.62	120.30
1	1A	706	C	N3-C4-C5	6.69	124.58	121.90
1	1A	809	U	C6-N1-C1'	-6.69	111.83	121.20
1	1A	1365	G	C5-N7-C8	-6.69	100.95	104.30
1	1A	2049	G	C2-N3-C4	6.69	115.25	111.90
1	1A	283	G	C8-N9-C4	-6.69	103.72	106.40
1	1A	2406	C	C2-N3-C4	-6.69	116.55	119.90
32	1a	896	C	C6-N1-C2	6.69	122.98	120.30
46	1n	3	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	1A	593	G	C5-C6-N1	6.69	114.84	111.50
1	1A	1298	G	N3-C4-N9	-6.69	121.99	126.00
1	1A	2074	G	N9-C4-C5	6.69	108.08	105.40
1	2A	614	U	C6-N1-C2	-6.69	116.99	121.00
1	2A	1681	G	N3-C4-N9	-6.69	121.99	126.00
1	1A	1346	U	N1-C2-N3	6.69	118.91	114.90
1	1A	793	A	C8-N9-C4	-6.68	103.13	105.80
1	1A	1669	G	C6-C5-N7	6.68	134.41	130.40
2	1B	115	G	C8-N9-C4	6.68	109.07	106.40
32	1a	204	U	C6-N1-C2	-6.68	116.99	121.00
32	2a	357	G	N3-C2-N2	-6.68	115.22	119.90
1	1A	1333	A	C8-N9-C4	-6.68	103.13	105.80
1	2A	94(A)	G	C8-N9-C4	-6.68	103.73	106.40
1	1A	1403	U	C5-C6-N1	-6.68	119.36	122.70
1	1A	1069	U	C5-C4-O4	-6.68	121.89	125.90
32	1a	115	G	P-O3'-C3'	6.68	127.72	119.70
32	1a	189(D)	C	N3-C2-O2	-6.68	117.22	121.90
1	2A	1828	G	O5'-P-OP1	-6.68	99.69	105.70
1	2A	2030	A	O5'-P-OP1	-6.68	99.69	105.70
1	1A	1178	A	N1-C2-N3	6.68	132.64	129.30
1	1A	1944	G	O5'-P-OP2	-6.68	99.69	105.70
1	1A	2183	C	C5-C6-N1	6.68	124.34	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	728	A	OP1-P-OP2	6.68	129.62	119.60
32	1a	807	A	C8-N9-C4	-6.68	103.13	105.80
1	2A	532	A	C8-N9-C4	-6.68	103.13	105.80
1	2A	2575	C	N3-C2-O2	-6.68	117.23	121.90
1	2A	2784	C	O5'-P-OP2	-6.68	99.69	105.70
3	2D	275	LYS	N-CA-C	-6.68	92.97	111.00
1	1A	2750	G	N1-C6-O6	-6.67	115.89	119.90
32	1a	690	G	OP1-P-OP2	6.67	129.61	119.60
1	2A	576	U	N1-C2-O2	-6.67	118.13	122.80
1	1A	802	C	C4-C5-C6	6.67	120.74	117.40
32	2a	431	A	O5'-P-OP1	-6.67	99.69	105.70
1	2A	572	A	N1-C6-N6	-6.67	114.60	118.60
1	1A	508	A	O5'-P-OP2	-6.67	99.70	105.70
1	1A	2358	A	N1-C2-N3	6.67	132.63	129.30
1	1A	2546	A	C5-C6-N6	-6.67	118.37	123.70
32	1a	326	G	N9-C4-C5	6.66	108.06	105.40
1	1A	314	G	O5'-P-OP1	-6.66	99.70	105.70
1	1A	15	G	C8-N9-C4	-6.66	103.74	106.40
1	1A	1621	C	N3-C4-C5	6.66	124.56	121.90
1	2A	679	C	N1-C2-O2	-6.66	114.90	118.90
1	2A	788	A	N1-C6-N6	6.66	122.60	118.60
1	2A	2237	G	C5-C6-O6	6.66	132.60	128.60
1	1A	590	A	N1-C2-N3	-6.66	125.97	129.30
1	1A	770	G	N1-C2-N2	-6.66	110.21	116.20
1	1A	1014	U	C4-C5-C6	-6.66	115.70	119.70
1	1A	1807	G	N3-C2-N2	6.66	124.56	119.90
1	1A	2020	G	N1-C6-O6	-6.66	115.91	119.90
1	1A	2503	U	C5-C4-O4	-6.66	121.91	125.90
32	1a	900	A	C2-N3-C4	6.66	113.93	110.60
32	1a	1243	C	C6-N1-C2	-6.66	117.64	120.30
32	1a	1486	G	C5-C6-O6	-6.66	124.61	128.60
1	2A	2773	C	C6-N1-C2	6.66	122.96	120.30
1	1A	107	G	N7-C8-N9	-6.65	109.77	113.10
32	2a	649	G	N3-C4-C5	6.65	131.93	128.60
1	1A	1237	G	C2-N3-C4	-6.65	108.57	111.90
1	1A	1422	C	N3-C4-N4	-6.65	113.34	118.00
1	1A	2284	U	OP2-P-O3'	6.65	119.83	105.20
1	1A	2592	U	C5-C6-N1	-6.65	119.37	122.70
32	1a	1169	A	C8-N9-C4	-6.65	103.14	105.80
1	2A	1363	C	O5'-P-OP2	-6.65	99.71	105.70
1	1A	2406	C	N1-C2-O2	-6.65	114.91	118.90
1	1A	2802	C	C2-N3-C4	-6.65	116.58	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1041	C	N1-C2-O2	6.65	122.89	118.90
1	1A	2010	C	C5-C6-N1	-6.65	117.68	121.00
1	1A	2568	C	N3-C4-C5	6.65	124.56	121.90
1	2A	271(P)	C	O5'-P-OP2	-6.65	99.72	105.70
1	1A	292	G	C4-C5-N7	6.65	113.46	110.80
1	1A	1822	A	OP1-P-OP2	-6.65	109.63	119.60
32	1a	1409	C	N1-C2-O2	6.65	122.89	118.90
1	2A	1253	A	N7-C8-N9	-6.65	110.48	113.80
1	1A	195	U	N1-C2-N3	6.64	118.89	114.90
1	1A	466	G	N1-C6-O6	6.64	123.89	119.90
1	1A	2457	G	OP1-P-OP2	6.64	129.57	119.60
1	2A	2783	G	N1-C6-O6	-6.64	115.91	119.90
1	1A	2447	A	O5'-P-OP1	-6.64	99.72	105.70
1	1A	1829	U	N3-C4-O4	-6.64	114.75	119.40
1	1A	436	C	O5'-P-OP2	6.64	118.67	110.70
1	2A	2058	A	C6-C5-N7	-6.64	127.65	132.30
1	1A	575	G	N3-C2-N2	6.64	124.55	119.90
1	1A	2291	G	C4-C5-N7	6.64	113.45	110.80
1	2A	1326	U	O5'-P-OP1	-6.64	99.73	105.70
1	2A	1652	A	O5'-P-OP1	-6.64	99.73	105.70
1	1A	2006	G	C6-C5-N7	6.63	134.38	130.40
1	1A	2375	C	N3-C4-N4	-6.63	113.36	118.00
32	1a	1479	C	OP1-P-O3'	6.63	119.80	105.20
1	2A	312	G	O5'-P-OP1	-6.63	99.73	105.70
1	1A	2839	C	C5-C6-N1	6.63	124.32	121.00
1	2A	2167	U	C6-N1-C2	-6.63	117.02	121.00
1	1A	302	A	P-O3'-C3'	6.63	127.66	119.70
1	1A	1186	U	N3-C2-O2	-6.63	117.56	122.20
32	1a	533	A	C4-C5-N7	6.63	114.01	110.70
1	2A	48	G	O5'-P-OP2	-6.63	99.73	105.70
1	1A	2358	A	C4-C5-C6	6.63	120.31	117.00
1	1A	747	G	N3-C2-N2	6.62	124.54	119.90
2	1B	100	A	OP1-P-OP2	6.62	129.54	119.60
1	2A	11	G	C4-C5-N7	6.62	113.45	110.80
32	2a	397	A	O5'-P-OP2	-6.62	99.74	105.70
1	1A	2576	A	C6-C5-N7	-6.62	127.66	132.30
1	2A	2385	C	N1-C2-O2	-6.62	114.93	118.90
32	2a	871	U	N1-C2-O2	6.62	127.44	122.80
1	1A	2225	U	C5-C6-N1	-6.62	119.39	122.70
32	1a	801	U	N1-C2-O2	6.62	127.44	122.80
32	1a	836	G	C4-C5-N7	6.62	113.45	110.80
1	2A	1087	G	C8-N9-C1'	6.62	135.61	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1365	G	N3-C2-N2	-6.62	115.27	119.90
1	1A	1181	G	N1-C6-O6	6.62	123.87	119.90
32	1a	204	U	N1-C2-O2	6.62	127.43	122.80
32	1a	1184	G	C4-C5-N7	6.62	113.45	110.80
1	2A	1076	C	C2-N1-C1'	6.62	126.08	118.80
32	2a	218	C	C6-N1-C2	-6.62	117.65	120.30
1	1A	1742	G	C5-N7-C8	-6.62	100.99	104.30
1	1A	1543	U	C5-C6-N1	-6.61	119.39	122.70
1	1A	2561	G	N3-C4-C5	-6.61	125.29	128.60
1	1A	2593	G	C4-C5-N7	6.61	113.44	110.80
32	1a	501	C	OP2-P-O3'	6.61	119.75	105.20
32	1a	1530	G	N1-C2-N2	6.61	122.15	116.20
1	2A	2679	A	OP2-P-O3'	6.61	119.75	105.20
1	1A	1831	C	N3-C2-O2	-6.61	117.27	121.90
1	1A	359	C	N3-C4-C5	-6.61	119.26	121.90
1	1A	418	G	C5-C6-N1	6.61	114.80	111.50
1	1A	1986	G	C4-C5-N7	6.61	113.44	110.80
1	1A	2284	U	C2-N3-C4	-6.61	123.04	127.00
1	2A	1073	A	P-O3'-C3'	6.61	127.63	119.70
1	1A	2217	C	OP1-P-O3'	6.60	119.73	105.20
1	1A	583	C	C4-C5-C6	6.60	120.70	117.40
1	1A	886	U	N3-C4-C5	6.60	118.56	114.60
2	1B	79	C	N3-C4-C5	6.60	124.54	121.90
32	2a	799	G	N1-C6-O6	-6.60	115.94	119.90
1	1A	790	G	N9-C4-C5	6.60	108.04	105.40
1	1A	1237	G	C4-C5-N7	-6.60	108.16	110.80
1	1A	1953	U	C4-C5-C6	-6.60	115.74	119.70
32	2a	618	C	OP1-P-O3'	6.60	119.72	105.20
32	1a	590	C	O5'-P-OP2	-6.60	99.76	105.70
1	1A	1611	C	C5-C4-N4	6.60	124.82	120.20
32	1a	563	A	N7-C8-N9	6.60	117.10	113.80
32	1a	769	G	OP2-P-O3'	6.60	119.72	105.20
32	2a	269	C	C6-N1-C2	6.60	122.94	120.30
1	1A	1708	G	N7-C8-N9	-6.60	109.80	113.10
1	1A	103	C	N3-C4-C5	6.59	124.54	121.90
1	1A	1700	G	OP1-P-O3'	6.59	119.71	105.20
32	1a	353	A	C5-N7-C8	-6.59	100.60	103.90
32	2a	898	G	N3-C4-C5	6.59	131.90	128.60
1	1A	1447	G	C5-C6-N1	-6.59	108.20	111.50
32	1a	804	U	C5-C4-O4	6.59	129.86	125.90
32	1a	819	A	C5-C6-N6	-6.59	118.43	123.70
2	2B	24	G	N1-C6-O6	6.59	123.86	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1333	A	N7-C8-N9	6.59	117.10	113.80
2	2B	14	U	O5'-P-OP2	-6.59	99.77	105.70
1	1A	1958	A	C4-C5-N7	6.59	113.99	110.70
1	2A	568	U	N3-C4-C5	6.59	118.55	114.60
1	2A	1904	G	O5'-P-OP2	-6.59	99.77	105.70
1	1A	428	A	N9-C4-C5	6.58	108.43	105.80
1	1A	1559	C	O5'-P-OP2	6.58	118.60	110.70
1	2A	2805	G	N1-C6-O6	-6.58	115.95	119.90
1	1A	1662	A	O5'-P-OP2	6.58	118.60	110.70
1	2A	1963	U	C2-N1-C1'	6.58	125.60	117.70
1	2A	2576	G	OP2-P-O3'	6.58	119.69	105.20
1	1A	2383	G	C2-N3-C4	6.58	115.19	111.90
1	1A	2432	C	N1-C2-O2	-6.58	114.95	118.90
1	2A	1244	G	C8-N9-C4	6.58	109.03	106.40
1	2A	1332	G	C5-C6-O6	-6.58	124.65	128.60
23	2I	21	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	2A	1780	A	C8-N9-C4	-6.58	103.17	105.80
32	2a	831	U	OP1-P-OP2	-6.58	109.73	119.60
1	1A	901	G	C5-C6-O6	6.58	132.55	128.60
1	1A	2129	C	C6-N1-C2	-6.58	117.67	120.30
32	1a	1136	U	C6-N1-C2	-6.58	117.05	121.00
1	2A	36	G	O5'-P-OP2	-6.58	99.78	105.70
32	2a	581	G	N1-C6-O6	6.58	123.85	119.90
1	1A	1475	G	N1-C6-O6	-6.58	115.95	119.90
32	1a	1021	G	N1-C6-O6	-6.58	115.95	119.90
1	1A	1234	A	N1-C6-N6	6.58	122.55	118.60
1	2A	741	G	O5'-P-OP1	-6.58	99.78	105.70
1	2A	1836	C	O5'-P-OP2	-6.58	99.78	105.70
1	1A	604	C	N1-C2-O2	-6.57	114.96	118.90
1	1A	2017	U	C5-C6-N1	-6.57	119.41	122.70
1	1A	2596	U	C2-N1-C1'	-6.57	109.81	117.70
1	2A	188	G	O5'-P-OP2	-6.57	99.78	105.70
1	2A	1065	U	O4'-C1'-N1	6.57	113.46	108.20
1	2A	1783	A	C2-N3-C4	6.57	113.89	110.60
32	1a	148	G	N1-C6-O6	-6.57	115.96	119.90
1	2A	1666	G	N1-C2-N2	-6.57	110.28	116.20
1	1A	910	A	OP2-P-O3'	6.57	119.66	105.20
1	2A	312	G	N1-C6-O6	6.57	123.84	119.90
1	2A	655	A	C8-N9-C4	-6.57	103.17	105.80
1	1A	215	G	N1-C2-N2	6.57	122.11	116.20
32	1a	1176	A	N1-C6-N6	-6.57	114.66	118.60
1	2A	2773	C	C5-C6-N1	-6.57	117.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	483	A	C6-N1-C2	6.57	122.54	118.60
1	1A	1242	G	N1-C6-O6	-6.57	115.96	119.90
1	1A	1757	C	C6-N1-C2	6.57	122.93	120.30
1	2A	789	A	N1-C6-N6	6.57	122.54	118.60
32	2a	775	G	OP2-P-O3'	6.57	119.65	105.20
32	2a	824	C	N3-C4-C5	-6.57	119.27	121.90
1	1A	749	G	OP1-P-OP2	6.57	129.45	119.60
1	1A	418	G	C8-N9-C4	6.56	109.03	106.40
1	1A	593	G	C2-N3-C4	6.56	115.18	111.90
1	1A	1692	G	N7-C8-N9	-6.56	109.82	113.10
1	1A	1862	G	C5-C6-O6	6.56	132.54	128.60
1	1A	2523	U	C5-C6-N1	-6.56	119.42	122.70
32	1a	286	G	O5'-P-OP1	-6.56	99.79	105.70
1	1A	424	G	C8-N9-C4	6.56	109.03	106.40
1	1A	1302	G	N7-C8-N9	-6.56	109.82	113.10
1	1A	360	C	C6-N1-C2	-6.56	117.68	120.30
1	1A	1368	A	C6-N1-C2	6.56	122.54	118.60
1	1A	483	A	C5-C6-N1	-6.56	114.42	117.70
32	1a	1500	A	N1-C6-N6	-6.56	114.67	118.60
32	1a	1505	G	N3-C4-N9	-6.56	122.07	126.00
1	2A	2319	G	C5-N7-C8	-6.56	101.02	104.30
32	2a	572	A	C4-N9-C1'	-6.56	114.50	126.30
32	2a	871	U	N3-C2-O2	-6.56	117.61	122.20
1	1A	2030	C	N1-C2-N3	6.55	123.79	119.20
1	1A	2881	C	N3-C4-C5	6.55	124.52	121.90
1	2A	752	A	OP2-P-O3'	6.55	119.62	105.20
1	1A	554	A	C8-N9-C4	-6.55	103.18	105.80
32	1a	57	G	C5-C6-O6	6.55	132.53	128.60
32	1a	801	U	N3-C2-O2	-6.55	117.61	122.20
1	2A	108	U	O5'-P-OP2	-6.55	99.80	105.70
1	1A	2762	A	C5-C6-N1	6.55	120.98	117.70
1	1A	596	G	C5-C6-O6	-6.55	124.67	128.60
1	1A	1105	G	C8-N9-C4	6.55	109.02	106.40
1	1A	1377	A	OP2-P-O3'	6.55	119.61	105.20
1	1A	2440	G	C6-N1-C2	-6.55	121.17	125.10
32	2a	1378	C	N3-C4-C5	-6.55	119.28	121.90
1	2A	660	G	C5-C6-O6	6.55	132.53	128.60
32	2a	115	G	O5'-P-OP2	-6.55	99.81	105.70
32	2a	262	A	O5'-P-OP2	-6.55	99.81	105.70
32	2a	618	C	N3-C4-C5	-6.55	119.28	121.90
32	2a	1139	G	C4-C5-N7	-6.55	108.18	110.80
1	1A	891	C	C2-N3-C4	-6.54	116.63	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1379	C	C2-N3-C4	-6.54	116.63	119.90
1	1A	2639	G	N7-C8-N9	-6.54	109.83	113.10
2	1B	41	U	C5-C4-O4	6.54	129.83	125.90
1	2A	739	G	C5-C6-O6	-6.54	124.67	128.60
32	2a	717	C	O5'-P-OP2	6.54	118.55	110.70
32	2a	1011	G	C4-C5-N7	-6.54	108.18	110.80
1	1A	802	C	C6-N1-C2	-6.54	117.68	120.30
1	2A	663	G	C8-N9-C4	6.54	109.02	106.40
1	1A	1683	C	N3-C2-O2	-6.54	117.32	121.90
32	1a	134	A	N1-C6-N6	6.54	122.52	118.60
1	1A	2052	A	C5-N7-C8	-6.54	100.63	103.90
1	2A	2576	G	C8-N9-C4	6.54	109.02	106.40
1	1A	2100	C	C5-C6-N1	-6.54	117.73	121.00
1	1A	2353	G	C8-N9-C4	-6.54	103.79	106.40
1	1A	472	G	N9-C4-C5	-6.53	102.79	105.40
1	1A	652	A	C2-N3-C4	6.53	113.87	110.60
1	1A	2577	A	C6-N1-C2	-6.53	114.68	118.60
1	1A	2630	G	N1-C6-O6	-6.53	115.98	119.90
2	1B	57	A	C4-C5-C6	-6.53	113.73	117.00
32	1a	655	A	O5'-P-OP2	-6.53	99.82	105.70
1	1A	752	A	C8-N9-C4	6.53	108.41	105.80
1	1A	1752	G	C8-N9-C4	-6.53	103.79	106.40
1	2A	2515	C	N1-C2-O2	-6.53	114.98	118.90
1	1A	565	C	N3-C4-C5	6.53	124.51	121.90
1	1A	1655	A	C5-N7-C8	6.53	107.17	103.90
1	1A	1690	G	C6-C5-N7	6.53	134.32	130.40
1	1A	616	G	C5-C6-O6	6.53	132.52	128.60
1	2A	2002	G	C5-N7-C8	6.53	107.56	104.30
32	1a	928	G	O5'-P-OP1	-6.53	99.82	105.70
1	2A	2827	C	N3-C2-O2	6.53	126.47	121.90
32	2a	902	G	N7-C8-N9	-6.53	109.84	113.10
1	2A	1574	C	C5-C6-N1	6.53	124.26	121.00
1	2A	1937	A	O4'-C1'-N9	6.53	113.42	108.20
1	2A	1966	A	C5-C6-N6	6.53	128.92	123.70
1	1A	2229	A	O4'-C1'-N9	6.52	113.42	108.20
1	1A	848	G	N7-C8-N9	6.52	116.36	113.10
1	2A	1097	U	C6-N1-C1'	-6.52	112.07	121.20
32	2a	289	G	OP1-P-OP2	-6.52	109.82	119.60
1	1A	2080	A	C8-N9-C4	6.52	108.41	105.80
1	1A	874	U	OP1-P-OP2	-6.52	109.82	119.60
1	1A	1285	G	C5-C6-N1	-6.52	108.24	111.50
1	1A	2037	A	O5'-P-OP2	-6.52	99.83	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2283	G	N3-C4-C5	-6.52	125.34	128.60
32	1a	1465	C	N1-C2-O2	-6.52	114.99	118.90
1	2A	2058	A	N1-C6-N6	6.52	122.51	118.60
1	1A	1924	C	OP2-P-O3'	6.52	119.54	105.20
1	2A	573	G	OP1-P-O3'	6.52	119.54	105.20
32	2a	38	G	C8-N9-C4	6.52	109.01	106.40
1	1A	745	C	O5'-P-OP2	-6.52	99.84	105.70
1	2A	1618	A	N1-C6-N6	-6.52	114.69	118.60
1	2A	2488	A	N1-C6-N6	6.52	122.51	118.60
1	1A	1359	U	O5'-P-OP1	-6.51	99.84	105.70
1	1A	1853	G	N1-C6-O6	-6.51	115.99	119.90
1	2A	297	C	C6-N1-C2	-6.51	117.69	120.30
1	1A	1378	G	C6-C5-N7	-6.51	126.49	130.40
1	1A	106	U	N3-C4-C5	6.51	118.51	114.60
1	1A	204	G	O5'-P-OP2	6.51	118.51	110.70
1	1A	2244	U	OP1-P-OP2	6.51	129.37	119.60
1	1A	2877	G	N1-C6-O6	6.51	123.81	119.90
32	2a	190	U	C6-N1-C2	-6.51	117.09	121.00
1	1A	1057	G	O5'-P-OP2	-6.51	99.84	105.70
1	2A	1047	G	N3-C4-C5	-6.51	125.35	128.60
1	1A	1495	G	C8-N9-C4	6.50	109.00	106.40
1	1A	1482	G	C5-C6-O6	6.50	132.50	128.60
1	2A	1652	A	C8-N9-C4	6.50	108.40	105.80
1	1A	1700	G	C8-N9-C4	-6.50	103.80	106.40
1	1A	1911	A	C2-N3-C4	-6.50	107.35	110.60
32	1a	1279	A	N7-C8-N9	6.50	117.05	113.80
1	1A	1537	G	C5-N7-C8	6.50	107.55	104.30
32	1a	753	A	OP1-P-O3'	6.50	119.50	105.20
1	1A	2288	G	C5-C6-N1	6.50	114.75	111.50
2	1B	98	G	O5'-P-OP2	-6.50	99.85	105.70
1	2A	920	G	N9-C4-C5	6.50	108.00	105.40
1	2A	1650	G	C8-N9-C4	-6.50	103.80	106.40
32	2a	1099	G	N3-C2-N2	-6.50	115.35	119.90
32	1a	576	G	C4-N9-C1'	6.50	134.94	126.50
1	1A	1371	G	N3-C2-N2	-6.49	115.35	119.90
1	1A	2671	G	C2-N3-C4	-6.49	108.65	111.90
1	1A	2609	G	C8-N9-C4	-6.49	103.80	106.40
1	2A	2553	G	C8-N9-C4	6.49	109.00	106.40
1	1A	491	G	C5-C6-N1	6.49	114.75	111.50
1	1A	2095	C	N3-C4-C5	6.49	124.50	121.90
1	1A	2262	G	O5'-P-OP2	-6.49	99.86	105.70
1	2A	1087	G	C4-N9-C1'	-6.49	118.06	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	115	G	N3-C4-C5	-6.49	125.36	128.60
1	2A	11	G	C5-C6-O6	-6.49	124.71	128.60
1	2A	237	C	OP2-P-O3'	6.49	119.48	105.20
1	2A	1766	U	O5'-P-OP2	-6.49	99.86	105.70
1	1A	1650	C	C5-C4-N4	-6.49	115.66	120.20
1	2A	1968	G	C5-C6-O6	-6.49	124.71	128.60
2	2B	41	U	C6-N1-C2	-6.49	117.11	121.00
1	1A	892	G	O5'-P-OP2	-6.48	99.86	105.70
1	1A	2165	C	C5-C6-N1	6.48	124.24	121.00
1	1A	2476	C	N1-C2-O2	-6.48	115.01	118.90
1	1A	359	C	C2-N3-C4	6.48	123.14	119.90
1	1A	2102	G	N1-C6-O6	-6.48	116.01	119.90
1	2A	845	G	O4'-C1'-N9	6.48	113.38	108.20
1	1A	1033	G	N9-C4-C5	6.48	107.99	105.40
1	1A	1959	A	O5'-P-OP2	-6.48	99.87	105.70
32	1a	1276	G	N7-C8-N9	6.48	116.34	113.10
1	2A	1650	G	N1-C6-O6	-6.48	116.01	119.90
32	2a	1158	C	N1-C2-O2	6.48	122.79	118.90
1	1A	2272	C	O5'-P-OP2	-6.48	99.87	105.70
1	1A	2292	G	C5-C6-O6	6.48	132.49	128.60
2	2B	115	G	N7-C8-N9	-6.48	109.86	113.10
1	1A	1822	A	OP2-P-O3'	6.47	119.44	105.20
1	2A	1323	U	OP1-P-O3'	6.47	119.44	105.20
1	2A	2182	G	N9-C4-C5	6.47	107.99	105.40
32	2a	343	U	O4'-C1'-N1	6.47	113.38	108.20
1	1A	1951	G	O5'-P-OP2	-6.47	99.87	105.70
1	1A	2251	G	N3-C2-N2	6.47	124.43	119.90
1	1A	2361	G	C8-N9-C4	6.47	108.99	106.40
1	1A	2627	U	N3-C4-O4	-6.47	114.87	119.40
32	1a	1054	C	C5-C6-N1	-6.47	117.76	121.00
1	1A	1204	C	N3-C4-N4	-6.47	113.47	118.00
1	1A	107	G	C6-C5-N7	6.47	134.28	130.40
1	1A	1390	G	N3-C2-N2	-6.47	115.37	119.90
1	1A	2618	C	C2-N3-C4	-6.47	116.67	119.90
1	2A	1388	G	C8-N9-C4	6.47	108.99	106.40
1	1A	2754	A	OP1-P-OP2	6.47	129.30	119.60
1	2A	1784	A	O5'-P-OP2	-6.47	99.88	105.70
1	1A	849	A	N1-C6-N6	-6.47	114.72	118.60
1	1A	1255	A	C8-N9-C4	-6.47	103.21	105.80
1	1A	2266	C	C6-N1-C2	-6.47	117.71	120.30
1	1A	1867	C	N3-C2-O2	-6.46	117.38	121.90
1	1A	2195	A	N1-C2-N3	6.46	132.53	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	383	U	N3-C2-O2	-6.46	117.67	122.20
1	2A	2179	C	C6-N1-C2	-6.46	117.71	120.30
1	2A	2358	G	O5'-P-OP2	-6.46	99.88	105.70
32	2a	1015	A	C8-N9-C4	-6.46	103.21	105.80
32	2a	1024	G	N1-C2-N2	6.46	122.02	116.20
1	1A	575	G	OP1-P-OP2	-6.46	109.91	119.60
32	1a	836	G	C5-C6-O6	-6.46	124.72	128.60
1	2A	157	U	N1-C2-O2	6.46	127.32	122.80
1	2A	2041	U	N3-C2-O2	6.46	126.72	122.20
1	1A	403	C	N1-C2-O2	6.46	122.78	118.90
1	1A	755	C	N3-C4-C5	6.46	124.48	121.90
1	1A	2623	U	N1-C2-O2	-6.46	118.28	122.80
1	1A	2632	C	OP1-P-OP2	6.46	129.29	119.60
32	1a	221	C	C6-N1-C2	-6.46	117.72	120.30
1	2A	1531	C	C6-N1-C2	-6.46	117.72	120.30
1	1A	940	C	C6-N1-C2	-6.46	117.72	120.30
1	1A	1302	G	C8-N9-C4	6.46	108.98	106.40
1	2A	2541	A	N1-C6-N6	6.46	122.48	118.60
1	1A	841	G	N1-C2-N2	-6.46	110.39	116.20
1	1A	2319	G	N1-C6-O6	6.46	123.78	119.90
1	1A	2741	U	N3-C4-O4	-6.46	114.88	119.40
32	1a	875	C	OP1-P-O3'	6.46	119.41	105.20
1	1A	1831	C	N1-C2-N3	6.46	123.72	119.20
32	1a	105	G	C4-C5-N7	6.46	113.38	110.80
1	2A	1689	A	C4-C5-N7	6.46	113.93	110.70
1	1A	2620	G	O5'-P-OP2	-6.46	99.89	105.70
1	1A	1816	A	N7-C8-N9	6.45	117.03	113.80
1	2A	2599	G	N1-C6-O6	-6.45	116.03	119.90
1	2A	753	C	N3-C4-N4	-6.45	113.48	118.00
32	2a	890	G	O4'-C1'-N9	6.45	113.36	108.20
1	1A	621	G	N1-C6-O6	-6.45	116.03	119.90
1	1A	1093	G	C4-N9-C1'	6.45	134.89	126.50
1	1A	2348	A	C5-C6-N6	-6.45	118.54	123.70
1	2A	510	C	OP1-P-OP2	6.45	129.27	119.60
1	2A	1963	U	N3-C2-O2	-6.45	117.69	122.20
1	1A	1147	U	N3-C2-O2	-6.45	117.69	122.20
1	1A	1270	C	N3-C4-C5	6.45	124.48	121.90
1	1A	2612	A	N9-C4-C5	6.45	108.38	105.80
32	1a	1084	G	O5'-P-OP2	-6.45	99.90	105.70
32	1a	399	G	N1-C6-O6	6.45	123.77	119.90
1	1A	2269	U	N1-C2-N3	6.44	118.77	114.90
1	2A	2128	C	N1-C2-O2	6.44	122.77	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	28	A	O5'-P-OP2	-6.44	99.90	105.70
1	1A	786	G	OP2-P-O3'	-6.44	91.03	105.20
1	1A	966	G	C5-C6-O6	6.44	132.47	128.60
1	2A	792	G	C2-N3-C4	6.44	115.12	111.90
1	2A	882	G	C4-N9-C1'	-6.44	118.13	126.50
1	1A	1429	C	N1-C2-O2	-6.44	115.04	118.90
1	1A	1806	U	C2-N3-C4	-6.44	123.14	127.00
1	1A	2621	U	C5-C6-N1	-6.44	119.48	122.70
32	1a	511	C	N3-C2-O2	-6.44	117.39	121.90
1	1A	621	G	OP2-P-O3'	6.44	119.36	105.20
1	1A	1511	C	N1-C2-O2	-6.44	115.04	118.90
1	1A	2262	G	C5-C6-O6	6.44	132.46	128.60
1	1A	2346	G	C5-C6-O6	-6.44	124.74	128.60
1	1A	1438	A	OP2-P-O3'	6.43	119.36	105.20
1	1A	2043	C	C6-N1-C2	6.43	122.87	120.30
32	1a	500	G	OP2-P-O3'	6.43	119.36	105.20
1	2A	35	G	N3-C2-N2	6.43	124.40	119.90
1	2A	127	A	O5'-P-OP2	-6.43	99.91	105.70
1	2A	2207	G	C4-C5-C6	6.43	122.66	118.80
32	2a	539	A	C8-N9-C4	-6.43	103.23	105.80
1	1A	1809	U	C6-N1-C2	6.43	124.86	121.00
1	1A	2112	G	C5-C6-O6	6.43	132.46	128.60
1	2A	1318	C	N1-C2-O2	-6.43	115.04	118.90
32	2a	662	G	N1-C6-O6	6.43	123.76	119.90
1	1A	1311	A	C8-N9-C4	-6.43	103.23	105.80
1	1A	1690	G	C5-C6-O6	6.43	132.46	128.60
1	1A	2115	G	C8-N9-C4	6.43	108.97	106.40
1	2A	2570	G	C4-C5-N7	-6.43	108.23	110.80
1	1A	813	C	C5-C6-N1	-6.43	117.79	121.00
1	2A	1280	G	OP2-P-O3'	6.43	119.34	105.20
1	2A	1905	C	O5'-P-OP2	-6.43	99.92	105.70
1	1A	2019	G	OP1-P-OP2	-6.43	109.96	119.60
1	1A	98	U	C6-N1-C1'	-6.42	112.21	121.20
1	1A	2222	C	C2-N3-C4	-6.42	116.69	119.90
1	1A	2579	G	O5'-P-OP1	-6.42	99.92	105.70
1	2A	254	G	C2-N3-C4	-6.42	108.69	111.90
1	2A	1497	U	C5-C6-N1	-6.42	119.49	122.70
1	1A	916	G	O5'-P-OP2	-6.42	99.92	105.70
1	2A	1653	G	OP1-P-OP2	6.42	129.24	119.60
1	2A	2463	C	O5'-P-OP2	-6.42	99.92	105.70
32	2a	802	A	C8-N9-C4	-6.42	103.23	105.80
1	1A	1299	A	C2-N3-C4	6.42	113.81	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2609	G	O5'-P-OP2	-6.42	99.92	105.70
1	1A	879	G	O5'-P-OP2	-6.42	99.92	105.70
1	1A	2573	A	N1-C6-N6	-6.42	114.75	118.60
2	1B	71	C	C5-C6-N1	-6.42	117.79	121.00
1	1A	2451	A	C6-N1-C2	6.42	122.45	118.60
32	1a	134	A	C5-C6-N6	-6.42	118.56	123.70
32	1a	366	C	OP1-P-OP2	6.42	129.22	119.60
32	2a	773	G	N3-C4-C5	6.42	131.81	128.60
1	1A	1604	C	C6-N1-C2	6.42	122.87	120.30
1	1A	1886	G	OP2-P-O3'	6.42	119.31	105.20
1	1A	2107	C	C2-N3-C4	-6.42	116.69	119.90
32	1a	190	U	OP1-P-OP2	-6.42	109.98	119.60
2	1B	1	U	C5-C4-O4	-6.41	122.05	125.90
1	1A	803	C	C4-C5-C6	6.41	120.61	117.40
1	1A	1356	G	C5-C6-O6	6.41	132.45	128.60
1	1A	1377	A	C8-N9-C4	-6.41	103.23	105.80
1	2A	1066	U	N1-C2-O2	-6.41	118.31	122.80
1	1A	1299	A	C8-N9-C4	6.41	108.36	105.80
32	1a	935	A	O5'-P-OP1	-6.41	99.93	105.70
1	2A	1992	G	O5'-P-OP2	-6.41	99.93	105.70
1	2A	2178	C	C6-N1-C2	-6.41	117.74	120.30
1	1A	105	C	N1-C2-O2	-6.41	115.06	118.90
1	1A	497	A	C8-N9-C4	-6.41	103.24	105.80
1	1A	1442	U	OP1-P-OP2	6.41	129.21	119.60
1	1A	1543	U	N3-C4-C5	6.41	118.44	114.60
1	2A	467	G	C5-N7-C8	6.41	107.50	104.30
1	1A	1411	A	N1-C6-N6	6.41	122.44	118.60
32	1a	1382	C	N3-C2-O2	-6.41	117.42	121.90
1	2A	2612	C	N3-C4-C5	6.41	124.46	121.90
32	2a	899	C	C6-N1-C2	6.41	122.86	120.30
32	2a	1125	U	N1-C2-O2	6.41	127.28	122.80
32	1a	528	C	C6-N1-C2	-6.40	117.74	120.30
1	2A	1252	G	O4'-C1'-N9	-6.40	103.08	108.20
32	2a	372	C	C2-N3-C4	6.40	123.10	119.90
1	1A	1020	C	N3-C2-O2	-6.40	117.42	121.90
32	1a	158	G	C8-N9-C1'	6.40	135.32	127.00
1	2A	1583	A	O5'-P-OP2	-6.40	99.94	105.70
1	1A	985	G	N3-C4-C5	-6.40	125.40	128.60
32	1a	143	A	O5'-P-OP1	-6.40	99.94	105.70
1	1A	918	U	N1-C2-O2	-6.40	118.32	122.80
32	1a	567	G	C8-N9-C4	-6.40	103.84	106.40
32	1a	820	U	C4-C5-C6	6.40	123.54	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	830	G	C5-C6-O6	-6.40	124.76	128.60
1	1A	1260	G	C5-C6-N1	6.40	114.70	111.50
1	1A	1876	G	C5-C6-O6	6.40	132.44	128.60
1	1A	2604	G	N1-C6-O6	-6.40	116.06	119.90
1	2A	1517	G	C5-C6-N1	-6.40	108.30	111.50
1	1A	2272	C	N3-C2-O2	-6.40	117.42	121.90
1	2A	784	A	OP1-P-O3'	6.40	119.27	105.20
1	1A	2295	C	N3-C4-C5	6.39	124.46	121.90
32	1a	603	U	O5'-P-OP2	6.39	118.37	110.70
1	2A	1328	G	C5-C6-O6	-6.39	124.76	128.60
1	1A	1633	A	C2-N3-C4	6.39	113.80	110.60
1	2A	1073	A	N1-C2-N3	6.39	132.50	129.30
2	2B	1	U	N1-C2-O2	6.39	127.27	122.80
32	2a	251	G	N3-C4-N9	6.39	129.84	126.00
1	2A	1983	C	N3-C4-N4	6.39	122.47	118.00
1	1A	572	A	N3-C4-C5	-6.39	122.33	126.80
1	1A	2053	A	C6-N1-C2	6.39	122.43	118.60
32	1a	813	U	OP1-P-OP2	-6.39	110.02	119.60
1	1A	617	U	C5-C6-N1	-6.39	119.51	122.70
1	1A	835	A	C4-C5-C6	6.39	120.19	117.00
1	2A	2850	A	N7-C8-N9	6.39	116.99	113.80
1	1A	1820	A	C8-N9-C4	6.39	108.36	105.80
1	2A	1091	G	C8-N9-C4	-6.39	103.84	106.40
1	2A	2145	C	C2-N3-C4	6.39	123.09	119.90
1	2A	2416	C	C6-N1-C2	-6.39	117.75	120.30
1	1A	1520	G	N3-C2-N2	6.38	124.37	119.90
1	1A	2072	C	OP2-P-O3'	6.38	119.25	105.20
2	1B	42	C	O5'-P-OP1	-6.38	99.95	105.70
1	2A	1354	A	O5'-P-OP2	-6.38	99.95	105.70
1	2A	1924	C	C6-N1-C2	-6.38	117.75	120.30
32	2a	458	C	N3-C2-O2	-6.38	117.43	121.90
32	1a	781	A	C4-C5-C6	-6.38	113.81	117.00
32	2a	442	C	C2-N1-C1'	6.38	125.82	118.80
32	1a	1370	G	C6-C5-N7	-6.38	126.57	130.40
32	2a	397	A	C8-N9-C4	-6.38	103.25	105.80
1	1A	751	G	C6-N1-C2	-6.38	121.27	125.10
1	1A	1725	G	N7-C8-N9	6.38	116.29	113.10
1	1A	2862	G	OP2-P-O3'	6.38	119.23	105.20
32	1a	1406	U	C2-N3-C4	-6.38	123.17	127.00
1	1A	1291	G	N9-C4-C5	6.38	107.95	105.40
1	1A	1823	G	N1-C6-O6	-6.38	116.07	119.90
1	1A	1856	A	C2-N3-C4	6.38	113.79	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2033	U	N3-C4-C5	-6.38	110.78	114.60
32	1a	901	A	N1-C6-N6	6.38	122.42	118.60
1	1A	354	A	N9-C1'-C2'	-6.38	104.99	112.00
1	1A	673	G	C5-C6-O6	6.37	132.42	128.60
1	1A	2260	C	N1-C2-O2	-6.37	115.08	118.90
2	1B	80	U	N3-C4-O4	-6.37	114.94	119.40
1	2A	2039	C	C6-N1-C2	-6.37	117.75	120.30
1	1A	1478	C	N1-C2-O2	-6.37	115.08	118.90
1	1A	2448	G	C5-C6-O6	6.37	132.42	128.60
32	1a	670	G	C4-C5-N7	-6.37	108.25	110.80
32	1a	1026	G	N7-C8-N9	6.37	116.28	113.10
1	2A	1617	C	C6-N1-C2	-6.37	117.75	120.30
1	2A	2475	C	C6-N1-C2	-6.37	117.75	120.30
1	2A	2896	C	C6-N1-C2	-6.37	117.75	120.30
1	1A	990	A	O5'-P-OP2	-6.37	99.97	105.70
1	1A	1024	G	N1-C6-O6	-6.37	116.08	119.90
1	1A	2092	G	C5-C6-O6	6.37	132.42	128.60
1	2A	652(T)	C	C5-C6-N1	6.37	124.19	121.00
1	2A	1606	G	OP1-P-O3'	6.37	119.22	105.20
1	1A	425	G	C2-N3-C4	-6.37	108.72	111.90
1	1A	441	C	O5'-P-OP2	-6.37	99.97	105.70
1	1A	874	U	N3-C4-C5	6.37	118.42	114.60
1	1A	2525	G	C6-N1-C2	6.37	128.92	125.10
1	2A	226	G	O4'-C1'-N9	6.37	113.30	108.20
32	1a	174	C	C5-C6-N1	6.37	124.18	121.00
1	2A	1913	A	N7-C8-N9	6.37	116.98	113.80
1	1A	196	A	C4-C5-N7	6.37	113.88	110.70
1	1A	369	A	C5-C6-N1	6.37	120.88	117.70
1	1A	843	C	N1-C2-N3	6.37	123.66	119.20
1	1A	1148	C	C5-C6-N1	6.37	124.18	121.00
1	1A	1316	C	N3-C4-N4	-6.37	113.54	118.00
32	1a	841	U	N1-C2-O2	6.37	127.26	122.80
1	2A	1586	A	O5'-P-OP2	6.37	118.34	110.70
1	2A	2783	G	C4-C5-N7	-6.37	108.25	110.80
1	1A	800	C	C5-C4-N4	6.36	124.65	120.20
1	1A	1739	U	C5-C6-N1	-6.36	119.52	122.70
1	1A	2419	G	C8-N9-C1'	-6.36	118.73	127.00
1	1A	2678	C	C6-N1-C2	-6.36	117.75	120.30
1	2A	675	A	C2-N3-C4	-6.36	107.42	110.60
1	2A	1373	A	N7-C8-N9	-6.36	110.62	113.80
32	2a	1406	U	O5'-P-OP1	6.36	118.33	110.70
1	1A	850	U	C5-C6-N1	-6.36	119.52	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1229	G	C5-C6-O6	6.36	132.42	128.60
1	1A	2102	G	C8-N9-C4	6.36	108.94	106.40
1	1A	2627	U	N1-C2-O2	6.36	127.25	122.80
32	1a	326	G	C5-C6-O6	6.36	132.42	128.60
1	2A	2689	U	N3-C2-O2	-6.36	117.75	122.20
1	1A	330	U	C2-N3-C4	6.36	130.82	127.00
1	2A	1032	A	O5'-P-OP2	-6.36	99.98	105.70
1	1A	836	A	OP1-P-OP2	-6.36	110.06	119.60
1	2A	2132	U	C5-C4-O4	6.36	129.72	125.90
1	1A	631	A	N1-C6-N6	-6.36	114.79	118.60
1	1A	1425	A	C4-C5-N7	6.36	113.88	110.70
1	1A	1653	C	N3-C4-N4	6.36	122.45	118.00
1	1A	1747	A	C8-N9-C4	6.36	108.34	105.80
1	1A	1861	C	N3-C4-C5	6.36	124.44	121.90
1	1A	1950	A	O5'-P-OP1	-6.36	99.98	105.70
1	1A	2207	C	N1-C2-O2	6.36	122.71	118.90
1	1A	2445	A	C2-N3-C4	6.36	113.78	110.60
1	1A	2790	G	C5-C6-N1	6.36	114.68	111.50
32	1a	576	G	C8-N9-C1'	-6.36	118.73	127.00
1	1A	497	A	N9-C4-C5	6.36	108.34	105.80
1	1A	762	G	N3-C4-N9	6.35	129.81	126.00
1	1A	1863	C	N1-C2-N3	6.35	123.65	119.20
32	2a	404	U	O5'-P-OP2	-6.35	99.98	105.70
1	1A	1668	G	OP1-P-OP2	6.35	129.13	119.60
32	1a	1035	A	C8-N9-C4	-6.35	103.26	105.80
1	1A	1573	G	C4-C5-N7	-6.35	108.26	110.80
1	1A	1993	A	C2-N3-C4	-6.35	107.42	110.60
1	1A	2457	G	N1-C6-O6	-6.35	116.09	119.90
1	1A	2565	G	N3-C4-N9	6.35	129.81	126.00
1	2A	100	G	C8-N9-C4	6.35	108.94	106.40
1	2A	958	U	N1-C2-N3	6.35	118.71	114.90
32	2a	533	A	O5'-P-OP2	6.35	118.32	110.70
32	1a	603	U	O5'-P-OP1	-6.35	99.99	105.70
1	2A	1497	U	N3-C4-O4	-6.35	114.96	119.40
1	1A	1965	U	N1-C2-N3	6.35	118.71	114.90
1	1A	2638	C	C6-N1-C2	6.35	122.84	120.30
32	1a	1097	C	N3-C2-O2	-6.35	117.46	121.90
1	2A	2058	A	C4-C5-C6	6.35	120.17	117.00
1	1A	87	G	N3-C2-N2	-6.34	115.46	119.90
1	1A	700	A	C5-C6-N6	-6.34	118.62	123.70
1	1A	700	A	N1-C6-N6	6.34	122.41	118.60
1	1A	2204	G	N3-C4-N9	-6.34	122.19	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	821	G	C6-C5-N7	-6.34	126.59	130.40
32	1a	1292	U	O5'-P-OP2	-6.34	99.99	105.70
1	1A	616	G	C4-C5-N7	-6.34	108.26	110.80
1	1A	2118	U	OP2-P-O3'	6.34	119.15	105.20
32	1a	773	G	N3-C4-N9	-6.34	122.19	126.00
1	2A	308	G	C5-C6-O6	-6.34	124.79	128.60
1	2A	2893	G	N3-C2-N2	6.34	124.34	119.90
1	1A	556	C	OP1-P-OP2	-6.34	110.09	119.60
1	1A	1312	G	C5-C6-O6	-6.34	124.80	128.60
1	2A	2336	A	O5'-P-OP2	-6.34	99.99	105.70
1	1A	1714	G	N1-C6-O6	-6.34	116.10	119.90
1	1A	1902	C	C6-N1-C2	-6.34	117.76	120.30
32	1a	68	G	O5'-P-OP2	-6.34	100.00	105.70
1	2A	1071	G	N1-C6-O6	6.34	123.70	119.90
1	2A	1362	C	O5'-P-OP1	-6.34	100.00	105.70
1	2A	2273	A	O5'-P-OP2	-6.34	99.99	105.70
1	1A	451	G	N1-C6-O6	-6.34	116.10	119.90
1	2A	602	G	O5'-P-OP2	-6.34	100.00	105.70
1	2A	1807	G	O5'-P-OP2	-6.34	100.00	105.70
1	1A	1756	U	N1-C2-O2	-6.34	118.36	122.80
32	2a	1030(D)	A	C8-N9-C4	-6.34	103.27	105.80
1	1A	1725	G	C6-N1-C2	-6.33	121.30	125.10
1	1A	677	C	C2-N3-C4	-6.33	116.73	119.90
1	1A	1293	A	N7-C8-N9	6.33	116.97	113.80
1	1A	2636	G	N3-C2-N2	6.33	124.33	119.90
32	1a	1150	U	C5-C6-N1	6.33	125.87	122.70
1	1A	733	G	N3-C2-N2	6.33	124.33	119.90
1	1A	1221	G	C8-N9-C1'	6.33	135.23	127.00
1	1A	2044	U	O5'-P-OP2	6.33	118.30	110.70
32	1a	625	G	O5'-P-OP1	-6.33	100.00	105.70
32	1a	1505	G	C4-C5-N7	-6.33	108.27	110.80
1	1A	255	G	C4-C5-N7	6.33	113.33	110.80
1	1A	330	U	C5-C4-O4	6.33	129.70	125.90
1	1A	364	A	O5'-P-OP1	-6.33	100.00	105.70
1	1A	1507	A	O4'-C1'-N9	6.33	113.26	108.20
1	1A	1977	U	C5-C6-N1	-6.33	119.54	122.70
1	1A	2283	G	N3-C2-N2	6.33	124.33	119.90
1	1A	1115	A	C8-N9-C4	6.33	108.33	105.80
1	2A	1670	C	OP1-P-O3'	6.33	119.11	105.20
32	2a	777	A	O5'-P-OP2	-6.33	100.01	105.70
32	2a	1375	A	C8-N9-C4	-6.33	103.27	105.80
1	1A	1340	U	C4-C5-C6	6.32	123.49	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2511	C	N3-C4-N4	6.32	122.43	118.00
32	1a	902	G	OP2-P-O3'	6.32	119.11	105.20
32	1a	1125	U	O5'-P-OP1	-6.32	100.01	105.70
1	2A	746	A	O5'-P-OP1	-6.32	100.01	105.70
1	2A	1062	G	O4'-C1'-N9	6.32	113.26	108.20
1	2A	1261	C	C2-N1-C1'	-6.32	111.84	118.80
1	1A	2523	U	C2-N3-C4	-6.32	123.21	127.00
1	1A	2582	G	C4-C5-N7	-6.32	108.27	110.80
1	2A	1992	G	C5-C6-O6	-6.32	124.81	128.60
1	1A	1635	C	N3-C4-C5	6.32	124.43	121.90
1	1A	1814	A	C6-C5-N7	6.32	136.72	132.30
1	1A	226	C	C2-N3-C4	-6.32	116.74	119.90
1	1A	486	A	C5-C6-N6	6.32	128.75	123.70
32	1a	1184	G	N1-C6-O6	6.32	123.69	119.90
1	2A	602	G	N3-C4-N9	6.32	129.79	126.00
1	1A	2828	G	C5-C6-O6	6.32	132.39	128.60
1	1A	2881	C	N3-C2-O2	6.32	126.32	121.90
1	1A	747	G	N1-C2-N2	-6.31	110.52	116.20
1	1A	1142	A	O4'-C1'-N9	6.31	113.25	108.20
1	1A	837	C	N3-C2-O2	6.31	126.32	121.90
1	1A	877	G	N1-C6-O6	-6.31	116.11	119.90
1	1A	1154	U	N3-C4-O4	6.31	123.82	119.40
1	1A	1662	A	O5'-P-OP1	-6.31	100.02	105.70
1	2A	1062	G	N7-C8-N9	6.31	116.26	113.10
1	1A	816	G	OP2-P-O3'	6.31	119.08	105.20
1	1A	906	G	C8-N9-C4	6.31	108.92	106.40
1	1A	2551	C	C6-N1-C2	6.31	122.82	120.30
4	1E	119	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	1A	740	C	N3-C2-O2	-6.31	117.48	121.90
1	1A	2091	G	C6-N1-C2	-6.31	121.31	125.10
1	1A	335	A	O5'-P-OP1	6.30	118.27	110.70
1	1A	640	A	OP1-P-OP2	6.30	129.06	119.60
1	1A	1383	G	C4-C5-N7	-6.30	108.28	110.80
1	1A	1833	A	O5'-P-OP2	6.30	118.27	110.70
1	1A	2023	A	C4-C5-N7	-6.30	107.55	110.70
1	1A	2201	C	C5-C6-N1	6.30	124.15	121.00
32	1a	1441	G	C5-C6-O6	6.30	132.38	128.60
1	2A	272(E)	G	C8-N9-C4	6.30	108.92	106.40
1	1A	365	G	N9-C4-C5	6.30	107.92	105.40
1	2A	395	U	N1-C2-O2	6.30	127.21	122.80
1	1A	578	U	O4'-C1'-N1	6.30	113.24	108.20
1	1A	1072	U	N3-C2-O2	-6.30	117.79	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1451	U	C5-C4-O4	6.30	129.68	125.90
1	1A	2227	G	N3-C4-C5	6.30	131.75	128.60
32	1a	663	A	O5'-P-OP1	-6.30	100.03	105.70
32	2a	1475	G	N7-C8-N9	6.30	116.25	113.10
1	1A	906	G	C4-N9-C1'	-6.30	118.31	126.50
1	2A	1323	U	N1-C2-O2	-6.30	118.39	122.80
1	1A	980	C	C4-C5-C6	6.30	120.55	117.40
1	1A	1814	A	C4-C5-C6	-6.30	113.85	117.00
32	2a	802	A	N7-C8-N9	6.30	116.95	113.80
1	1A	744	C	N3-C4-N4	-6.30	113.59	118.00
1	1A	2277	U	N3-C4-C5	-6.30	110.82	114.60
1	1A	2308	U	N3-C4-O4	6.30	123.81	119.40
1	1A	2400	A	C8-N9-C4	-6.30	103.28	105.80
1	1A	2475	C	C2-N3-C4	-6.30	116.75	119.90
1	1A	2879	G	C8-N9-C4	-6.30	103.88	106.40
1	1A	821	A	N1-C6-N6	-6.29	114.82	118.60
1	2A	366	C	N1-C2-O2	-6.29	115.12	118.90
1	2A	1427	A	C6-N1-C2	-6.29	114.82	118.60
1	1A	505	A	C5-C6-N6	6.29	128.74	123.70
1	1A	1845	G	C5-C6-O6	-6.29	124.82	128.60
1	1A	2072	C	N1-C2-O2	-6.29	115.12	118.90
1	1A	2411	G	O5'-P-OP2	-6.29	100.03	105.70
32	1a	814	A	O5'-P-OP2	6.29	118.25	110.70
1	2A	1595	G	O5'-P-OP1	-6.29	100.03	105.70
1	1A	480	A	N9-C4-C5	6.29	108.32	105.80
1	1A	722	A	C4-C5-N7	6.29	113.84	110.70
1	1A	1031	C	O5'-P-OP2	-6.29	100.04	105.70
1	1A	2079	A	C5-N7-C8	6.29	107.05	103.90
32	1a	768	A	N9-C4-C5	-6.29	103.28	105.80
1	2A	33	U	N1-C2-O2	6.29	127.20	122.80
1	2A	1283	G	C8-N9-C4	6.29	108.92	106.40
1	2A	2074	U	C5-C6-N1	6.29	125.85	122.70
1	1A	2272	C	C5-C4-N4	6.29	124.60	120.20
1	1A	8	A	O5'-P-OP2	6.29	118.25	110.70
1	1A	500	G	N1-C6-O6	-6.29	116.13	119.90
1	1A	1410	G	N1-C6-O6	-6.29	116.13	119.90
32	1a	1521	G	OP1-P-OP2	6.29	129.03	119.60
1	2A	1187	G	O5'-P-OP1	6.29	118.25	110.70
1	1A	594	A	C2-N3-C4	6.29	113.74	110.60
1	1A	666	C	C5-C6-N1	6.29	124.14	121.00
1	1A	799	A	N9-C4-C5	-6.29	103.29	105.80
1	1A	850	U	N3-C2-O2	-6.29	117.80	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2137	G	N3-C4-C5	-6.29	125.46	128.60
11	1P	39	LYS	CD-CE-NZ	-6.29	97.25	111.70
1	2A	988	A	C4-C5-N7	6.29	113.84	110.70
1	2A	1445(A)	C	O5'-P-OP1	-6.29	100.04	105.70
32	2a	1482	G	N1-C6-O6	-6.29	116.13	119.90
1	1A	214	A	O5'-P-OP1	6.28	118.24	110.70
1	1A	1833	A	N7-C8-N9	-6.28	110.66	113.80
19	1X	73	ARG	NE-CZ-NH1	-6.28	117.16	120.30
32	1a	1411	C	C6-N1-C2	6.28	122.81	120.30
1	1A	194	G	N1-C2-N2	-6.28	110.55	116.20
1	1A	476	G	N9-C4-C5	-6.28	102.89	105.40
1	1A	477	C	C2-N3-C4	-6.28	116.76	119.90
1	1A	786	G	C5-C6-O6	-6.28	124.83	128.60
1	2A	1256	G	N9-C4-C5	-6.28	102.89	105.40
1	2A	1662	C	C2-N3-C4	-6.28	116.76	119.90
32	2a	1452	C	N1-C2-O2	6.28	122.67	118.90
1	2A	35	G	N1-C2-N2	-6.28	110.55	116.20
32	2a	798	G	C8-N9-C4	-6.28	103.89	106.40
1	1A	292	G	N3-C4-C5	6.28	131.74	128.60
1	1A	1709	C	C6-N1-C2	6.28	122.81	120.30
1	1A	1958	A	N9-C4-C5	-6.28	103.29	105.80
32	1a	1513	A	N1-C2-N3	-6.28	126.16	129.30
1	2A	1450(A)	C	C6-N1-C2	-6.28	117.79	120.30
1	1A	573	G	C8-N9-C4	-6.28	103.89	106.40
1	1A	2029	C	C5-C4-N4	6.28	124.59	120.20
1	1A	2619	G	C5-C6-O6	6.28	132.37	128.60
1	2A	226	G	C5-C6-O6	-6.28	124.83	128.60
32	2a	1037	C	C6-N1-C2	-6.27	117.79	120.30
2	1B	102	A	N1-C2-N3	6.27	132.44	129.30
32	1a	449	C	N1-C2-O2	6.27	122.66	118.90
1	1A	553	A	N3-C4-N9	6.27	132.41	127.40
32	1a	163	C	C6-N1-C2	-6.27	117.79	120.30
32	1a	284	G	C8-N9-C4	6.27	108.91	106.40
1	2A	1838	C	C4-C5-C6	6.27	120.53	117.40
1	2A	2372	G	N1-C6-O6	6.27	123.66	119.90
1	1A	1921	G	C5-C6-N1	6.27	114.63	111.50
32	1a	1436	U	C5-C4-O4	-6.27	122.14	125.90
1	1A	2802	C	C6-N1-C1'	6.27	128.32	120.80
32	1a	1466	C	C6-N1-C2	-6.27	117.79	120.30
1	1A	1104	G	C5-C6-O6	-6.26	124.84	128.60
1	1A	1221	G	C6-C5-N7	6.26	134.16	130.40
1	1A	1256	U	O5'-P-OP2	6.26	118.22	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2273	C	C6-N1-C2	-6.26	117.79	120.30
1	2A	2162	G	C4-N9-C1'	6.26	134.64	126.50
1	2A	2238	G	C5-C6-O6	-6.26	124.84	128.60
32	1a	187	C	C5-C6-N1	6.26	124.13	121.00
1	2A	1518	U	C5-C4-O4	6.26	129.66	125.90
1	1A	734	C	C2-N3-C4	-6.26	116.77	119.90
1	1A	960	C	O5'-P-OP2	-6.26	100.06	105.70
1	1A	1391	C	N1-C2-O2	6.26	122.66	118.90
2	2B	33	G	N1-C6-O6	6.26	123.66	119.90
1	1A	498	A	O5'-P-OP2	-6.26	100.07	105.70
32	1a	1514	C	C6-N1-C2	-6.26	117.80	120.30
32	1a	670	G	C5-C6-O6	6.26	132.35	128.60
1	1A	2279	A	OP1-P-OP2	6.26	128.99	119.60
32	1a	780	A	N1-C2-N3	-6.26	126.17	129.30
32	1a	1062	U	N3-C2-O2	-6.26	117.82	122.20
1	1A	1522	G	N9-C4-C5	6.25	107.90	105.40
1	2A	391	G	C5-C6-N1	6.25	114.63	111.50
1	1A	2591	C	C5-C6-N1	-6.25	117.87	121.00
1	1A	2858	G	N7-C8-N9	-6.25	109.97	113.10
32	1a	404	U	C2-N1-C1'	6.25	125.20	117.70
1	2A	1437	C	N1-C2-O2	6.25	122.65	118.90
32	2a	295	C	C5-C6-N1	-6.25	117.87	121.00
1	2A	806	C	N1-C2-O2	-6.25	115.15	118.90
1	1A	234	G	OP1-P-O3'	6.25	118.95	105.20
1	1A	820	U	C6-N1-C2	6.25	124.75	121.00
1	1A	1690	G	C4-C5-N7	-6.25	108.30	110.80
1	2A	1791	A	N7-C8-N9	6.25	116.92	113.80
1	2A	1826	G	N1-C6-O6	-6.25	116.15	119.90
1	1A	413	G	N7-C8-N9	6.25	116.22	113.10
1	1A	515	G	N1-C6-O6	6.25	123.65	119.90
1	1A	1130	A	C4-C5-N7	-6.25	107.58	110.70
1	1A	2610	A	N1-C6-N6	-6.25	114.85	118.60
32	1a	1019	C	C6-N1-C2	-6.25	117.80	120.30
1	1A	1437	U	C2-N3-C4	-6.25	123.25	127.00
1	1A	1533	G	OP1-P-O3'	6.25	118.94	105.20
1	2A	2603	G	O5'-P-OP1	6.25	118.19	110.70
1	1A	2324	U	O5'-P-OP2	6.24	118.19	110.70
1	2A	2744	G	O5'-P-OP2	-6.24	100.08	105.70
1	1A	2802	C	N3-C4-N4	-6.24	113.63	118.00
32	1a	1529	G	O4'-C1'-N9	6.24	113.19	108.20
1	2A	57	C	C6-N1-C2	-6.24	117.80	120.30
1	2A	2177	C	C2-N1-C1'	6.24	125.67	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1495	U	C2-N3-C4	6.24	130.75	127.00
1	1A	492	A	C5-C6-N1	6.24	120.82	117.70
1	1A	802	C	N3-C4-C5	-6.24	119.40	121.90
32	1a	874	G	N7-C8-N9	-6.24	109.98	113.10
32	1a	919	A	N1-C6-N6	-6.24	114.86	118.60
32	1a	1243	C	N1-C2-O2	-6.24	115.16	118.90
1	2A	645	C	C2-N3-C4	6.24	123.02	119.90
1	2A	655	A	N7-C8-N9	6.24	116.92	113.80
1	1A	1024	G	C4-C5-N7	-6.24	108.31	110.80
32	1a	687	A	P-O3'-C3'	6.24	127.19	119.70
32	1a	1053	G	C8-N9-C4	6.24	108.89	106.40
1	2A	1091	G	N3-C4-C5	-6.24	125.48	128.60
1	2A	2613	U	N3-C2-O2	-6.24	117.83	122.20
2	2B	1	U	C5-C6-N1	6.24	125.82	122.70
1	1A	1411	A	C5-C6-N6	-6.24	118.71	123.70
32	1a	93	G	C2-N3-C4	6.24	115.02	111.90
1	2A	408	G	O5'-P-OP2	-6.24	100.09	105.70
1	1A	89	U	C5-C6-N1	-6.23	119.58	122.70
1	1A	2634	C	N3-C4-C5	6.23	124.39	121.90
32	1a	781	A	C4-C5-N7	6.23	113.82	110.70
1	2A	2422	A	C2-N3-C4	-6.23	107.48	110.60
1	1A	1340	U	C5-C6-N1	-6.23	119.58	122.70
1	1A	2568	C	C2-N3-C4	-6.23	116.78	119.90
1	2A	483	A	OP1-P-OP2	6.23	128.95	119.60
1	1A	1953	U	N3-C4-C5	6.23	118.34	114.60
1	2A	988	A	N7-C8-N9	6.23	116.92	113.80
1	2A	2426	A	N9-C4-C5	-6.23	103.31	105.80
32	2a	1500	A	C6-N1-C2	6.23	122.34	118.60
1	2A	1477	A	O5'-P-OP2	-6.23	100.09	105.70
1	2A	2804	C	C6-N1-C2	-6.23	117.81	120.30
1	1A	82	G	C5-C6-O6	-6.23	124.86	128.60
1	1A	791	G	C5-C6-O6	6.23	132.34	128.60
1	1A	2234	G	N3-C4-C5	6.23	131.71	128.60
1	1A	2245	U	N3-C2-O2	-6.23	117.84	122.20
1	2A	1340	U	C2-N3-C4	-6.23	123.26	127.00
1	2A	1689	A	C5-C6-N6	-6.23	118.72	123.70
1	1A	201	G	O5'-P-OP1	6.23	118.17	110.70
1	1A	1091	A	N1-C6-N6	-6.23	114.86	118.60
32	1a	1054	C	N3-C4-N4	-6.23	113.64	118.00
1	1A	1228	G	N1-C6-O6	-6.22	116.17	119.90
2	2B	54	G	C8-N9-C4	-6.22	103.91	106.40
32	2a	848	C	C6-N1-C2	-6.22	117.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	171	A	O5'-P-OP2	6.22	118.17	110.70
1	1A	1573	G	N3-C2-N2	-6.22	115.54	119.90
1	2A	572	A	N9-C4-C5	6.22	108.29	105.80
1	2A	587	C	O4'-C1'-N1	-6.22	103.22	108.20
1	1A	1690	G	C2-N3-C4	6.22	115.01	111.90
1	1A	1851	U	N1-C2-N3	6.22	118.63	114.90
32	1a	191	G	C4-C5-N7	-6.22	108.31	110.80
32	1a	1348	U	O5'-P-OP2	-6.22	100.10	105.70
1	1A	641	G	N1-C2-N2	-6.22	110.60	116.20
1	2A	1652	A	N3-C4-C5	6.22	131.15	126.80
1	2A	2505	G	C8-N9-C4	-6.22	103.91	106.40
1	1A	594	A	O5'-P-OP1	-6.22	100.10	105.70
1	2A	614	U	N3-C2-O2	-6.22	117.85	122.20
1	2A	2142	C	O4'-C1'-N1	6.22	113.17	108.20
1	1A	821	A	C2-N3-C4	6.22	113.71	110.60
1	1A	2858	G	N9-C4-C5	6.22	107.89	105.40
1	2A	192	C	N3-C4-N4	6.22	122.35	118.00
1	1A	546	G	N1-C6-O6	-6.21	116.17	119.90
32	2a	810	C	N3-C4-C5	6.21	124.39	121.90
1	2A	250	G	N1-C6-O6	-6.21	116.17	119.90
32	2a	560	U	C5-C6-N1	6.21	125.81	122.70
1	1A	1183	G	C4-C5-N7	-6.21	108.31	110.80
1	1A	1995	G	OP1-P-OP2	6.21	128.92	119.60
1	1A	2703	C	N3-C4-C5	6.21	124.38	121.90
1	2A	964	C	O5'-P-OP2	-6.21	100.11	105.70
1	2A	2425	A	N7-C8-N9	6.21	116.91	113.80
32	2a	1085	U	O5'-P-OP1	-6.21	100.11	105.70
1	1A	1766	G	N3-C2-N2	6.21	124.25	119.90
1	1A	2455	C	N1-C2-O2	-6.21	115.17	118.90
1	1A	2460	A	C2-N3-C4	6.21	113.70	110.60
1	2A	1394	U	O5'-P-OP2	6.21	118.15	110.70
1	1A	217	A	C4-N9-C1'	-6.21	115.13	126.30
1	1A	1989	C	O5'-P-OP2	-6.21	100.11	105.70
1	2A	1610	A	N1-C6-N6	6.21	122.32	118.60
32	2a	883	C	C4-C5-C6	6.21	120.50	117.40
1	1A	1455	C	C5-C6-N1	-6.21	117.90	121.00
1	1A	387	G	N3-C4-N9	-6.20	122.28	126.00
1	1A	1006	C	OP1-P-OP2	6.20	128.91	119.60
1	2A	415	A	O5'-P-OP1	6.20	118.14	110.70
32	2a	189(J)	G	C8-N9-C4	6.20	108.88	106.40
1	1A	1430	A	N9-C4-C5	6.20	108.28	105.80
1	1A	1736	A	C8-N9-C4	-6.20	103.32	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	251	A	C4-C5-C6	6.20	120.10	117.00
1	2A	1121	C	O5'-P-OP2	-6.20	100.12	105.70
1	2A	1992	G	N3-C4-N9	6.20	129.72	126.00
1	2A	2113	U	C5-C6-N1	6.20	125.80	122.70
1	2A	2334	G	C5-C6-O6	-6.20	124.88	128.60
32	2a	534	U	O5'-P-OP2	-6.20	100.12	105.70
32	2a	1528	U	C6-N1-C2	6.20	124.72	121.00
1	1A	61	C	OP1-P-OP2	6.20	128.90	119.60
1	1A	554	A	C5-N7-C8	-6.20	100.80	103.90
1	1A	1250	U	C5-C4-O4	-6.20	122.18	125.90
1	1A	1391	C	N3-C2-O2	-6.20	117.56	121.90
1	1A	2283	G	N3-C4-N9	6.20	129.72	126.00
1	1A	2776	G	OP2-P-O3'	6.20	118.83	105.20
32	1a	353	A	C4-C5-N7	6.20	113.80	110.70
32	2a	792	A	O4'-C1'-N9	6.20	113.16	108.20
1	1A	406	G	N7-C8-N9	-6.20	110.00	113.10
1	1A	2101	U	N1-C2-O2	-6.20	118.46	122.80
1	2A	12	U	C6-N1-C2	-6.20	117.28	121.00
32	2a	45	U	C6-N1-C2	6.20	124.72	121.00
32	2a	93	G	O4'-C1'-N9	6.20	113.16	108.20
32	2a	1182	G	N3-C4-C5	6.20	131.70	128.60
1	1A	1371	G	C4-C5-N7	-6.20	108.32	110.80
1	1A	1556	A	N1-C6-N6	6.20	122.32	118.60
1	1A	2429	C	N3-C4-C5	-6.20	119.42	121.90
1	1A	2639	G	N1-C6-O6	6.20	123.62	119.90
32	1a	901	A	N1-C2-N3	6.20	132.40	129.30
32	2a	1391	U	C5-C4-O4	6.20	129.62	125.90
32	2a	1501	C	N1-C2-O2	-6.20	115.18	118.90
1	1A	2368	C	N3-C2-O2	6.19	126.24	121.90
32	1a	487	A	C8-N9-C4	6.19	108.28	105.80
32	2a	1465	C	N3-C4-N4	6.19	122.33	118.00
1	1A	992	G	N9-C4-C5	6.19	107.88	105.40
1	1A	2134	G	C2-N3-C4	6.19	115.00	111.90
1	1A	2546	A	N1-C6-N6	6.19	122.31	118.60
32	1a	545	C	O5'-P-OP1	-6.19	100.13	105.70
32	1a	1258	G	C2-N3-C4	6.19	115.00	111.90
1	2A	1047	G	C2-N3-C4	6.19	115.00	111.90
1	2A	2207	G	C5-N7-C8	-6.19	101.20	104.30
1	1A	1050	C	C5-C6-N1	-6.19	117.90	121.00
1	1A	2048	C	N3-C4-N4	6.19	122.33	118.00
1	1A	2449	U	C5-C6-N1	-6.19	119.61	122.70
1	1A	2579	G	N1-C6-O6	-6.19	116.19	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	895	G	C5-C6-O6	6.19	132.31	128.60
1	2A	1700	A	O5'-P-OP2	6.19	118.13	110.70
1	2A	2206	G	C8-N9-C4	6.19	108.88	106.40
1	2A	2268	A	O5'-P-OP1	-6.19	100.13	105.70
1	1A	1696	G	C8-N9-C4	-6.19	103.92	106.40
1	2A	584	C	N1-C2-O2	-6.19	115.19	118.90
1	2A	1336	A	N1-C6-N6	-6.19	114.89	118.60
32	2a	1030	C	C6-N1-C2	-6.19	117.83	120.30
32	2a	1062	U	N3-C2-O2	-6.19	117.87	122.20
32	1a	971	G	C5-C6-N1	-6.19	108.41	111.50
1	1A	1440	U	O5'-P-OP2	6.18	118.12	110.70
1	1A	2050	U	C5-C4-O4	6.18	129.61	125.90
1	1A	2654	G	C8-N9-C4	-6.18	103.93	106.40
1	2A	80	G	N1-C6-O6	-6.18	116.19	119.90
1	1A	215	G	N3-C4-N9	-6.18	122.29	126.00
32	1a	1046	A	C5-C6-N6	-6.18	118.75	123.70
1	2A	1813	G	C8-N9-C4	6.18	108.87	106.40
1	1A	1283	A	N9-C4-C5	6.18	108.27	105.80
1	1A	2082	A	C5-C6-N6	6.18	128.64	123.70
32	1a	1436	U	N1-C2-N3	6.18	118.61	114.90
1	2A	1170	G	C5-C6-N1	-6.18	108.41	111.50
1	2A	2140	C	C2-N3-C4	6.18	122.99	119.90
1	1A	2249	G	N1-C2-N2	-6.18	110.64	116.20
1	1A	2691	A	C2-N3-C4	6.18	113.69	110.60
30	18	42	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	2A	678	C	C2-N3-C4	-6.18	116.81	119.90
1	2A	704	G	O4'-C1'-N9	6.18	113.14	108.20
1	2A	741	G	N3-C4-N9	-6.18	122.29	126.00
32	2a	1510	U	C5-C4-O4	-6.18	122.19	125.90
1	1A	909	G	OP2-P-O3'	6.18	118.79	105.20
32	1a	157	G	C4-C5-N7	-6.18	108.33	110.80
1	1A	1151	U	C6-N1-C2	6.18	124.70	121.00
1	1A	2092	G	O5'-P-OP2	-6.18	100.14	105.70
1	2A	791	C	C5-C6-N1	-6.18	117.91	121.00
1	2A	1670	C	N3-C4-C5	-6.18	119.43	121.90
1	1A	1298	G	C2-N3-C4	-6.17	108.81	111.90
1	2A	2017	U	O5'-P-OP1	-6.17	100.14	105.70
32	2a	301	G	O5'-P-OP1	6.17	118.11	110.70
1	1A	555	G	C4-C5-N7	6.17	113.27	110.80
1	1A	1567	G	N7-C8-N9	6.17	116.19	113.10
1	2A	271(Y)	U	O4'-C1'-N1	6.17	113.14	108.20
1	1A	1343	C	N1-C2-O2	-6.17	115.20	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	647	C	C6-N1-C2	-6.17	117.83	120.30
32	1a	452	A	O4'-C1'-N9	6.17	113.13	108.20
32	1a	718	G	O5'-P-OP2	6.17	118.10	110.70
32	1a	1151	A	OP1-P-OP2	6.17	128.85	119.60
1	2A	1838	C	N1-C2-N3	6.17	123.52	119.20
1	2A	2263	C	N3-C2-O2	6.17	126.22	121.90
1	2A	2346	A	O5'-P-OP1	-6.17	100.15	105.70
1	2A	2592	G	N1-C6-O6	-6.17	116.20	119.90
1	1A	12	U	C6-N1-C2	-6.17	117.30	121.00
1	1A	842	C	N3-C4-N4	-6.17	113.68	118.00
1	1A	1375	U	N3-C4-O4	-6.17	115.08	119.40
1	1A	1543	U	O4'-C1'-N1	6.17	113.13	108.20
1	2A	2392	A	O5'-P-OP1	-6.17	100.15	105.70
32	1a	174	C	N3-C2-O2	-6.17	117.58	121.90
1	2A	44	G	O5'-P-OP2	-6.17	100.15	105.70
32	2a	1063	C	C6-N1-C2	-6.17	117.83	120.30
1	1A	504	A	N7-C8-N9	6.16	116.88	113.80
1	2A	915	C	N1-C2-O2	6.16	122.60	118.90
1	2A	1837	C	O5'-P-OP1	-6.16	100.15	105.70
1	1A	448	U	N1-C2-O2	-6.16	118.49	122.80
1	2A	1231	G	C5-C6-N1	-6.16	108.42	111.50
32	2a	768	A	N1-C2-N3	6.16	132.38	129.30
1	1A	860	U	N3-C4-O4	-6.16	115.09	119.40
1	1A	1669	G	C4-C5-N7	-6.16	108.33	110.80
1	1A	1911	A	OP1-P-OP2	6.16	128.84	119.60
1	1A	2091	G	O5'-P-OP1	6.16	118.09	110.70
32	1a	754	C	N3-C2-O2	-6.16	117.59	121.90
1	2A	50	U	C6-N1-C2	6.16	124.70	121.00
1	2A	1320	C	C2-N3-C4	-6.16	116.82	119.90
1	2A	1320	C	C6-N1-C2	6.16	122.76	120.30
1	2A	1997	G	OP2-P-O3'	6.16	118.75	105.20
32	2a	876	G	C6-C5-N7	6.16	134.10	130.40
1	1A	372	G	O5'-P-OP2	-6.16	100.16	105.70
1	1A	2590	G	N1-C6-O6	-6.16	116.20	119.90
1	2A	1005	C	O5'-P-OP1	-6.16	100.16	105.70
1	1A	2782	C	N1-C2-O2	-6.16	115.21	118.90
1	1A	2835	C	C6-N1-C2	6.16	122.76	120.30
32	1a	1252	A	N1-C6-N6	-6.16	114.91	118.60
1	2A	2508	G	C5-C6-N1	6.16	114.58	111.50
32	2a	820	U	N1-C2-O2	-6.16	118.49	122.80
32	1a	1134	G	C8-N9-C4	-6.16	103.94	106.40
1	1A	31	C	N1-C2-O2	-6.15	115.21	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1054	C	N3-C4-C5	-6.15	119.44	121.90
1	2A	2786	U	C5-C6-N1	6.15	125.78	122.70
1	1A	826	U	N1-C2-O2	-6.15	118.49	122.80
1	1A	2106	C	N3-C4-C5	6.15	124.36	121.90
1	1A	2257	U	C5-C6-N1	-6.15	119.62	122.70
1	1A	2682	A	O4'-C1'-N9	-6.15	103.28	108.20
1	1A	1965	U	C5-C6-N1	-6.15	119.63	122.70
1	1A	8	A	OP1-P-OP2	-6.14	110.38	119.60
1	1A	86	C	N3-C4-C5	6.14	124.36	121.90
1	1A	481	C	N1-C2-O2	-6.14	115.21	118.90
1	1A	562	C	C5-C6-N1	-6.14	117.93	121.00
1	1A	751	G	N1-C6-O6	6.14	123.59	119.90
1	1A	863	C	N3-C2-O2	-6.14	117.60	121.90
1	1A	1383	G	C6-N1-C2	-6.14	121.41	125.10
1	1A	1804	A	C8-N9-C4	6.14	108.26	105.80
32	2a	517	G	C8-N9-C4	-6.14	103.94	106.40
1	1A	99	G	C8-N9-C4	6.14	108.86	106.40
1	1A	476	G	C5-C6-O6	-6.14	124.91	128.60
1	1A	782	A	C5-C6-N6	6.14	128.61	123.70
1	1A	1556	A	O4'-C1'-N9	6.14	113.11	108.20
1	1A	2368	C	N3-C4-C5	6.14	124.36	121.90
1	2A	1365	A	C6-N1-C2	-6.14	114.92	118.60
1	2A	2129	C	C5-C6-N1	6.14	124.07	121.00
1	1A	24	G	C5-N7-C8	6.14	107.37	104.30
1	1A	417	A	N9-C4-C5	-6.14	103.34	105.80
1	1A	649	C	C5-C6-N1	-6.14	117.93	121.00
1	1A	1279	C	C2-N3-C4	-6.14	116.83	119.90
1	1A	1369	U	N1-C2-N3	6.14	118.58	114.90
1	1A	2088	C	C4-C5-C6	6.14	120.47	117.40
1	2A	1246	A	C8-N9-C4	6.14	108.26	105.80
1	1A	34	C	OP1-P-OP2	6.14	128.81	119.60
1	1A	2713	C	C2-N3-C4	-6.14	116.83	119.90
32	2a	1028	C	C2-N1-C1'	6.14	125.55	118.80
1	1A	1397	C	OP1-P-O3'	6.14	118.70	105.20
2	1B	93	G	C8-N9-C4	-6.14	103.94	106.40
32	1a	139	G	OP1-P-OP2	-6.14	110.39	119.60
1	2A	1696	G	C5-C6-O6	-6.14	124.92	128.60
1	2A	1928	A	O5'-P-OP1	-6.14	100.18	105.70
1	1A	1110	C	N1-C2-O2	6.13	122.58	118.90
1	1A	1204	C	C5-C6-N1	-6.13	117.93	121.00
1	1A	1458	A	O5'-P-OP1	6.13	118.06	110.70
1	1A	2004	C	N3-C4-N4	-6.13	113.71	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1246	A	C2-N3-C4	-6.13	107.53	110.60
1	1A	1626	A	O5'-P-OP2	-6.13	100.18	105.70
1	1A	349	G	N1-C6-O6	6.13	123.58	119.90
1	2A	90	U	N3-C4-O4	-6.13	115.11	119.40
1	2A	417	C	O5'-P-OP1	-6.13	100.18	105.70
1	2A	529	A	O4'-C1'-N9	6.13	113.10	108.20
1	2A	2058	A	C5-C6-N6	-6.13	118.80	123.70
1	1A	1314	A	C4-C5-C6	6.13	120.06	117.00
1	2A	1682	G	N1-C6-O6	-6.13	116.22	119.90
1	1A	529	U	O5'-P-OP1	-6.13	100.18	105.70
1	1A	2258	G	C5-N7-C8	6.13	107.36	104.30
32	1a	880	C	O5'-P-OP2	-6.13	100.18	105.70
32	2a	1331	G	O4'-C1'-N9	6.13	113.10	108.20
32	1a	863	U	C6-N1-C1'	6.13	129.78	121.20
1	2A	562	U	N1-C2-N3	6.13	118.58	114.90
1	2A	958	U	N3-C2-O2	-6.13	117.91	122.20
1	1A	2443	U	N3-C4-O4	-6.12	115.11	119.40
1	1A	1658	C	C4-C5-C6	6.12	120.46	117.40
1	1A	1831	C	C4-C5-C6	6.12	120.46	117.40
1	1A	2428	C	N3-C4-C5	6.12	124.35	121.90
1	1A	2607	G	C4-C5-N7	-6.12	108.35	110.80
1	1A	45	C	C2-N1-C1'	-6.12	112.07	118.80
1	1A	1234	A	O5'-P-OP2	-6.12	100.19	105.70
1	1A	2654	G	C5-C6-O6	6.12	132.27	128.60
1	2A	464	U	OP1-P-OP2	-6.12	110.42	119.60
1	2A	1359	A	C2-N3-C4	6.12	113.66	110.60
1	2A	975	C	C6-N1-C2	-6.12	117.85	120.30
1	2A	1405	U	O5'-P-OP2	-6.12	100.19	105.70
2	2B	24	G	N3-C4-N9	6.12	129.67	126.00
32	2a	918	A	N1-C6-N6	-6.12	114.93	118.60
1	1A	660	C	N1-C2-N3	6.12	123.48	119.20
1	1A	2590	G	C4-C5-N7	-6.12	108.35	110.80
32	1a	866	C	OP1-P-OP2	6.12	128.78	119.60
1	1A	1039	G	C5-C6-O6	6.12	132.27	128.60
1	2A	251	A	C6-N1-C2	-6.12	114.93	118.60
1	2A	1108	U	C6-N1-C2	-6.12	117.33	121.00
1	1A	1097	G	C5-C6-N1	-6.11	108.44	111.50
1	1A	2562	G	C8-N9-C4	-6.11	103.95	106.40
32	1a	261	U	N1-C2-O2	-6.11	118.52	122.80
1	2A	118	A	O5'-P-OP1	-6.11	100.20	105.70
1	2A	575	A	O5'-P-OP2	6.11	118.04	110.70
1	1A	1097	G	O5'-P-OP2	6.11	118.03	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1742	G	N7-C8-N9	6.11	116.16	113.10
1	2A	349	G	C5-C6-O6	6.11	132.27	128.60
1	1A	191	U	C5-C6-N1	-6.11	119.64	122.70
1	1A	326	C	N3-C2-O2	-6.11	117.62	121.90
1	1A	1211	U	C4-C5-C6	6.11	123.37	119.70
1	2A	216	A	C2-N3-C4	-6.11	107.54	110.60
1	2A	1657	C	OP2-P-O3'	6.11	118.64	105.20
1	2A	125	G	C8-N9-C4	-6.11	103.96	106.40
1	1A	23	G	N3-C2-N2	-6.11	115.62	119.90
1	1A	251	A	N1-C6-N6	6.11	122.26	118.60
1	1A	2187	G	C2-N3-C4	6.11	114.95	111.90
1	2A	1656	C	O5'-P-OP2	-6.11	100.20	105.70
1	2A	2296	U	N3-C2-O2	-6.11	117.93	122.20
23	2I	21	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	1A	96	C	N1-C2-N3	6.10	123.47	119.20
1	1A	1848	G	O5'-P-OP2	-6.10	100.21	105.70
1	1A	1884	A	C8-N9-C4	6.10	108.24	105.80
1	2A	989	G	OP2-P-O3'	6.10	118.63	105.20
1	1A	2061	C	O5'-P-OP2	-6.10	100.21	105.70
1	1A	2767	U	N3-C2-O2	-6.10	117.93	122.20
1	2A	1775	U	N1-C2-N3	6.10	118.56	114.90
2	1B	50	G	C6-C5-N7	6.10	134.06	130.40
32	2a	664	G	N9-C4-C5	6.10	107.84	105.40
1	1A	495	G	C5-N7-C8	6.10	107.35	104.30
1	1A	1816	A	N1-C6-N6	6.10	122.26	118.60
1	1A	2600	G	N1-C6-O6	-6.10	116.24	119.90
32	1a	644	G	C6-C5-N7	6.10	134.06	130.40
1	2A	529	A	N3-C4-C5	6.10	131.07	126.80
1	1A	1262	C	C2-N3-C4	-6.10	116.85	119.90
1	1A	1361	C	O5'-P-OP2	-6.10	100.21	105.70
1	1A	1823	G	N7-C8-N9	-6.10	110.05	113.10
32	2a	454	C	N3-C2-O2	-6.10	117.63	121.90
1	1A	726	C	C5-C6-N1	-6.10	117.95	121.00
1	2A	761	A	C5-N7-C8	6.10	106.95	103.90
1	1A	724	A	N1-C6-N6	-6.09	114.94	118.60
1	1A	1956	C	O5'-P-OP2	-6.09	100.22	105.70
1	2A	62	C	C5-C6-N1	-6.09	117.95	121.00
1	2A	1040	C	C6-N1-C2	6.09	122.74	120.30
1	2A	2005	A	N1-C2-N3	-6.09	126.25	129.30
1	2A	2013	A	C2-N3-C4	-6.09	107.55	110.60
32	2a	266	G	C2'-C3'-O3'	6.09	123.45	113.70
1	2A	532	A	N7-C8-N9	6.09	116.85	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2473	U	N3-C2-O2	-6.09	117.94	122.20
1	1A	1567	G	O5'-P-OP1	6.09	118.01	110.70
1	1A	2511	C	N1-C2-O2	-6.09	115.25	118.90
1	1A	2735	G	N3-C4-N9	6.09	129.66	126.00
1	2A	1092	C	C2-N3-C4	6.09	122.95	119.90
1	2A	1499	C	OP2-P-O3'	6.09	118.60	105.20
1	1A	1598	C	C4-C5-C6	6.09	120.44	117.40
1	1A	2597	U	N1-C2-N3	6.09	118.55	114.90
2	2B	64	C	C6-N1-C2	6.09	122.74	120.30
1	1A	320	C	N1-C2-O2	-6.09	115.25	118.90
1	2A	97	C	C5-C6-N1	-6.09	117.96	121.00
32	2a	810	C	C6-N1-C2	6.09	122.73	120.30
1	1A	1548	C	C6-N1-C2	-6.09	117.86	120.30
1	1A	2448	G	N9-C4-C5	6.09	107.83	105.40
32	1a	481	G	N3-C4-N9	6.09	129.65	126.00
32	1a	1495	U	C5-C6-N1	6.09	125.74	122.70
1	2A	331	A	N1-C6-N6	-6.09	114.95	118.60
1	2A	1247	A	C2-N3-C4	-6.09	107.56	110.60
1	2A	1466	G	C8-N9-C4	6.09	108.83	106.40
1	2A	2062	A	C6-N1-C2	-6.09	114.95	118.60
1	2A	2763	G	N3-C4-N9	6.09	129.65	126.00
32	2a	1253	G	O5'-P-OP2	-6.09	100.22	105.70
1	1A	1254	G	N3-C2-N2	-6.08	115.64	119.90
1	1A	1482	G	OP1-P-OP2	-6.08	110.47	119.60
1	2A	1073	A	O5'-P-OP2	-6.08	100.23	105.70
1	1A	243	G	C4-C5-N7	-6.08	108.37	110.80
32	1a	781	A	C8-N9-C4	6.08	108.23	105.80
32	2a	1203	C	C6-N1-C2	6.08	122.73	120.30
1	1A	1661	C	C6-N1-C2	-6.08	117.87	120.30
1	1A	618	C	C4-C5-C6	-6.08	114.36	117.40
1	1A	2323	A	N1-C6-N6	-6.08	114.95	118.60
1	2A	2319	G	C2-N3-C4	-6.08	108.86	111.90
1	1A	395	C	C6-N1-C2	6.08	122.73	120.30
1	1A	583	C	C5-C4-N4	6.08	124.45	120.20
1	1A	1068	G	C6-N1-C2	6.08	128.75	125.10
1	2A	1807	G	N7-C8-N9	-6.08	110.06	113.10
1	1A	203	G	O5'-P-OP2	-6.07	100.23	105.70
1	1A	1117	G	N3-C4-C5	-6.07	125.56	128.60
32	1a	135	C	OP1-P-OP2	-6.07	110.49	119.60
1	2A	988	A	C5-C6-N6	-6.07	118.84	123.70
1	1A	902	G	N9-C4-C5	-6.07	102.97	105.40
1	1A	1354	A	C8-N9-C4	-6.07	103.37	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1203	G	N9-C4-C5	-6.07	102.97	105.40
1	1A	1646	C	C2-N3-C4	-6.07	116.86	119.90
1	1A	1811	A	O5'-P-OP2	-6.07	100.24	105.70
1	2A	2834	G	C5-C6-O6	6.07	132.24	128.60
1	1A	1403	U	N3-C2-O2	-6.07	117.95	122.20
1	1A	1600	A	OP2-P-O3'	6.07	118.55	105.20
1	1A	1843	A	N1-C6-N6	-6.07	114.96	118.60
1	2A	507	A	C5-N7-C8	-6.07	100.86	103.90
1	1A	167	G	N9-C4-C5	6.07	107.83	105.40
1	1A	586	G	N3-C2-N2	-6.07	115.65	119.90
1	1A	697	C	C2-N1-C1'	6.07	125.47	118.80
1	1A	1291	G	C4-C5-N7	-6.07	108.37	110.80
1	1A	1802	C	C2-N3-C4	-6.07	116.87	119.90
32	2a	548	G	N1-C6-O6	6.07	123.54	119.90
32	1a	78	G	O4'-C1'-N9	6.07	113.05	108.20
1	1A	748	G	C8-N9-C4	6.06	108.83	106.40
1	1A	1392	G	N1-C6-O6	-6.06	116.26	119.90
10	1O	104	ARG	NE-CZ-NH1	6.06	123.33	120.30
32	1a	624	C	C6-N1-C2	-6.06	117.88	120.30
32	1a	1210	C	C6-N1-C2	6.06	122.72	120.30
1	2A	44	G	OP1-P-OP2	6.06	128.69	119.60
1	2A	734	A	C2-N3-C4	-6.06	107.57	110.60
32	2a	1086	U	N1-C2-O2	6.06	127.04	122.80
1	1A	274	U	N1-C2-N3	-6.06	111.26	114.90
2	1B	59	A	C6-N1-C2	-6.06	114.96	118.60
32	1a	1052	U	N3-C2-O2	-6.06	117.96	122.20
1	2A	1087	G	N3-C4-C5	6.06	131.63	128.60
1	1A	843	C	N1-C2-O2	-6.06	115.27	118.90
1	1A	2419	G	C4-N9-C1'	6.06	134.38	126.50
1	1A	2623	U	N3-C4-O4	6.06	123.64	119.40
1	1A	516	G	N9-C4-C5	6.06	107.82	105.40
32	1a	105	G	N9-C4-C5	-6.06	102.98	105.40
32	1a	1406	U	O5'-P-OP2	-6.06	100.25	105.70
1	2A	2207	G	C8-N9-C4	-6.06	103.98	106.40
1	1A	174	U	O5'-P-OP2	-6.06	100.25	105.70
1	1A	1537	G	N7-C8-N9	-6.06	110.07	113.10
1	2A	878	A	C8-N9-C4	-6.06	103.38	105.80
1	1A	725	C	C4-C5-C6	6.05	120.43	117.40
1	1A	1851	U	C5-C4-O4	6.05	129.53	125.90
2	1B	13	A	C8-N9-C4	6.05	108.22	105.80
1	2A	1501	C	N3-C4-C5	-6.05	119.48	121.90
1	2A	2827	C	C2-N3-C4	-6.05	116.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	269	C	C2-N1-C1'	-6.05	112.14	118.80
1	1A	1640	G	C8-N9-C4	-6.05	103.98	106.40
1	1A	1918	G	C5-C6-O6	6.05	132.23	128.60
1	2A	798	G	C5-C6-O6	6.05	132.23	128.60
1	2A	1865	G	N9-C4-C5	6.05	107.82	105.40
1	1A	722	A	C6-C5-N7	-6.05	128.06	132.30
1	1A	779	C	N1-C2-N3	6.05	123.43	119.20
1	1A	979	G	C5-N7-C8	6.05	107.33	104.30
1	1A	1138	C	O4'-C1'-N1	6.05	113.04	108.20
1	1A	2839	C	OP2-P-O3'	6.05	118.51	105.20
32	1a	174	C	OP1-P-O3'	6.05	118.51	105.20
1	2A	935	C	O5'-P-OP2	-6.05	100.26	105.70
1	2A	1091	G	C2-N3-C4	6.05	114.92	111.90
1	2A	2751	G	N3-C4-C5	6.05	131.62	128.60
1	1A	20	C	N3-C4-N4	-6.05	113.77	118.00
1	1A	274	U	C5-C6-N1	6.05	125.72	122.70
1	1A	2287	C	C4-C5-C6	6.05	120.42	117.40
1	2A	2302	G	N9-C4-C5	6.05	107.82	105.40
1	1A	271	U	N3-C4-O4	-6.05	115.17	119.40
1	1A	780	G	N7-C8-N9	-6.05	110.08	113.10
1	1A	2250	G	OP1-P-OP2	6.05	128.67	119.60
1	1A	2476	C	N3-C4-C5	6.05	124.32	121.90
1	1A	107	G	C5-N7-C8	6.04	107.32	104.30
1	1A	2804	C	N3-C4-N4	6.04	122.23	118.00
1	1A	2891	C	OP1-P-OP2	6.04	128.67	119.60
32	1a	309	G	OP1-P-O3'	6.04	118.50	105.20
1	2A	1420	U	P-O3'-C3'	6.04	126.95	119.70
1	1A	952	G	C8-N9-C1'	6.04	134.85	127.00
1	1A	2047	C	O5'-P-OP2	-6.04	100.26	105.70
32	1a	622	A	N1-C6-N6	-6.04	114.97	118.60
32	1a	889	A	O5'-P-OP1	-6.04	100.26	105.70
1	1A	1536	A	N1-C6-N6	-6.04	114.97	118.60
32	1a	1523	G	OP1-P-OP2	6.04	128.66	119.60
1	2A	1646	C	OP1-P-O3'	6.04	118.49	105.20
32	2a	351	G	C2-N3-C4	-6.04	108.88	111.90
1	1A	354	A	C5-C6-N1	-6.04	114.68	117.70
1	1A	1512	G	O5'-P-OP2	-6.04	100.26	105.70
1	1A	2356	U	O4'-C1'-N1	-6.04	103.37	108.20
1	2A	50	U	O5'-P-OP1	-6.04	100.26	105.70
1	2A	2513	G	C2-N3-C4	6.04	114.92	111.90
1	1A	1137	G	N1-C6-O6	-6.04	116.28	119.90
1	1A	1742	G	N1-C6-O6	6.04	123.52	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1838	G	N9-C1'-C2'	-6.04	105.36	112.00
1	2A	1031	G	N1-C6-O6	6.04	123.52	119.90
1	2A	1235	G	C8-N9-C4	-6.04	103.98	106.40
32	2a	883	C	O5'-P-OP1	-6.04	100.27	105.70
1	1A	2165	C	C2-N3-C4	6.04	122.92	119.90
1	2A	1082	U	N3-C2-O2	-6.04	117.97	122.20
1	2A	1250	G	O5'-P-OP2	-6.04	100.27	105.70
1	1A	2239	A	N1-C2-N3	-6.04	126.28	129.30
2	1B	108	U	C5-C4-O4	6.04	129.52	125.90
32	1a	1300	G	C8-N9-C4	6.04	108.81	106.40
1	2A	2302	G	C4-C5-N7	-6.04	108.39	110.80
1	1A	164	G	N3-C2-N2	6.03	124.12	119.90
1	1A	1833	A	C5-C6-N6	-6.03	118.87	123.70
1	1A	1884	A	O5'-P-OP1	-6.03	100.27	105.70
1	1A	1958	A	N7-C8-N9	6.03	116.82	113.80
1	2A	2036	C	O5'-P-OP1	-6.03	100.27	105.70
1	1A	196	A	C5-C6-N6	-6.03	118.88	123.70
1	1A	1221	G	N1-C2-N2	6.03	121.63	116.20
1	1A	2802	C	N3-C4-C5	6.03	124.31	121.90
32	2a	1115	C	N3-C4-C5	-6.03	119.49	121.90
1	1A	1369	U	C2-N3-C4	-6.03	123.38	127.00
1	1A	1414	G	N1-C6-O6	-6.03	116.28	119.90
1	2A	2879	C	N3-C4-N4	6.03	122.22	118.00
1	1A	1133	G	C2-N3-C4	6.03	114.91	111.90
32	1a	226	G	N7-C8-N9	-6.03	110.09	113.10
1	2A	1251	C	C5-C6-N1	6.03	124.01	121.00
1	1A	852	G	C2-N3-C4	6.03	114.91	111.90
1	1A	1548	C	OP2-P-O3'	6.03	118.45	105.20
1	1A	2007	G	C5-N7-C8	6.03	107.31	104.30
1	2A	143	G	C4-C5-N7	-6.03	108.39	110.80
1	2A	694	U	N3-C2-O2	6.02	126.42	122.20
1	2A	2668	G	N1-C6-O6	-6.02	116.29	119.90
1	1A	50	G	C6-N1-C2	-6.02	121.49	125.10
1	1A	2065	C	OP2-P-O3'	6.02	118.45	105.20
1	2A	1233	C	O5'-P-OP1	-6.02	100.28	105.70
1	1A	179	A	C6-N1-C2	6.02	122.21	118.60
1	1A	594	A	N1-C6-N6	-6.02	114.99	118.60
1	1A	1128	U	C6-N1-C2	-6.02	117.39	121.00
1	1A	2551	C	C2-N3-C4	-6.02	116.89	119.90
32	1a	811	C	C6-N1-C2	6.02	122.71	120.30
32	1a	1475	G	N1-C6-O6	6.02	123.51	119.90
1	2A	753	C	O5'-P-OP2	6.02	117.92	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1537	G	N3-C4-C5	-6.02	125.59	128.60
1	1A	758	G	C6-C5-N7	-6.02	126.79	130.40
1	2A	1687	G	C5-C6-O6	6.02	132.21	128.60
1	1A	68	C	O5'-P-OP1	-6.01	100.29	105.70
1	1A	1909	C	O5'-P-OP2	6.01	117.92	110.70
1	2A	1618	A	C5-C6-N6	6.01	128.51	123.70
1	2A	2893	G	C5-C6-N1	6.01	114.51	111.50
32	2a	1221	G	C8-N9-C4	6.01	108.81	106.40
1	1A	579	G	C8-N9-C4	-6.01	104.00	106.40
1	1A	1132	A	C2-N3-C4	6.01	113.61	110.60
1	1A	2579	G	C8-N9-C4	6.01	108.81	106.40
1	1A	1014	U	N1-C2-N3	-6.01	111.29	114.90
1	1A	1711	A	C8-N9-C4	-6.01	103.40	105.80
32	1a	353	A	OP2-P-O3'	6.01	118.42	105.20
1	2A	9	U	N3-C4-C5	-6.01	110.99	114.60
32	2a	383	A	C8-N9-C4	6.01	108.20	105.80
32	2a	1189	C	C6-N1-C2	6.01	122.70	120.30
1	1A	1921	G	C5-N7-C8	-6.01	101.30	104.30
1	1A	2624	C	C2-N3-C4	6.01	122.91	119.90
1	2A	1054	A	O4'-C1'-N9	6.01	113.01	108.20
2	2B	115	G	N1-C6-O6	6.01	123.51	119.90
1	2A	527	C	C6-N1-C1'	6.01	128.01	120.80
1	1A	82	G	N1-C6-O6	6.01	123.50	119.90
1	1A	760	G	C8-N9-C4	6.01	108.80	106.40
1	1A	954	C	C6-N1-C2	6.01	122.70	120.30
1	2A	743	G	N1-C6-O6	-6.01	116.30	119.90
1	2A	1170	G	N7-C8-N9	6.01	116.10	113.10
1	1A	1807	G	N1-C2-N2	-6.00	110.80	116.20
1	1A	74	G	C8-N9-C4	6.00	108.80	106.40
1	1A	986	A	N7-C8-N9	6.00	116.80	113.80
1	1A	1853	G	C5-C6-O6	6.00	132.20	128.60
1	1A	1986	G	N3-C4-N9	6.00	129.60	126.00
1	1A	2122	G	C8-N9-C4	6.00	108.80	106.40
1	1A	2514	G	C2-N3-C4	-6.00	108.90	111.90
1	1A	2514	G	N3-C2-N2	6.00	124.10	119.90
1	2A	250	G	C6-C5-N7	6.00	134.00	130.40
1	2A	2105	C	C2-N3-C4	6.00	122.90	119.90
32	2a	1486	G	OP2-P-O3'	6.00	118.40	105.20
1	1A	1042	A	N7-C8-N9	-6.00	110.80	113.80
1	2A	177	G	O4'-C1'-N9	6.00	113.00	108.20
1	2A	679	C	N3-C2-O2	6.00	126.10	121.90
1	2A	792	G	N1-C2-N3	-6.00	120.30	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1343	G	N1-C6-O6	-6.00	116.30	119.90
1	1A	1439	A	N9-C4-C5	6.00	108.20	105.80
1	1A	2726	A	N1-C6-N6	-6.00	115.00	118.60
32	1a	394	G	O5'-P-OP1	-6.00	100.30	105.70
1	2A	906	G	C5-C6-N1	-6.00	108.50	111.50
32	2a	1100	C	C2-N1-C1'	-6.00	112.20	118.80
32	2a	1477	C	OP2-P-O3'	6.00	118.39	105.20
1	2A	2858	C	C6-N1-C2	6.00	122.70	120.30
1	2A	911	A	OP1-P-O3'	5.99	118.39	105.20
32	2a	686	U	N3-C2-O2	-5.99	118.00	122.20
32	2a	704	A	C2-N3-C4	5.99	113.60	110.60
1	1A	476	G	C5-C6-N1	5.99	114.50	111.50
1	1A	1573	G	N9-C4-C5	5.99	107.80	105.40
32	1a	226	G	N9-C4-C5	-5.99	103.00	105.40
1	2A	2385	C	OP1-P-OP2	5.99	128.59	119.60
1	2A	2895	U	C6-N1-C2	-5.99	117.41	121.00
1	1A	479	C	O5'-P-OP1	-5.99	100.31	105.70
1	1A	1001	G	C6-N1-C2	5.99	128.69	125.10
1	1A	2245	U	N3-C4-O4	-5.99	115.21	119.40
32	1a	78	G	N1-C2-N2	5.99	121.59	116.20
1	1A	533	G	N3-C2-N2	-5.99	115.71	119.90
1	1A	722	A	N9-C4-C5	-5.99	103.41	105.80
1	1A	791	G	C4-C5-N7	-5.99	108.40	110.80
1	1A	2025	G	C5-C6-O6	5.99	132.19	128.60
1	1A	2448	G	C4-C5-N7	-5.99	108.41	110.80
32	1a	325	A	C8-N9-C4	5.99	108.19	105.80
1	2A	983	A	C8-N9-C4	5.99	108.19	105.80
1	2A	1770	G	C5-C6-N1	5.99	114.49	111.50
44	2l	29	GLY	N-CA-C	-5.99	98.13	113.10
1	1A	716	G	N7-C8-N9	-5.99	110.11	113.10
1	1A	2902	G	N9-C4-C5	-5.99	103.00	105.40
32	1a	1151	A	O5'-P-OP2	-5.99	100.31	105.70
1	2A	655	A	C4-C5-C6	5.99	119.99	117.00
1	2A	1420	U	C2-N1-C1'	-5.99	110.52	117.70
32	1a	114	U	OP1-P-OP2	5.99	128.58	119.60
32	1a	332	G	O5'-P-OP1	-5.99	100.31	105.70
1	2A	416	C	O5'-P-OP2	-5.99	100.31	105.70
1	2A	474	G	OP2-P-O3'	5.99	118.37	105.20
2	2B	8	U	N3-C2-O2	5.99	126.39	122.20
32	2a	404	U	C5-C6-N1	5.99	125.69	122.70
1	1A	1264	G	N9-C4-C5	-5.98	103.01	105.40
1	1A	2031	G	N1-C2-N2	5.98	121.59	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	166	G	N1-C6-O6	-5.98	116.31	119.90
1	1A	505	A	N1-C6-N6	-5.98	115.01	118.60
1	1A	1861	C	C5-C4-N4	-5.98	116.01	120.20
1	1A	2574	U	N1-C2-O2	5.98	126.99	122.80
1	2A	1804	C	C5-C6-N1	5.98	123.99	121.00
32	2a	343	U	C4-C5-C6	-5.98	116.11	119.70
1	1A	2194	U	C4-C5-C6	5.98	123.29	119.70
32	1a	115	G	C8-N9-C4	-5.98	104.01	106.40
32	1a	971	G	O5'-P-OP2	-5.98	100.32	105.70
32	1a	1094	G	O5'-P-OP1	-5.98	100.32	105.70
1	2A	2822	G	C8-N9-C4	5.98	108.79	106.40
32	2a	776	G	C6-C5-N7	-5.98	126.81	130.40
1	1A	124	A	OP2-P-O3'	5.98	118.35	105.20
1	2A	445	C	N3-C2-O2	5.98	126.08	121.90
1	1A	840	A	O5'-P-OP2	-5.98	100.32	105.70
1	2A	2010	G	OP1-P-OP2	-5.98	110.64	119.60
32	2a	1108	G	C8-N9-C1'	-5.98	119.23	127.00
1	1A	1807	G	C6-C5-N7	-5.98	126.81	130.40
32	2a	1511	G	OP2-P-O3'	5.98	118.35	105.20
1	1A	183	G	O5'-P-OP2	-5.97	100.32	105.70
32	1a	189(A)	C	O5'-P-OP1	5.97	117.87	110.70
1	2A	2723	C	C6-N1-C2	-5.97	117.91	120.30
32	2a	1100	C	N1-C2-O2	-5.97	115.31	118.90
1	1A	647	G	C5-C6-O6	5.97	132.18	128.60
1	1A	1256	U	OP1-P-OP2	-5.97	110.64	119.60
1	1A	2095	C	C2-N3-C4	-5.97	116.91	119.90
1	1A	2698	G	C4-C5-N7	5.97	113.19	110.80
32	1a	1493	A	C2-N3-C4	5.97	113.59	110.60
32	2a	618	C	C2-N3-C4	5.97	122.89	119.90
1	1A	1550	C	O5'-P-OP2	-5.97	100.33	105.70
1	2A	11	G	C5-N7-C8	-5.97	101.31	104.30
32	2a	1362	C	C6-N1-C2	-5.97	117.91	120.30
1	1A	776	G	C5-N7-C8	-5.97	101.31	104.30
1	1A	933	C	N1-C2-O2	5.97	122.48	118.90
1	1A	1355	G	N3-C2-N2	-5.97	115.72	119.90
1	1A	1709	C	N3-C4-C5	5.97	124.29	121.90
1	1A	1806	U	N1-C2-O2	-5.97	118.62	122.80
1	1A	697	C	C5-C6-N1	5.97	123.98	121.00
1	1A	508	A	N1-C2-N3	5.97	132.28	129.30
1	1A	537	G	N7-C8-N9	-5.97	110.12	113.10
1	2A	674	G	N1-C6-O6	-5.97	116.32	119.90
1	1A	781	A	N1-C6-N6	5.96	122.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	878	G	N1-C2-N3	5.96	127.48	123.90
1	1A	1492	C	C6-N1-C2	-5.96	117.91	120.30
1	1A	2238	C	C5-C6-N1	-5.96	118.02	121.00
2	2B	13	A	O5'-P-OP2	-5.96	100.33	105.70
32	2a	701	C	O5'-P-OP2	-5.96	100.33	105.70
1	1A	1192	C	N1-C2-O2	-5.96	115.32	118.90
1	1A	2155	G	O4'-C1'-N9	5.96	112.97	108.20
32	1a	1382	C	N1-C2-O2	5.96	122.48	118.90
1	2A	911	A	OP1-P-OP2	5.96	128.54	119.60
1	1A	281	G	C5-C6-O6	5.96	132.18	128.60
1	1A	1692	G	N1-C2-N3	-5.96	120.32	123.90
1	1A	2764	G	O4'-C1'-N9	5.96	112.97	108.20
1	2A	2829	C	C6-N1-C2	5.96	122.69	120.30
32	1a	607	A	N1-C6-N6	5.96	122.18	118.60
1	1A	1059	C	N3-C4-N4	-5.96	113.83	118.00
1	1A	2006	G	N3-C4-N9	-5.96	122.42	126.00
1	1A	2527	C	C5-C4-N4	-5.96	116.03	120.20
32	1a	899	C	C6-N1-C2	5.96	122.68	120.30
1	2A	2599	G	C4-C5-N7	-5.96	108.42	110.80
32	2a	993	G	C4-N9-C1'	5.96	134.25	126.50
46	2n	44	LEU	CA-CB-CG	5.96	129.00	115.30
1	1A	1184	G	N9-C4-C5	5.96	107.78	105.40
1	1A	1853	G	N1-C2-N2	-5.96	110.84	116.20
1	1A	2640	C	C5-C4-N4	-5.96	116.03	120.20
32	1a	521	G	OP1-P-OP2	5.96	128.53	119.60
1	1A	255	G	C5-C6-N1	5.96	114.48	111.50
1	1A	1248	G	C5-C6-O6	-5.96	125.03	128.60
1	1A	1299	A	C4-C5-N7	-5.96	107.72	110.70
1	1A	2512	U	N1-C2-O2	5.96	126.97	122.80
1	1A	968	U	C2-N3-C4	-5.95	123.43	127.00
32	1a	681	C	N1-C2-O2	-5.95	115.33	118.90
1	2A	1883	G	C5-N7-C8	5.95	107.28	104.30
1	1A	987	G	N3-C2-N2	5.95	124.06	119.90
1	1A	1539	C	C2-N3-C4	-5.95	116.92	119.90
1	1A	2368	C	N1-C2-O2	-5.95	115.33	118.90
1	1A	2394	G	C8-N9-C4	-5.95	104.02	106.40
32	1a	57	G	N1-C6-O6	-5.95	116.33	119.90
1	2A	1657	C	OP1-P-O3'	-5.95	92.11	105.20
1	1A	308	U	C5-C4-O4	-5.95	122.33	125.90
1	1A	1080	G	N3-C2-N2	-5.95	115.74	119.90
1	1A	1148	C	N3-C2-O2	-5.95	117.74	121.90
1	1A	1611	C	O5'-P-OP2	-5.95	100.35	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1821	C	OP1-P-O3'	5.95	118.29	105.20
1	1A	2537	G	OP2-P-O3'	5.95	118.29	105.20
32	2a	134	A	N9-C4-C5	-5.95	103.42	105.80
1	1A	557	A	C5-C6-N6	5.95	128.46	123.70
1	1A	114	C	C5-C4-N4	5.95	124.36	120.20
1	1A	246	A	O5'-P-OP1	5.95	117.83	110.70
1	1A	821	A	N9-C4-C5	5.95	108.18	105.80
1	1A	1006	C	O5'-P-OP1	5.95	117.83	110.70
32	1a	73	G	N1-C6-O6	-5.95	116.33	119.90
32	1a	926	G	N9-C4-C5	5.95	107.78	105.40
1	1A	1727	U	N3-C4-C5	5.94	118.17	114.60
1	1A	1804	A	N9-C1'-C2'	-5.94	105.46	112.00
1	1A	2165	C	C6-N1-C2	-5.94	117.92	120.30
32	1a	1181	G	C6-N1-C2	5.94	128.67	125.10
32	1a	1486	G	N3-C4-C5	5.94	131.57	128.60
1	2A	193	U	N3-C2-O2	5.94	126.36	122.20
1	2A	1076	C	N1-C1'-C2'	5.94	121.73	114.00
32	2a	46	G	N1-C6-O6	5.94	123.47	119.90
1	1A	35	G	C4-C5-N7	-5.94	108.42	110.80
1	1A	794	U	N3-C4-C5	-5.94	111.03	114.60
1	1A	847	A	O5'-P-OP1	-5.94	100.35	105.70
1	1A	2068	G	N7-C8-N9	-5.94	110.13	113.10
32	1a	189(L)	G	N3-C4-C5	-5.94	125.63	128.60
32	1a	363	A	O5'-P-OP2	-5.94	100.35	105.70
1	2A	1690	A	N9-C4-C5	-5.94	103.42	105.80
1	1A	96	C	N3-C2-O2	-5.94	117.74	121.90
1	1A	461	U	C2-N3-C4	-5.94	123.44	127.00
1	1A	1769	G	C6-C5-N7	5.94	133.96	130.40
1	1A	2714	U	N3-C2-O2	5.94	126.36	122.20
1	2A	1089	G	O4'-C1'-N9	5.94	112.95	108.20
1	2A	1815	A	N9-C4-C5	5.94	108.18	105.80
1	2A	2475	C	N3-C4-C5	-5.94	119.52	121.90
32	2a	122	G	C6-N1-C2	-5.94	121.53	125.10
1	1A	696	C	C5-C6-N1	5.94	123.97	121.00
1	2A	1092	C	C6-N1-C2	-5.94	117.92	120.30
1	2A	2248	C	O5'-P-OP2	-5.94	100.36	105.70
32	2a	876	G	N1-C6-O6	-5.94	116.34	119.90
1	1A	164	G	N1-C2-N2	-5.94	110.86	116.20
1	1A	815	G	C8-N9-C4	-5.94	104.03	106.40
1	1A	1085	G	C8-N9-C4	5.94	108.78	106.40
1	2A	803	U	N3-C2-O2	-5.94	118.04	122.20
32	2a	909	A	C5-C6-N6	-5.94	118.95	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1840	A	N1-C6-N6	-5.94	115.04	118.60
1	1A	2020	G	N9-C4-C5	5.94	107.77	105.40
1	2A	421	U	O5'-P-OP2	-5.94	100.36	105.70
1	1A	595	A	C5-N7-C8	5.93	106.87	103.90
1	1A	748	G	N1-C6-O6	-5.93	116.34	119.90
1	1A	860	U	C2-N3-C4	-5.93	123.44	127.00
1	1A	1762	G	N3-C4-N9	-5.93	122.44	126.00
1	1A	2863	C	O5'-P-OP2	-5.93	100.36	105.70
32	2a	1472	U	O5'-P-OP2	-5.93	100.36	105.70
1	1A	515	G	N1-C2-N2	5.93	121.54	116.20
1	1A	1747	A	O4'-C1'-N9	-5.93	103.45	108.20
1	1A	2047	C	N3-C2-O2	5.93	126.05	121.90
1	1A	2720	G	C8-N9-C4	5.93	108.77	106.40
1	1A	360	C	C5-C4-N4	5.93	124.35	120.20
1	1A	533	G	OP1-P-OP2	5.93	128.50	119.60
1	1A	600	G	C4-C5-N7	-5.93	108.43	110.80
1	1A	1532	A	O5'-P-OP2	-5.93	100.36	105.70
1	1A	1692	G	C4-C5-N7	-5.93	108.43	110.80
1	2A	204	A	O5'-P-OP2	-5.93	100.36	105.70
1	1A	854	U	C6-N1-C2	-5.93	117.44	121.00
1	1A	1304	C	N3-C2-O2	-5.93	117.75	121.90
1	1A	2335	G	N3-C2-N2	5.93	124.05	119.90
32	1a	536	C	C6-N1-C2	-5.93	117.93	120.30
32	1a	1063	C	N1-C2-O2	5.93	122.46	118.90
32	1a	1457	G	C8-N9-C4	5.93	108.77	106.40
32	2a	574	A	O5'-P-OP1	5.93	117.82	110.70
1	1A	2480	G	C5-C6-O6	-5.93	125.04	128.60
1	2A	271(W)	G	C5-C6-N1	-5.93	108.54	111.50
1	2A	602	G	N3-C4-C5	-5.93	125.64	128.60
1	1A	407	U	C2-N3-C4	-5.93	123.44	127.00
1	1A	2084	A	C8-N9-C4	5.93	108.17	105.80
32	1a	802	A	C5-C6-N6	-5.93	118.96	123.70
1	2A	1834	U	N1-C2-O2	5.93	126.95	122.80
1	1A	1666	G	N3-C2-N2	5.92	124.05	119.90
1	1A	1862	G	OP2-P-O3'	5.92	118.23	105.20
32	1a	1273	G	C8-N9-C4	5.92	108.77	106.40
1	2A	193	U	C5-C6-N1	-5.92	119.74	122.70
1	2A	2123	G	N3-C4-N9	5.92	129.55	126.00
1	1A	1816	A	C4-C5-N7	5.92	113.66	110.70
32	1a	825	G	C5-C6-N1	5.92	114.46	111.50
1	2A	365	C	C4-C5-C6	5.92	120.36	117.40
1	1A	122	G	N1-C2-N2	-5.92	110.87	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	180	A	OP1-P-O3'	-5.92	92.17	105.20
1	1A	1843	A	C8-N9-C4	-5.92	103.43	105.80
32	1a	649	G	O5'-P-OP2	-5.92	100.37	105.70
32	1a	1442	G	C8-N9-C4	-5.92	104.03	106.40
1	1A	808	A	C2-N3-C4	5.92	113.56	110.60
1	1A	1245	C	C5-C6-N1	-5.92	118.04	121.00
1	1A	2297	C	N3-C2-O2	-5.92	117.76	121.90
1	1A	2506	G	C5-C6-O6	5.92	132.15	128.60
1	1A	713	G	N7-C8-N9	-5.92	110.14	113.10
1	1A	1482	G	C8-N9-C4	-5.92	104.03	106.40
1	2A	2036	C	OP1-P-OP2	5.92	128.48	119.60
1	2A	2339	G	O5'-P-OP2	-5.92	100.37	105.70
1	1A	877	G	C4-C5-N7	-5.92	108.43	110.80
1	1A	2040	G	O5'-P-OP1	-5.92	100.38	105.70
32	1a	552	U	C5-C6-N1	-5.92	119.74	122.70
1	2A	1378	A	O5'-P-OP1	-5.92	100.38	105.70
1	1A	1171	G	N3-C2-N2	-5.92	115.76	119.90
1	1A	1702	A	C5-C6-N6	5.92	128.43	123.70
1	1A	2776	G	C4-C5-N7	5.92	113.17	110.80
32	1a	1065	U	P-O3'-C3'	5.92	126.80	119.70
1	1A	716	G	O4'-C1'-N9	-5.91	103.47	108.20
1	1A	1320	A	N1-C6-N6	5.91	122.15	118.60
1	1A	1708	G	C5-N7-C8	5.91	107.26	104.30
1	1A	2291	G	N1-C6-O6	5.91	123.45	119.90
1	2A	1935	G	C5-C6-O6	-5.91	125.05	128.60
1	1A	1359	U	O4'-C1'-N1	5.91	112.93	108.20
1	1A	2138	G	C8-N9-C4	-5.91	104.04	106.40
1	1A	2640	C	C2-N3-C4	-5.91	116.94	119.90
13	1R	67	LEU	CB-CG-CD2	-5.91	100.95	111.00
32	1a	542	G	C8-N9-C4	-5.91	104.04	106.40
32	1a	834	C	O5'-P-OP2	-5.91	100.38	105.70
1	2A	1899	G	C8-N9-C4	-5.91	104.04	106.40
1	1A	1820	A	N3-C4-C5	5.91	130.94	126.80
1	1A	1850	A	C4-C5-C6	5.91	119.95	117.00
32	1a	533	A	C6-N1-C2	-5.91	115.06	118.60
1	2A	1883	G	N3-C4-N9	5.91	129.54	126.00
1	1A	2283	G	OP2-P-O3'	5.91	118.19	105.20
1	1A	2638	C	N3-C2-O2	5.91	126.03	121.90
32	1a	719	C	C4-C5-C6	5.91	120.35	117.40
1	2A	250	G	N9-C4-C5	5.91	107.76	105.40
1	2A	417	C	N3-C4-N4	5.91	122.13	118.00
1	2A	866	A	N9-C4-C5	-5.91	103.44	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	280	C	C6-N1-C2	5.91	122.66	120.30
32	2a	1287	A	N1-C6-N6	-5.91	115.06	118.60
1	1A	2220	A	C5-N7-C8	5.90	106.85	103.90
2	1B	89	G	N1-C6-O6	5.90	123.44	119.90
1	2A	234	C	C6-N1-C2	-5.90	117.94	120.30
1	2A	780	G	O5'-P-OP2	-5.90	100.39	105.70
32	2a	22	G	C8-N9-C4	-5.90	104.04	106.40
1	1A	844	C	C6-N1-C2	5.90	122.66	120.30
1	1A	1119	A	O4'-C1'-N9	5.90	112.92	108.20
1	1A	1309	U	OP2-P-O3'	5.90	118.19	105.20
1	1A	1725	G	C5-N7-C8	-5.90	101.35	104.30
1	1A	2046	G	N7-C8-N9	-5.90	110.15	113.10
1	1A	2597	U	N3-C4-O4	-5.90	115.27	119.40
1	1A	2728	C	C6-N1-C2	5.90	122.66	120.30
1	1A	2745	G	C4-C5-N7	-5.90	108.44	110.80
32	1a	1087	G	N3-C4-C5	-5.90	125.65	128.60
1	2A	116	C	N1-C2-O2	-5.90	115.36	118.90
1	2A	1650	G	N9-C4-C5	5.90	107.76	105.40
1	2A	2318	G	C4-N9-C1'	5.90	134.17	126.50
32	2a	687	A	P-O3'-C3'	5.90	126.78	119.70
1	1A	1171	G	N1-C2-N3	5.90	127.44	123.90
1	1A	1455	C	C2-N3-C4	-5.90	116.95	119.90
1	1A	2023	A	C5-N7-C8	5.90	106.85	103.90
1	1A	2657	G	N7-C8-N9	5.90	116.05	113.10
1	2A	1536	C	C6-N1-C2	-5.90	117.94	120.30
32	2a	438	G	N3-C2-N2	5.90	124.03	119.90
32	2a	647	C	C5-C6-N1	5.90	123.95	121.00
1	1A	2698	G	N3-C2-N2	5.90	124.03	119.90
2	1B	55	U	OP1-P-OP2	5.90	128.45	119.60
32	1a	33	A	O5'-P-OP2	-5.90	100.39	105.70
1	1A	164	G	C5-C6-N1	5.90	114.45	111.50
1	1A	947	A	N1-C6-N6	5.90	122.14	118.60
1	1A	1346	U	N3-C2-O2	-5.90	118.07	122.20
1	1A	1627	A	C4-C5-N7	5.90	113.65	110.70
1	1A	1640	G	N9-C4-C5	5.90	107.76	105.40
1	1A	2602	A	OP2-P-O3'	5.90	118.17	105.20
1	2A	780	G	N1-C6-O6	5.90	123.44	119.90
1	2A	2476	A	C8-N9-C4	-5.90	103.44	105.80
1	2A	2611	U	OP2-P-O3'	5.90	118.17	105.20
32	2a	721	G	N1-C6-O6	5.90	123.44	119.90
1	2A	1602	U	N3-C4-C5	5.90	118.14	114.60
1	2A	2307	G	C5-C6-O6	-5.90	125.06	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1790	A	N1-C2-N3	5.89	132.25	129.30
1	1A	1821	C	C2-N3-C4	-5.89	116.95	119.90
1	1A	1951	G	C5-C6-O6	5.89	132.14	128.60
32	1a	674	G	OP1-P-O3'	5.89	118.17	105.20
1	2A	2167	U	C5-C4-O4	5.89	129.44	125.90
1	2A	2185	C	N3-C2-O2	-5.89	117.77	121.90
32	2a	1373	G	C8-N9-C4	-5.89	104.04	106.40
1	1A	542	C	C2-N3-C4	-5.89	116.95	119.90
1	1A	1867	C	C6-N1-C2	-5.89	117.94	120.30
2	1B	90	A	N1-C2-N3	-5.89	126.35	129.30
32	1a	848	C	C5-C6-N1	5.89	123.95	121.00
1	2A	2810	A	N1-C6-N6	5.89	122.14	118.60
32	2a	531	U	N1-C2-O2	5.89	126.92	122.80
1	1A	1051	C	C5-C4-N4	5.89	124.32	120.20
1	2A	31	C	O5'-P-OP1	-5.89	100.40	105.70
1	2A	2852	G	C8-N9-C4	5.89	108.76	106.40
1	1A	2240	G	N9-C4-C5	5.89	107.76	105.40
32	1a	486	U	N3-C2-O2	-5.89	118.08	122.20
1	1A	1132	A	C8-N9-C4	-5.89	103.44	105.80
1	1A	2588	G	N1-C6-O6	-5.89	116.37	119.90
1	1A	2697	G	OP2-P-O3'	5.89	118.15	105.20
1	2A	920	G	C8-N9-C4	-5.89	104.05	106.40
1	2A	2223	G	O5'-P-OP2	-5.89	100.40	105.70
1	1A	1637	G	C5-C6-O6	5.89	132.13	128.60
1	1A	1862	G	C8-N9-C4	-5.89	104.05	106.40
32	1a	343	U	N3-C2-O2	-5.89	118.08	122.20
1	1A	2831	A	N1-C2-N3	5.88	132.24	129.30
1	1A	870	G	N9-C4-C5	5.88	107.75	105.40
1	1A	2636	G	C5-C6-N1	5.88	114.44	111.50
1	2A	645	C	N1-C2-O2	5.88	122.43	118.90
32	2a	372	C	N1-C2-O2	5.88	122.43	118.90
32	2a	709	G	N7-C8-N9	5.88	116.04	113.10
1	1A	847	A	C5-C6-N6	5.88	128.40	123.70
1	1A	1062	G	OP1-P-OP2	-5.88	110.78	119.60
1	1A	1692	G	C2-N3-C4	5.88	114.84	111.90
32	1a	984	C	C6-N1-C2	5.88	122.65	120.30
1	1A	2458	G	C2-N3-C4	5.88	114.84	111.90
1	1A	2529	C	C5-C4-N4	-5.88	116.09	120.20
1	2A	2162	G	C8-N9-C1'	-5.88	119.36	127.00
1	2A	2615	U	N3-C4-C5	5.88	118.13	114.60
32	2a	1274	G	C8-N9-C4	-5.88	104.05	106.40
1	1A	1924	C	O5'-P-OP1	-5.88	100.41	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	700	G	O5'-P-OP2	-5.88	100.41	105.70
32	1a	1170	A	C8-N9-C4	-5.88	103.45	105.80
32	2a	1103	C	C6-N1-C2	-5.88	117.95	120.30
1	1A	2314	G	O5'-P-OP2	-5.87	100.41	105.70
1	2A	214	G	C2-N3-C4	5.87	114.84	111.90
1	2A	2429	G	O5'-P-OP2	-5.87	100.41	105.70
1	1A	102	U	N1-C2-O2	-5.87	118.69	122.80
1	1A	2439	C	C2-N1-C1'	-5.87	112.34	118.80
32	1a	340	U	C6-N1-C2	5.87	124.52	121.00
32	1a	900	A	N1-C2-N3	-5.87	126.36	129.30
1	2A	2420	C	C6-N1-C2	5.87	122.65	120.30
1	1A	869	U	N1-C2-N3	5.87	118.42	114.90
1	1A	2007	G	N7-C8-N9	-5.87	110.17	113.10
1	1A	2024	G	C5-C6-O6	5.87	132.12	128.60
2	1B	117	G	O5'-P-OP1	5.87	117.74	110.70
1	2A	1115	G	C8-N9-C4	5.87	108.75	106.40
1	1A	34	C	N3-C4-C5	-5.87	119.55	121.90
1	1A	2245	U	OP1-P-OP2	5.87	128.40	119.60
1	1A	2802	C	C5-C6-N1	-5.87	118.07	121.00
32	1a	1035	A	N7-C8-N9	5.87	116.73	113.80
1	2A	27	G	OP1-P-OP2	-5.87	110.80	119.60
1	2A	212	G	OP2-P-O3'	5.87	118.11	105.20
1	2A	1063	G	C4-N9-C1'	5.87	134.13	126.50
1	2A	1076	C	C2-N3-C4	5.87	122.83	119.90
1	2A	2817	G	N1-C6-O6	-5.87	116.38	119.90
32	2a	656	C	C6-N1-C2	-5.87	117.95	120.30
1	1A	1221	G	OP1-P-O3'	5.87	118.11	105.20
1	2A	2148	G	N3-C4-N9	5.87	129.52	126.00
1	1A	24	G	C4-C5-N7	-5.87	108.45	110.80
1	1A	966	G	N1-C2-N2	-5.87	110.92	116.20
1	1A	1980	C	N1-C2-O2	-5.87	115.38	118.90
1	1A	2618	C	C5-C6-N1	-5.87	118.07	121.00
1	1A	2775	G	C8-N9-C4	5.87	108.75	106.40
1	2A	2299	G	N1-C6-O6	5.87	123.42	119.90
1	2A	2316	C	C6-N1-C2	-5.87	117.95	120.30
32	2a	1023	G	N7-C8-N9	5.87	116.03	113.10
1	1A	35	G	C5-C6-O6	5.86	132.12	128.60
1	1A	565	C	C2-N3-C4	-5.86	116.97	119.90
1	1A	1701	A	O5'-P-OP2	5.86	117.74	110.70
1	1A	2606	C	C6-N1-C2	5.86	122.64	120.30
2	1B	75	G	N1-C2-N3	5.86	127.42	123.90
1	2A	1650	G	C5-C6-O6	5.86	132.12	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	25	19	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	1A	1319	U	OP1-P-OP2	5.86	128.39	119.60
1	1A	1922	A	C2-N3-C4	5.86	113.53	110.60
1	1A	1981	G	C5-N7-C8	5.86	107.23	104.30
32	1a	227	G	N3-C2-N2	5.86	124.00	119.90
1	2A	2596	U	N1-C2-N3	5.86	118.42	114.90
32	2a	575	G	O4'-C1'-N9	-5.86	103.51	108.20
32	2a	698	G	C5-C6-O6	-5.86	125.08	128.60
32	2a	904	C	N3-C2-O2	5.86	126.00	121.90
1	1A	101	A	C6-C5-N7	-5.86	128.20	132.30
2	1B	109	C	OP1-P-OP2	5.86	128.39	119.60
32	1a	1037	C	C4-C5-C6	5.86	120.33	117.40
1	2A	2275	C	O4'-C1'-N1	-5.86	103.51	108.20
1	2A	2296	U	N1-C2-O2	5.86	126.90	122.80
2	2B	26	A	O5'-P-OP2	5.86	117.73	110.70
1	1A	249	G	O5'-P-OP1	-5.86	100.43	105.70
32	1a	49	U	N1-C2-O2	5.86	126.90	122.80
1	1A	1011	G	C5-C6-O6	5.86	132.12	128.60
32	2a	396	G	N1-C6-O6	5.86	123.42	119.90
1	1A	1528	U	N1-C2-O2	-5.86	118.70	122.80
1	1A	2016	C	N1-C2-O2	-5.86	115.39	118.90
1	1A	2569	G	C4-C5-N7	-5.86	108.46	110.80
1	1A	2619	G	C8-N9-C4	-5.86	104.06	106.40
1	1A	2714	U	C6-N1-C2	5.86	124.51	121.00
2	1B	106	G	C8-N9-C4	5.86	108.74	106.40
32	1a	1003	G	C8-N9-C4	-5.86	104.06	106.40
1	1A	115	G	N1-C2-N3	5.85	127.41	123.90
1	1A	2354	C	OP1-P-OP2	-5.85	110.82	119.60
1	1A	803	C	C5-C6-N1	-5.85	118.07	121.00
1	1A	1694	G	C6-N1-C2	-5.85	121.59	125.10
1	1A	2179	G	N1-C6-O6	-5.85	116.39	119.90
32	1a	767	A	N1-C2-N3	5.85	132.23	129.30
1	2A	513	A	N7-C8-N9	5.85	116.73	113.80
1	2A	691	C	C6-N1-C2	-5.85	117.96	120.30
32	2a	115	G	P-O3'-C3'	5.85	126.72	119.70
32	2a	398	C	C5-C4-N4	5.85	124.30	120.20
1	1A	499	G	OP2-P-O3'	5.85	118.07	105.20
1	1A	1054	C	C2-N1-C1'	5.85	125.24	118.80
1	1A	1360	C	C2-N3-C4	-5.85	116.97	119.90
1	1A	2171	G	C8-N9-C1'	5.85	134.61	127.00
1	1A	194	G	N3-C4-N9	5.85	129.51	126.00
1	1A	1690	G	N7-C8-N9	-5.85	110.17	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1994	A	N7-C8-N9	5.85	116.72	113.80
1	1A	2260	C	OP2-P-O3'	5.85	118.07	105.20
32	1a	621	A	N1-C6-N6	-5.85	115.09	118.60
32	1a	1480	G	C5-C6-O6	5.85	132.11	128.60
1	2A	1247	A	O5'-P-OP2	5.85	117.72	110.70
1	2A	1899	G	N7-C8-N9	5.85	116.03	113.10
32	2a	266	G	N3-C4-N9	5.85	129.51	126.00
1	1A	2485	U	C6-N1-C1'	-5.85	113.01	121.20
2	1B	99	G	N7-C8-N9	-5.85	110.18	113.10
1	2A	226	G	N1-C2-N2	5.85	121.46	116.20
1	2A	1662	C	N3-C4-N4	-5.85	113.91	118.00
32	2a	865	A	N7-C8-N9	5.85	116.72	113.80
32	1a	1345	U	O4'-C1'-N1	5.84	112.88	108.20
32	1a	1403	C	C6-N1-C2	-5.84	117.96	120.30
1	2A	639	U	C5-C6-N1	-5.84	119.78	122.70
1	2A	1017	G	O5'-P-OP1	-5.84	100.44	105.70
1	2A	1681	G	C5-N7-C8	-5.84	101.38	104.30
1	2A	2596	U	C5-C6-N1	-5.84	119.78	122.70
32	1a	1415	G	OP1-P-O3'	5.84	118.05	105.20
1	2A	1859	A	O5'-P-OP2	-5.84	100.44	105.70
1	1A	2006	G	N9-C4-C5	5.84	107.74	105.40
1	1A	2224	C	N1-C2-O2	-5.84	115.39	118.90
1	1A	2653	G	O4'-C1'-N9	-5.84	103.53	108.20
32	1a	509	A	C8-N9-C4	-5.84	103.46	105.80
32	1a	821	G	C5-C6-O6	-5.84	125.09	128.60
1	2A	190	A	O5'-P-OP2	-5.84	100.44	105.70
1	2A	1309	G	N1-C6-O6	5.84	123.41	119.90
1	2A	2207	G	C5-C6-N1	-5.84	108.58	111.50
1	2A	2255	G	C8-N9-C4	-5.84	104.06	106.40
1	1A	193	A	OP1-P-O3'	5.84	118.05	105.20
1	1A	2467	G	N3-C4-C5	-5.84	125.68	128.60
32	1a	346	G	C2-N3-C4	5.84	114.82	111.90
32	1a	1112	C	OP2-P-O3'	5.84	118.05	105.20
1	1A	1083	G	C5-C6-O6	-5.84	125.10	128.60
1	1A	1681	A	C5-C6-N6	5.84	128.37	123.70
32	2a	530	G	N3-C2-N2	5.84	123.99	119.90
1	1A	1690	G	C5-N7-C8	5.84	107.22	104.30
1	1A	1006	C	N1-C2-O2	-5.83	115.40	118.90
32	2a	1370	G	N3-C4-N9	5.83	129.50	126.00
1	1A	724	A	C5-N7-C8	5.83	106.82	103.90
1	1A	733	G	O5'-P-OP1	-5.83	100.45	105.70
1	1A	1183	G	C5-N7-C8	5.83	107.22	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1354	A	C5-C6-N1	-5.83	114.78	117.70
1	1A	1681	A	N1-C6-N6	-5.83	115.10	118.60
32	1a	1515	C	OP1-P-OP2	5.83	128.35	119.60
32	2a	266	G	C4-C5-C6	5.83	122.30	118.80
32	2a	343	U	C5-C6-N1	-5.83	119.78	122.70
1	1A	1317	G	C5-C6-O6	-5.83	125.10	128.60
32	1a	260	G	C5-C6-N1	-5.83	108.58	111.50
1	2A	808	G	C5-C6-N1	5.83	114.42	111.50
1	2A	1616	A	C8-N9-C4	-5.83	103.47	105.80
1	1A	2274	U	OP1-P-OP2	-5.83	110.86	119.60
1	1A	2475	C	N3-C4-N4	-5.83	113.92	118.00
1	2A	2137	C	N1-C2-O2	5.83	122.40	118.90
1	1A	731	G	N3-C4-C5	-5.83	125.69	128.60
1	1A	1620	G	OP2-P-O3'	5.83	118.02	105.20
1	1A	2519	C	C6-N1-C2	-5.83	117.97	120.30
1	1A	2826	C	OP2-P-O3'	5.83	118.02	105.20
1	1A	2880	C	C6-N1-C2	-5.83	117.97	120.30
1	1A	2900	G	C5-C6-O6	-5.83	125.10	128.60
2	1B	79	C	C2-N3-C4	-5.83	116.99	119.90
2	1B	115	G	C2-N3-C4	-5.83	108.99	111.90
1	2A	445	C	OP1-P-O3'	5.83	118.02	105.20
1	2A	900	A	P-O3'-C3'	5.83	126.69	119.70
1	2A	1497	U	C5-C4-O4	5.83	129.40	125.90
1	1A	360	C	N3-C4-C5	-5.83	119.57	121.90
1	1A	1838	G	C2-N3-C4	-5.83	108.99	111.90
1	2A	745	G	OP1-P-OP2	-5.83	110.86	119.60
1	2A	2182	G	N3-C4-N9	-5.83	122.50	126.00
1	1A	460	C	N3-C2-O2	-5.83	117.82	121.90
1	1A	2479	C	O5'-P-OP2	-5.83	100.46	105.70
1	1A	2621	U	C6-N1-C2	5.83	124.50	121.00
32	1a	297	G	C8-N9-C4	5.83	108.73	106.40
32	2a	266	G	C6-C5-N7	-5.83	126.91	130.40
1	1A	20	C	C4-C5-C6	5.82	120.31	117.40
1	1A	1449	C	C2-N3-C4	-5.82	116.99	119.90
1	1A	1456	G	N3-C4-N9	-5.82	122.51	126.00
1	1A	1728	G	N3-C4-N9	-5.82	122.51	126.00
1	1A	2125	C	C2-N3-C4	5.82	122.81	119.90
32	1a	1442	G	N1-C6-O6	-5.82	116.41	119.90
1	2A	1632	A	N7-C8-N9	-5.82	110.89	113.80
1	1A	2611	G	N3-C4-N9	-5.82	122.51	126.00
32	2a	901	A	N1-C2-N3	5.82	132.21	129.30
1	1A	2537	G	N3-C2-N2	5.82	123.97	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1006	C	N1-C2-O2	5.82	122.39	118.90
1	2A	1466	G	N7-C8-N9	-5.82	110.19	113.10
1	2A	2549	G	OP1-P-OP2	5.82	128.33	119.60
1	2A	2852	G	N9-C4-C5	-5.82	103.07	105.40
32	2a	122	G	N3-C4-C5	-5.82	125.69	128.60
1	1A	1714	G	C4-C5-N7	-5.82	108.47	110.80
1	1A	115	G	C6-N1-C2	-5.82	121.61	125.10
1	1A	213	G	O5'-P-OP2	-5.82	100.46	105.70
1	1A	731	G	N1-C2-N3	-5.82	120.41	123.90
1	1A	906	G	N3-C4-C5	5.82	131.51	128.60
1	1A	2280	A	C8-N9-C4	-5.82	103.47	105.80
23	11	61	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	2A	576	U	N1-C2-N3	5.82	118.39	114.90
1	2A	1332	G	N1-C6-O6	5.82	123.39	119.90
1	1A	2074	G	C8-N9-C4	-5.82	104.07	106.40
1	1A	2239	A	C2-N3-C4	5.82	113.51	110.60
32	1a	1437	C	O5'-P-OP1	-5.82	100.47	105.70
1	1A	2641	A	C5-N7-C8	-5.81	100.99	103.90
1	1A	2056	U	C5-C4-O4	5.81	129.39	125.90
32	2a	1134	G	N3-C4-C5	-5.81	125.69	128.60
1	1A	174	U	C2-N3-C4	-5.81	123.51	127.00
1	1A	209	G	C5-C6-O6	-5.81	125.11	128.60
1	1A	1151	U	C4-C5-C6	-5.81	116.21	119.70
1	1A	2370	G	N1-C6-O6	-5.81	116.41	119.90
1	2A	1954	G	OP1-P-OP2	5.81	128.32	119.60
1	1A	2560	G	N9-C4-C5	5.81	107.72	105.40
1	1A	2651	A	C8-N9-C4	5.81	108.12	105.80
32	1a	794	A	C5-C6-N1	-5.81	114.80	117.70
32	1a	1030(C)	G	C8-N9-C4	-5.81	104.08	106.40
1	2A	417	C	C6-N1-C2	-5.81	117.98	120.30
1	2A	2462	U	O5'-P-OP2	-5.81	100.47	105.70
1	2A	2807	G	N3-C4-N9	-5.81	122.51	126.00
1	1A	2403	G	OP1-P-OP2	5.81	128.31	119.60
1	1A	566	C	OP1-P-OP2	5.80	128.31	119.60
1	1A	1375	U	O5'-P-OP1	5.80	117.67	110.70
1	1A	2083	G	C2-N3-C4	5.80	114.80	111.90
1	2A	2085	C	C6-N1-C2	5.80	122.62	120.30
1	2A	2175	C	C2-N1-C1'	-5.80	112.42	118.80
32	2a	860	A	O5'-P-OP2	5.80	117.67	110.70
1	1A	1232	G	C4-C5-N7	5.80	113.12	110.80
1	1A	588	C	C6-N1-C2	-5.80	117.98	120.30
1	1A	2759	U	C5-C6-N1	-5.80	119.80	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1037	C	N3-C4-C5	-5.80	119.58	121.90
32	1a	1527	C	N3-C4-N4	5.80	122.06	118.00
1	1A	1178	A	OP1-P-OP2	5.80	128.30	119.60
1	2A	1264	G	OP1-P-OP2	5.80	128.30	119.60
32	2a	1152	A	C8-N9-C4	-5.80	103.48	105.80
1	1A	201	G	N3-C4-C5	5.80	131.50	128.60
2	1B	56	G	O5'-P-OP1	5.80	117.66	110.70
32	1a	158	G	C4-C5-N7	-5.80	108.48	110.80
32	1a	454	C	O5'-P-OP2	-5.80	100.48	105.70
32	1a	575	G	O4'-C1'-N9	-5.80	103.56	108.20
32	1a	732	C	N3-C4-N4	-5.80	113.94	118.00
1	2A	774	A	C8-N9-C4	-5.80	103.48	105.80
32	2a	351	G	N3-C4-C5	5.80	131.50	128.60
32	2a	1108	G	N3-C4-C5	-5.80	125.70	128.60
1	1A	596	G	C6-N1-C2	-5.79	121.62	125.10
1	1A	795	G	C5-C6-N1	5.79	114.40	111.50
1	1A	473	A	N1-C2-N3	5.79	132.20	129.30
1	1A	1823	G	C4-C5-N7	-5.79	108.48	110.80
1	1A	2245	U	C5-C4-O4	5.79	129.38	125.90
1	1A	2620	G	N9-C1'-C2'	-5.79	105.63	112.00
1	2A	1775	U	N1-C2-O2	-5.79	118.75	122.80
1	2A	2057	A	O5'-P-OP1	5.79	117.65	110.70
1	2A	2208	A	O4'-C1'-N9	5.79	112.83	108.20
1	2A	846	C	C6-N1-C2	5.79	122.62	120.30
1	2A	2318	G	N7-C8-N9	5.79	116.00	113.10
1	2A	2559	C	C6-N1-C2	5.79	122.62	120.30
32	2a	1139	G	C5-N7-C8	5.79	107.20	104.30
1	1A	563	G	C8-N9-C4	-5.79	104.08	106.40
32	1a	1299	A	C8-N9-C4	-5.79	103.48	105.80
1	2A	1244	G	N9-C4-C5	-5.79	103.08	105.40
1	2A	2009	G	N3-C4-N9	-5.79	122.53	126.00
1	1A	1653	C	C5-C4-N4	-5.79	116.15	120.20
1	1A	1869	C	O5'-P-OP2	-5.79	100.49	105.70
1	1A	2319	G	C5-C6-O6	-5.79	125.13	128.60
1	1A	2352	G	O5'-P-OP2	-5.79	100.49	105.70
1	1A	2358	A	C2-N3-C4	-5.79	107.70	110.60
1	1A	2434	A	N7-C8-N9	5.79	116.69	113.80
1	2A	455	C	N1-C2-O2	5.79	122.37	118.90
1	2A	942	G	C8-N9-C4	5.79	108.72	106.40
1	2A	1085	A	C8-N9-C4	5.79	108.11	105.80
1	1A	849	A	C8-N9-C4	-5.79	103.48	105.80
1	1A	1728	G	C5-N7-C8	-5.79	101.41	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2063	U	OP2-P-O3'	5.79	117.93	105.20
1	1A	2552	C	N3-C4-N4	-5.79	113.95	118.00
1	2A	203	C	C6-N1-C2	5.79	122.61	120.30
1	2A	1997	G	C5'-C4'-O4'	5.79	116.04	109.10
1	2A	2783	G	N9-C4-C5	5.79	107.71	105.40
1	1A	435	G	C5-N7-C8	5.78	107.19	104.30
1	1A	859	C	N3-C2-O2	5.78	125.95	121.90
1	1A	1472	G	C4-C5-N7	5.78	113.11	110.80
1	2A	1652	A	OP1-P-OP2	5.78	128.28	119.60
1	2A	1769	G	C4-C5-N7	5.78	113.11	110.80
1	2A	2197	U	N1-C2-O2	5.78	126.85	122.80
1	2A	2780	G	O4'-C1'-N9	-5.78	103.57	108.20
32	2a	768	A	C2-N3-C4	-5.78	107.71	110.60
1	1A	819	C	C2-N3-C4	-5.78	117.01	119.90
1	1A	2783	G	C5-C6-O6	-5.78	125.13	128.60
1	1A	1427	G	C4-C5-N7	-5.78	108.49	110.80
2	1B	117	G	O5'-P-OP2	-5.78	100.50	105.70
1	2A	232	G	C8-N9-C4	5.78	108.71	106.40
1	2A	867	C	C6-N1-C2	5.78	122.61	120.30
1	2A	1863	G	C8-N9-C4	5.78	108.71	106.40
1	1A	1303	C	C5-C6-N1	-5.78	118.11	121.00
1	1A	2239	A	C8-N9-C4	-5.78	103.49	105.80
1	2A	2416	C	N3-C4-C5	-5.78	119.59	121.90
1	1A	1433	C	N3-C2-O2	-5.78	117.86	121.90
1	1A	2674	A	N7-C8-N9	5.78	116.69	113.80
1	2A	248	G	N9-C4-C5	5.78	107.71	105.40
1	2A	784	A	C8-N9-C4	5.78	108.11	105.80
1	2A	2508	G	O5'-P-OP2	5.78	117.63	110.70
1	1A	1068	G	N3-C4-C5	5.78	131.49	128.60
1	1A	1316	C	C2-N1-C1'	-5.78	112.45	118.80
1	1A	1648	U	C5-C6-N1	-5.78	119.81	122.70
1	1A	2452	C	OP1-P-OP2	5.78	128.26	119.60
1	2A	698	C	OP1-P-OP2	5.78	128.26	119.60
1	2A	788	A	C6-C5-N7	-5.78	128.26	132.30
1	2A	1655	A	N7-C8-N9	-5.78	110.91	113.80
1	2A	2836	U	N3-C2-O2	-5.78	118.16	122.20
1	2A	2506	U	O4'-C1'-N1	5.77	112.82	108.20
1	1A	2029	C	N3-C4-C5	5.77	124.21	121.90
1	1A	2620	G	N3-C2-N2	-5.77	115.86	119.90
1	1A	2654	G	N3-C2-N2	5.77	123.94	119.90
32	1a	776	G	N9-C4-C5	-5.77	103.09	105.40
1	2A	145	G	C8-N9-C4	5.77	108.71	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1047	G	N3-C4-N9	5.77	129.46	126.00
1	1A	2514	G	C5-N7-C8	-5.77	101.42	104.30
1	2A	1208	C	N1-C2-O2	-5.77	115.44	118.90
1	2A	2467	C	N3-C2-O2	-5.77	117.86	121.90
2	2B	1	U	C2-N1-C1'	5.77	124.62	117.70
1	1A	1947	C	O5'-P-OP1	-5.77	100.51	105.70
1	1A	2572	C	N1-C2-N3	5.77	123.24	119.20
29	17	10	ARG	NE-CZ-NH2	-5.77	117.42	120.30
32	1a	142	G	C4-N9-C1'	-5.77	119.00	126.50
32	1a	1385	G	O5'-P-OP2	-5.77	100.51	105.70
1	2A	738	G	N1-C6-O6	-5.77	116.44	119.90
1	2A	2858	C	N3-C4-C5	5.77	124.21	121.90
32	2a	189(A)	C	C6-N1-C2	5.77	122.61	120.30
32	2a	833	U	N3-C2-O2	-5.77	118.16	122.20
1	1A	475	A	N7-C8-N9	-5.77	110.92	113.80
1	1A	703	G	C2-N3-C4	-5.77	109.02	111.90
1	1A	770	G	N3-C4-N9	5.77	129.46	126.00
1	1A	1306	G	C2-N3-C4	-5.77	109.02	111.90
1	1A	2514	G	N1-C2-N2	-5.77	111.01	116.20
1	1A	2789	A	C5-C6-N6	5.77	128.31	123.70
32	1a	1391	U	N3-C2-O2	-5.77	118.16	122.20
1	2A	481	G	O5'-P-OP1	5.77	117.62	110.70
1	2A	2599	G	C5-N7-C8	5.77	107.18	104.30
1	1A	35	G	OP2-P-O3'	5.77	117.89	105.20
32	1a	696	A	C5-C6-N6	-5.77	119.09	123.70
1	1A	1022	C	OP2-P-O3'	5.76	117.88	105.20
1	1A	2384	G	C5-C6-O6	-5.76	125.14	128.60
1	2A	878	A	N7-C8-N9	5.76	116.68	113.80
1	2A	1076	C	C5-C6-N1	5.76	123.88	121.00
32	2a	662	G	C5-C6-O6	-5.76	125.14	128.60
1	2A	1251	C	OP1-P-OP2	5.76	128.24	119.60
32	2a	623	C	C5-C4-N4	-5.76	116.17	120.20
1	1A	651	U	C6-N1-C2	-5.76	117.54	121.00
1	1A	1870	G	O5'-P-OP2	-5.76	100.52	105.70
1	2A	8	A	O5'-P-OP2	5.76	117.61	110.70
1	2A	2893	G	N9-C4-C5	-5.76	103.10	105.40
1	1A	1640	G	N3-C4-N9	-5.76	122.54	126.00
1	1A	1867	C	N1-C2-O2	5.76	122.36	118.90
1	1A	2134	G	N3-C4-N9	5.76	129.46	126.00
1	1A	2416	C	OP2-P-O3'	5.76	117.87	105.20
1	2A	94(A)	G	C6-N1-C2	-5.76	121.64	125.10
1	2A	97	C	C6-N1-C2	5.76	122.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	192	C	N3-C4-C5	5.76	124.20	121.90
2	1B	81	G	C5-C6-O6	5.76	132.06	128.60
1	2A	349	G	C4-C5-N7	-5.76	108.50	110.80
1	2A	2805	G	N3-C2-N2	5.76	123.93	119.90
1	1A	436	C	C2-N3-C4	-5.76	117.02	119.90
1	1A	572	A	C2-N3-C4	5.76	113.48	110.60
1	1A	2291	G	C5-C6-O6	-5.76	125.15	128.60
32	1a	339	C	C5-C6-N1	-5.76	118.12	121.00
32	1a	971	G	N3-C4-N9	-5.76	122.55	126.00
32	2a	1290	G	C8-N9-C4	-5.76	104.10	106.40
1	1A	35	G	N7-C8-N9	-5.75	110.22	113.10
1	1A	500	G	C5-C6-O6	5.75	132.05	128.60
1	1A	2418	U	C5-C6-N1	-5.75	119.82	122.70
1	1A	2513	C	C2-N1-C1'	-5.75	112.47	118.80
1	2A	515	A	O5'-P-OP1	-5.75	100.52	105.70
1	1A	533	G	O5'-P-OP1	-5.75	100.52	105.70
1	1A	1646	C	C5-C6-N1	-5.75	118.12	121.00
1	1A	2409	G	C5-C6-O6	-5.75	125.15	128.60
32	1a	1181	G	N3-C4-C5	5.75	131.48	128.60
1	2A	460	A	N1-C6-N6	5.75	122.05	118.60
32	2a	47	C	OP1-P-O3'	5.75	117.86	105.20
32	2a	872	A	C8-N9-C4	-5.75	103.50	105.80
1	1A	782	A	O5'-P-OP1	-5.75	100.52	105.70
1	1A	877	G	C5-C6-O6	5.75	132.05	128.60
1	1A	1278	G	C2-N3-C4	5.75	114.78	111.90
1	1A	1978	U	N1-C2-N3	5.75	118.35	114.90
2	1B	27	C	C6-N1-C2	5.75	122.60	120.30
32	1a	299	G	N9-C4-C5	-5.75	103.10	105.40
1	2A	464	U	C2-N3-C4	-5.75	123.55	127.00
1	2A	570	G	C5-C6-N1	5.75	114.38	111.50
2	2B	2	C	N1-C2-O2	5.75	122.35	118.90
1	1A	1700	G	C2'-C3'-O3'	5.75	122.90	113.70
1	1A	418	G	N1-C2-N3	5.75	127.35	123.90
1	1A	2179	G	C4-C5-N7	-5.75	108.50	110.80
2	1B	101	G	N1-C6-O6	5.75	123.35	119.90
32	1a	795	C	N3-C2-O2	5.75	125.92	121.90
1	2A	2032	G	C6-N1-C2	-5.75	121.65	125.10
32	2a	630	G	N7-C8-N9	5.75	115.97	113.10
1	1A	30	G	C5-N7-C8	5.75	107.17	104.30
1	1A	733	G	N7-C8-N9	-5.75	110.23	113.10
1	1A	1056	A	C2-N3-C4	-5.75	107.73	110.60
1	1A	1306	G	C5-C6-O6	5.75	132.05	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1798	U	OP2-P-O3'	5.75	117.84	105.20
1	2A	2540	C	O5'-P-OP2	-5.75	100.53	105.70
32	1a	1067	A	N9-C4-C5	5.75	108.10	105.80
1	2A	1178	C	C6-N1-C2	5.75	122.60	120.30
1	2A	1445(A)	C	C6-N1-C2	-5.75	118.00	120.30
1	1A	462	C	N1-C2-O2	-5.74	115.45	118.90
1	1A	837	C	C5-C4-N4	-5.74	116.18	120.20
1	1A	1076	G	N7-C8-N9	-5.74	110.23	113.10
1	1A	1102	G	C4-C5-N7	5.74	113.10	110.80
1	1A	1336	C	N3-C4-C5	-5.74	119.60	121.90
32	1a	162	A	N1-C6-N6	5.74	122.05	118.60
32	1a	428	G	O5'-P-OP2	-5.74	100.53	105.70
32	2a	281	G	C6-C5-N7	-5.74	126.95	130.40
1	1A	2194	U	N1-C2-N3	5.74	118.34	114.90
32	1a	1495	U	C6-N1-C2	-5.74	117.56	121.00
1	2A	2641	G	OP2-P-O3'	5.74	117.83	105.20
1	1A	2080	A	N7-C8-N9	-5.74	110.93	113.80
2	1B	69	G	OP2-P-O3'	5.74	117.83	105.20
32	1a	794	A	C6-N1-C2	5.74	122.04	118.60
1	2A	195	A	P-O3'-C3'	5.74	126.59	119.70
1	2A	666	G	N1-C6-O6	5.74	123.34	119.90
32	2a	1065	U	P-O3'-C3'	5.74	126.59	119.70
1	1A	468	G	C5-C6-O6	-5.74	125.16	128.60
1	1A	1155	C	C6-N1-C2	-5.74	118.00	120.30
1	1A	1253	C	C2-N3-C4	-5.74	117.03	119.90
1	1A	1959	A	OP1-P-OP2	5.74	128.21	119.60
1	1A	2302	G	N1-C6-O6	-5.74	116.46	119.90
1	1A	2464	C	C2-N3-C4	-5.74	117.03	119.90
1	1A	2623	U	C4-C5-C6	5.74	123.14	119.70
1	1A	2692	C	C6-N1-C2	-5.74	118.00	120.30
2	2B	22	U	C6-N1-C2	-5.74	117.56	121.00
1	1A	1240	G	C8-N9-C4	-5.74	104.11	106.40
1	1A	2779	G	C5-C6-O6	5.74	132.04	128.60
1	1A	2640	C	O5'-P-OP2	-5.74	100.54	105.70
32	1a	141	A	O5'-P-OP2	-5.74	100.54	105.70
1	2A	1632	A	C5-N7-C8	5.74	106.77	103.90
1	1A	981	C	N1-C2-O2	-5.73	115.46	118.90
1	1A	1191	C	C6-N1-C2	5.73	122.59	120.30
1	2A	864	G	OP1-P-OP2	-5.73	111.00	119.60
1	1A	974	G	OP1-P-OP2	-5.73	111.00	119.60
1	1A	1007	G	N3-C2-N2	-5.73	115.89	119.90
1	1A	1370	G	N1-C2-N2	-5.73	111.04	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1650	C	O5'-P-OP1	-5.73	100.54	105.70
1	1A	1696	G	OP2-P-O3'	5.73	117.81	105.20
32	1a	1082	G	N9-C4-C5	-5.73	103.11	105.40
1	1A	1299	A	C6-N1-C2	-5.73	115.16	118.60
1	1A	1675	U	N3-C2-O2	-5.73	118.19	122.20
1	1A	2055	A	OP1-P-OP2	-5.73	111.00	119.60
1	2A	207	A	N1-C2-N3	5.73	132.16	129.30
1	2A	1926	U	C6-N1-C1'	5.73	129.22	121.20
2	2B	5	C	C5-C6-N1	-5.73	118.14	121.00
32	1a	169	C	C5-C6-N1	-5.73	118.14	121.00
1	1A	1816	A	C8-N9-C4	-5.73	103.51	105.80
1	1A	2025	G	C5-N7-C8	5.73	107.16	104.30
32	1a	607	A	C4-C5-C6	5.73	119.86	117.00
32	1a	1524	C	C5-C6-N1	-5.73	118.14	121.00
1	2A	906	G	C6-N1-C2	5.73	128.54	125.10
1	2A	1427	A	C5-C6-N1	5.73	120.56	117.70
32	2a	1014	A	N7-C8-N9	5.73	116.66	113.80
1	1A	952	G	C6-C5-N7	5.73	133.84	130.40
1	1A	177	G	C5-C6-O6	5.72	132.03	128.60
1	1A	765	A	C6-C5-N7	-5.72	128.29	132.30
1	1A	852	G	N3-C4-C5	-5.72	125.74	128.60
1	1A	2602	A	C8-N9-C4	5.72	108.09	105.80
32	1a	1033	G	N3-C2-N2	5.72	123.91	119.90
32	1a	1532	U	C6-N1-C2	-5.72	117.56	121.00
1	2A	1124	C	O5'-P-OP1	-5.72	100.55	105.70
1	2A	1577	C	O5'-P-OP2	-5.72	100.55	105.70
32	2a	795	C	N3-C2-O2	-5.72	117.89	121.90
1	1A	657	A	O5'-P-OP2	5.72	117.57	110.70
1	1A	902	G	C4-C5-N7	5.72	113.09	110.80
1	1A	989	G	C4-N9-C1'	5.72	133.94	126.50
1	1A	1966	U	N3-C4-C5	5.72	118.03	114.60
1	1A	2402	U	C4-C5-C6	5.72	123.13	119.70
1	1A	2442	A	O5'-P-OP2	-5.72	100.55	105.70
1	1A	2902	G	C6-N1-C2	5.72	128.53	125.10
2	1B	71	C	C4-C5-C6	5.72	120.26	117.40
1	2A	363(E)	U	C5-C4-O4	-5.72	122.47	125.90
1	2A	1806	C	C2-N1-C1'	-5.72	112.50	118.80
1	2A	2588	G	N1-C6-O6	5.72	123.33	119.90
32	2a	115	G	N1-C6-O6	-5.72	116.47	119.90
32	2a	458	C	N1-C2-O2	5.72	122.33	118.90
1	1A	1358	U	N3-C4-O4	-5.72	115.39	119.40
32	1a	446	G	C5-C6-O6	-5.72	125.17	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	883	G	C6-C5-N7	5.72	133.83	130.40
1	1A	476	G	OP1-P-OP2	5.72	128.18	119.60
1	1A	569	G	N7-C8-N9	5.72	115.96	113.10
1	1A	1870	G	OP1-P-OP2	5.72	128.18	119.60
1	1A	2053	A	C5-C6-N1	-5.72	114.84	117.70
1	1A	2633	A	N1-C2-N3	-5.72	126.44	129.30
32	1a	699	C	N3-C2-O2	-5.72	117.90	121.90
1	2A	1082	U	N1-C2-O2	5.72	126.80	122.80
32	2a	518	C	C6-N1-C2	-5.72	118.01	120.30
32	1a	647	C	N3-C4-C5	-5.72	119.61	121.90
1	2A	2532	G	C5-C6-O6	-5.72	125.17	128.60
32	2a	500	G	C5-C6-O6	-5.72	125.17	128.60
1	1A	491	G	C5-C6-O6	-5.72	125.17	128.60
1	1A	1480	A	N1-C2-N3	5.72	132.16	129.30
1	2A	956	G	C2-N3-C4	-5.72	109.04	111.90
1	1A	283	G	N3-C2-N2	-5.71	115.90	119.90
1	1A	1200	G	N1-C2-N3	5.71	127.33	123.90
1	1A	2596	U	C6-N1-C1'	5.71	129.20	121.20
1	1A	2814	C	C6-N1-C2	-5.71	118.01	120.30
32	1a	1054	C	C5-C4-N4	5.71	124.20	120.20
1	2A	647	G	C8-N9-C4	-5.71	104.11	106.40
1	2A	759	G	O5'-P-OP1	-5.71	100.56	105.70
1	2A	2250	G	N1-C6-O6	-5.71	116.47	119.90
32	2a	1495	U	C6-N1-C2	-5.71	117.57	121.00
32	1a	1513	A	C5-C6-N1	5.71	120.56	117.70
32	2a	1452	C	N3-C2-O2	-5.71	117.90	121.90
1	1A	2713	C	N1-C2-N3	5.71	123.20	119.20
32	1a	482	A	OP1-P-O3'	5.71	117.77	105.20
32	2a	1152	A	N7-C8-N9	5.71	116.66	113.80
1	1A	1104	G	C8-N9-C4	5.71	108.68	106.40
1	1A	2138	G	C8-N9-C1'	-5.71	119.58	127.00
32	2a	230	G	N3-C2-N2	-5.71	115.90	119.90
1	1A	838	C	N3-C4-C5	5.71	124.18	121.90
1	1A	932	C	O5'-P-OP1	5.71	117.55	110.70
1	1A	1749	G	OP2-P-O3'	5.71	117.76	105.20
1	1A	2298	A	C4-C5-C6	5.71	119.85	117.00
1	1A	2612	A	N1-C2-N3	5.71	132.15	129.30
1	2A	330	A	O4'-C1'-N9	5.71	112.77	108.20
1	2A	960	A	N1-C6-N6	5.71	122.03	118.60
1	2A	1332	G	C6-C5-N7	-5.71	126.97	130.40
2	2B	30	C	N3-C4-C5	-5.71	119.62	121.90
2	1B	4	C	N1-C2-O2	-5.71	115.48	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	123	G	C8-N9-C4	5.71	108.68	106.40
1	2A	2372	G	C5-C6-O6	-5.71	125.18	128.60
32	2a	354	G	O5'-P-OP2	-5.71	100.56	105.70
1	1A	976	G	O5'-P-OP2	-5.70	100.57	105.70
1	1A	2346	G	OP2-P-O3'	5.70	117.75	105.20
2	1B	55	U	N1-C2-O2	-5.70	118.81	122.80
5	1F	53	THR	N-CA-CB	-5.70	99.47	110.30
1	2A	421	U	OP1-P-O3'	5.70	117.75	105.20
1	2A	756	C	C6-N1-C2	-5.70	118.02	120.30
1	2A	1379	A	N1-C6-N6	5.70	122.02	118.60
1	2A	1847	A	O5'-P-OP1	5.70	117.54	110.70
1	2A	1959	G	OP2-P-O3'	5.70	117.75	105.20
1	2A	2432	A	N9-C4-C5	-5.70	103.52	105.80
2	2B	27	C	N1-C2-O2	5.70	122.32	118.90
1	1A	2902	G	C4-C5-C6	-5.70	115.38	118.80
32	1a	820	U	N1-C2-N3	5.70	118.32	114.90
1	2A	531	C	C5-C6-N1	-5.70	118.15	121.00
1	2A	2138	C	N3-C4-C5	-5.70	119.62	121.90
1	1A	2745	G	N9-C4-C5	5.70	107.68	105.40
1	2A	2168	G	C8-N9-C4	-5.70	104.12	106.40
1	1A	451	G	C6-C5-N7	5.70	133.82	130.40
1	1A	1262	C	N1-C2-N3	5.70	123.19	119.20
1	1A	1358	U	C5-C6-N1	-5.70	119.85	122.70
1	1A	1994	A	C2-N3-C4	-5.70	107.75	110.60
1	1A	2134	G	N1-C6-O6	-5.70	116.48	119.90
1	1A	882	A	C2-N3-C4	5.70	113.45	110.60
1	1A	2092	G	N1-C6-O6	-5.70	116.48	119.90
1	1A	2116	G	N1-C6-O6	-5.70	116.48	119.90
13	1R	67	LEU	CA-CB-CG	5.70	128.40	115.30
32	1a	266	G	C4-N9-C1'	5.70	133.91	126.50
32	1a	1283	G	C8-N9-C4	-5.70	104.12	106.40
1	2A	508	G	N1-C6-O6	5.70	123.32	119.90
1	1A	308	U	N3-C4-O4	5.70	123.39	119.40
1	2A	1071	G	C5-C6-N1	-5.70	108.65	111.50
1	2A	2319	G	C4-C5-N7	5.70	113.08	110.80
1	2A	2517	C	O5'-P-OP2	-5.70	100.57	105.70
32	2a	1222	G	C5-C6-O6	-5.70	125.18	128.60
1	2A	2804	C	C5-C6-N1	5.69	123.85	121.00
32	2a	576	G	C8-N9-C4	5.69	108.68	106.40
1	1A	369	A	C6-N1-C2	-5.69	115.18	118.60
1	1A	1138	C	N3-C4-C5	5.69	124.18	121.90
1	1A	1775	C	C6-N1-C2	-5.69	118.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1884	A	N7-C8-N9	-5.69	110.95	113.80
1	2A	2238	G	N3-C2-N2	-5.69	115.92	119.90
32	2a	278	G	N1-C6-O6	-5.69	116.48	119.90
32	2a	485	G	N3-C4-N9	5.69	129.42	126.00
32	2a	1401	G	C8-N9-C4	5.69	108.68	106.40
1	1A	610	C	OP1-P-O3'	5.69	117.72	105.20
1	1A	1487	G	O5'-P-OP2	-5.69	100.58	105.70
1	1A	2550	C	C2-N3-C4	-5.69	117.06	119.90
1	1A	2622	C	N3-C4-N4	5.69	121.98	118.00
32	1a	394	G	C8-N9-C4	-5.69	104.12	106.40
32	1a	507	C	N1-C2-O2	5.69	122.31	118.90
32	2a	1487	G	N3-C2-N2	-5.69	115.92	119.90
1	1A	60	G	N3-C4-N9	-5.69	122.59	126.00
1	1A	2191	A	C4-C5-C6	-5.69	114.16	117.00
1	1A	121	G	OP1-P-OP2	5.69	128.13	119.60
1	1A	645	G	C2-N3-C4	5.69	114.74	111.90
1	1A	1126	C	C2-N3-C4	5.69	122.74	119.90
1	1A	1700	G	OP2-P-O3'	-5.69	92.69	105.20
1	1A	2511	C	C5-C6-N1	5.69	123.84	121.00
32	1a	613	C	O5'-P-OP2	-5.69	100.58	105.70
32	1a	938	A	O5'-P-OP1	-5.69	100.58	105.70
32	1a	1406	U	N3-C4-O4	-5.69	115.42	119.40
1	2A	1271	G	N9-C4-C5	-5.69	103.12	105.40
1	2A	1618	A	N9-C4-C5	5.69	108.08	105.80
32	2a	796	C	C6-N1-C2	5.69	122.58	120.30
1	1A	42	G	C4-C5-N7	5.69	113.07	110.80
1	1A	1210	G	N7-C8-N9	-5.69	110.26	113.10
1	1A	1788	U	N3-C2-O2	5.69	126.18	122.20
1	1A	1854	G	OP2-P-O3'	5.69	117.71	105.20
1	1A	2580	C	N3-C4-N4	5.69	121.98	118.00
1	1A	747	G	C5-C6-O6	5.68	132.01	128.60
1	1A	2250	G	C5'-C4'-O4'	-5.68	102.28	109.10
1	1A	2580	C	OP2-P-O3'	5.68	117.70	105.20
32	1a	821	G	N1-C6-O6	5.68	123.31	119.90
1	2A	1630	G	C4-C5-N7	-5.68	108.53	110.80
1	2A	2538	C	O5'-P-OP1	-5.68	100.58	105.70
1	1A	96	C	N3-C4-C5	-5.68	119.63	121.90
1	1A	579	G	C5-C6-O6	5.68	132.01	128.60
1	1A	2273	C	N3-C2-O2	-5.68	117.92	121.90
1	1A	2569	G	C5-N7-C8	5.68	107.14	104.30
32	1a	576	G	N1-C2-N2	-5.68	111.09	116.20
1	2A	493	G	O5'-P-OP1	-5.68	100.59	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1269	A	C2-N3-C4	-5.68	107.76	110.60
32	2a	52	G	C4-C5-N7	5.68	113.07	110.80
1	1A	992	G	C4-C5-N7	-5.68	108.53	110.80
1	1A	2423	A	C5-N7-C8	-5.68	101.06	103.90
32	1a	1182	G	N1-C6-O6	-5.68	116.49	119.90
32	2a	352	C	OP2-P-O3'	5.68	117.70	105.20
1	1A	495	G	N1-C2-N2	5.68	121.31	116.20
1	1A	641	G	OP2-P-O3'	5.68	117.69	105.20
1	1A	807	G	N1-C2-N2	-5.68	111.09	116.20
1	1A	2088	C	N3-C4-C5	-5.68	119.63	121.90
1	1A	2738	A	C5-N7-C8	-5.68	101.06	103.90
1	2A	2233	U	N1-C2-O2	-5.68	118.83	122.80
1	2A	2838	G	N3-C2-N2	-5.68	115.92	119.90
32	2a	686	U	C2-N3-C4	-5.68	123.59	127.00
1	1A	2007	G	N1-C6-O6	-5.68	116.49	119.90
32	1a	220	G	N3-C4-C5	-5.68	125.76	128.60
1	1A	1168	G	C5-C6-N1	5.68	114.34	111.50
1	1A	1184	G	C4-C5-N7	-5.68	108.53	110.80
1	2A	2046	G	N9-C4-C5	-5.68	103.13	105.40
1	2A	2275	C	C5'-C4'-O4'	-5.68	102.29	109.10
32	2a	411	A	C8-N9-C4	-5.68	103.53	105.80
32	2a	1484	C	N3-C4-C5	5.68	124.17	121.90
1	1A	1201	A	C5-C6-N6	-5.67	119.16	123.70
32	1a	595	G	C8-N9-C1'	-5.67	119.62	127.00
1	2A	1572	A	O5'-P-OP2	-5.67	100.59	105.70
32	2a	52	G	N9-C4-C5	-5.67	103.13	105.40
32	2a	509	A	C8-N9-C4	-5.67	103.53	105.80
32	1a	1030	C	C2-N3-C4	5.67	122.74	119.90
32	1a	1062	U	O5'-P-OP2	-5.67	100.59	105.70
1	1A	199	C	OP2-P-O3'	5.67	117.68	105.20
1	1A	1845	G	C6-C5-N7	-5.67	127.00	130.40
1	1A	2023	A	N1-C6-N6	-5.67	115.20	118.60
1	1A	2283	G	N1-C2-N2	-5.67	111.10	116.20
1	1A	2406	C	N1-C2-N3	5.67	123.17	119.20
2	1B	111	G	N1-C6-O6	-5.67	116.50	119.90
32	1a	133	U	N3-C2-O2	5.67	126.17	122.20
32	1a	831	U	C6-N1-C2	-5.67	117.60	121.00
1	1A	1314	A	N1-C2-N3	5.67	132.13	129.30
32	1a	596	C	N3-C2-O2	-5.67	117.93	121.90
1	2A	1763	G	C4-C5-N7	-5.67	108.53	110.80
1	1A	353	G	O4'-C1'-N9	-5.67	103.67	108.20
1	1A	1279	C	N3-C4-C5	5.67	124.17	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	490	G	O5'-P-OP2	-5.67	100.60	105.70
1	2A	1056	G	N1-C6-O6	5.67	123.30	119.90
1	2A	1104	C	C2-N1-C1'	-5.67	112.56	118.80
1	2A	1863	G	N9-C4-C5	-5.67	103.13	105.40
1	2A	2162	G	N3-C4-N9	5.67	129.40	126.00
1	1A	213	G	N1-C6-O6	-5.67	116.50	119.90
1	1A	1474	C	N1-C2-O2	-5.67	115.50	118.90
1	1A	1649	A	N1-C2-N3	-5.67	126.47	129.30
1	1A	1684	A	OP2-P-O3'	5.67	117.67	105.20
1	1A	2054	G	C5-C6-N1	-5.67	108.67	111.50
1	1A	2740	G	C8-N9-C4	-5.67	104.13	106.40
1	2A	260	G	C4-C5-N7	-5.67	108.53	110.80
1	2A	669	G	OP1-P-OP2	-5.67	111.10	119.60
32	2a	93	G	C4-N9-C1'	-5.67	119.13	126.50
32	2a	1442	G	N3-C4-C5	-5.67	125.77	128.60
32	1a	329	A	N1-C6-N6	5.67	122.00	118.60
1	1A	12	U	N3-C2-O2	-5.66	118.23	122.20
1	1A	2158	C	C2-N1-C1'	5.66	125.03	118.80
1	1A	2516	U	N3-C4-O4	-5.66	115.44	119.40
1	1A	2697	G	O5'-P-OP2	-5.66	100.60	105.70
1	2A	2378	A	N3-C4-N9	5.66	131.93	127.40
1	2A	2725	A	C2-N3-C4	-5.66	107.77	110.60
32	2a	833	U	OP2-P-O3'	5.66	117.66	105.20
1	1A	283	G	C4-C5-N7	-5.66	108.53	110.80
1	1A	702	A	O4'-C1'-N9	5.66	112.73	108.20
1	1A	1655	A	N1-C2-N3	-5.66	126.47	129.30
32	2a	902	G	C4-C5-N7	-5.66	108.53	110.80
1	1A	31	C	C6-N1-C2	-5.66	118.04	120.30
1	1A	1447	G	N3-C4-N9	-5.66	122.60	126.00
1	1A	1829	U	C2-N3-C4	-5.66	123.60	127.00
1	2A	227	A	N1-C2-N3	5.66	132.13	129.30
32	2a	1445	C	C6-N1-C2	5.66	122.56	120.30
1	1A	648	G	C5-C6-N1	5.66	114.33	111.50
1	1A	770	G	N3-C2-N2	5.66	123.86	119.90
1	1A	1630	A	C4-C5-C6	-5.66	114.17	117.00
1	1A	2193	A	N9-C4-C5	-5.66	103.54	105.80
1	1A	2737	C	OP2-P-O3'	5.66	117.65	105.20
1	2A	228	A	N3-C4-N9	-5.66	122.87	127.40
1	2A	630	G	N1-C6-O6	-5.66	116.50	119.90
1	2A	690	G	C5-N7-C8	5.66	107.13	104.30
1	2A	1416	G	C4-N9-C1'	-5.66	119.14	126.50
1	2A	1992	G	O4'-C1'-N9	-5.66	103.67	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	142	G	N1-C2-N2	-5.66	111.11	116.20
1	1A	1590	C	N3-C2-O2	5.66	125.86	121.90
1	1A	2262	G	N1-C6-O6	-5.66	116.51	119.90
1	2A	2681	C	N3-C2-O2	-5.66	117.94	121.90
1	1A	46	C	C6-N1-C2	-5.66	118.04	120.30
1	1A	1802	C	C4-C5-C6	5.66	120.23	117.40
1	2A	2707	G	N1-C6-O6	5.66	123.29	119.90
32	2a	64	G	N1-C6-O6	5.66	123.29	119.90
32	2a	892	A	C6-N1-C2	-5.66	115.21	118.60
32	2a	1015	A	N7-C8-N9	5.66	116.63	113.80
1	1A	1834	A	N7-C8-N9	-5.65	110.97	113.80
1	1A	2080	A	C5-N7-C8	5.65	106.73	103.90
18	1W	23	LEU	CB-CG-CD2	-5.65	101.39	111.00
1	2A	217	G	N1-C6-O6	-5.65	116.51	119.90
1	1A	1341	C	N1-C2-O2	5.65	122.29	118.90
32	1a	899	C	N1-C2-O2	-5.65	115.51	118.90
32	2a	884	U	OP1-P-OP2	5.65	128.08	119.60
1	1A	1465	A	N1-C2-N3	-5.65	126.47	129.30
32	1a	734	G	OP2-P-O3'	5.65	117.63	105.20
1	2A	221	A	C5'-C4'-C3'	-5.65	106.96	116.00
1	2A	1296	G	O5'-P-OP2	-5.65	100.61	105.70
1	2A	1651	G	N1-C6-O6	-5.65	116.51	119.90
1	1A	130	G	N7-C8-N9	-5.65	110.28	113.10
1	1A	2188	G	C6-C5-N7	5.65	133.79	130.40
1	2A	2353	G	N1-C6-O6	5.65	123.29	119.90
32	2a	1098	C	O5'-P-OP1	-5.65	100.62	105.70
1	1A	1455	C	OP1-P-O3'	-5.65	92.77	105.20
1	1A	2015	U	C5-C6-N1	-5.65	119.88	122.70
1	1A	2620	G	C6-N1-C2	-5.65	121.71	125.10
9	1N	138	LEU	CB-CG-CD1	-5.65	101.40	111.00
32	1a	1419	G	C6-N1-C2	5.65	128.49	125.10
1	2A	2895	U	C5-C6-N1	5.65	125.52	122.70
1	1A	175	G	C5-C6-O6	5.65	131.99	128.60
1	1A	553	A	C2-N3-C4	5.65	113.42	110.60
1	1A	1472	G	C6-C5-N7	-5.65	127.01	130.40
1	1A	2525	G	C5-C6-O6	5.65	131.99	128.60
1	1A	2530	A	C4-C5-C6	5.65	119.82	117.00
1	2A	1313	U	OP1-P-OP2	-5.65	111.13	119.60
1	1A	61	C	O5'-P-OP2	-5.64	100.62	105.70
1	2A	2074	U	C6-N1-C2	-5.64	117.61	121.00
1	2A	2501	C	C6-N1-C2	5.64	122.56	120.30
32	2a	1442(A)	G	N1-C6-O6	5.64	123.29	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2843	G	N3-C4-C5	-5.64	125.78	128.60
1	2A	752	A	N7-C8-N9	5.64	116.62	113.80
1	2A	1236	G	N1-C6-O6	-5.64	116.51	119.90
32	2a	1274	G	N7-C8-N9	5.64	115.92	113.10
1	1A	1009	C	O5'-P-OP2	-5.64	100.62	105.70
1	1A	1307	C	N3-C4-C5	5.64	124.16	121.90
1	1A	2099	A	O5'-P-OP2	5.64	117.47	110.70
1	2A	1616	A	N7-C8-N9	5.64	116.62	113.80
1	1A	1622	C	C6-N1-C2	-5.64	118.04	120.30
1	1A	1833	A	C8-N9-C4	5.64	108.06	105.80
1	1A	2131	U	N1-C2-N3	5.64	118.28	114.90
32	1a	1197	G	N3-C4-N9	5.64	129.38	126.00
1	2A	2891	G	N1-C6-O6	5.64	123.28	119.90
1	1A	479	C	O5'-P-OP2	5.64	117.47	110.70
1	1A	2466	G	OP1-P-OP2	5.64	128.06	119.60
32	1a	266	G	P-O3'-C3'	5.64	126.47	119.70
1	2A	676	A	OP2-P-O3'	5.64	117.60	105.20
1	2A	2331	G	C8-N9-C4	5.64	108.66	106.40
32	2a	771	G	N3-C4-C5	5.64	131.42	128.60
1	1A	729	G	N1-C6-O6	-5.64	116.52	119.90
1	1A	1252	C	N3-C2-O2	-5.64	117.95	121.90
1	1A	2650	G	N3-C4-C5	-5.64	125.78	128.60
3	1D	260	ARG	NE-CZ-NH2	-5.64	117.48	120.30
32	1a	148	G	N3-C4-N9	5.64	129.38	126.00
32	1a	754	C	N3-C4-N4	-5.64	114.06	118.00
1	2A	482	A	C4-C5-C6	5.64	119.82	117.00
1	1A	757	G	C8-N9-C4	5.63	108.65	106.40
3	1D	60	ARG	NE-CZ-NH1	-5.63	117.48	120.30
32	1a	312	C	C6-N1-C2	5.63	122.55	120.30
1	2A	2144	U	C6-N1-C2	-5.63	117.62	121.00
1	2A	2821	A	N9-C4-C5	-5.63	103.55	105.80
32	2a	397	A	C4-C5-C6	5.63	119.82	117.00
1	1A	1627	A	N9-C4-C5	-5.63	103.55	105.80
1	1A	2405	A	OP1-P-OP2	5.63	128.05	119.60
1	1A	2561	G	C2-N3-C4	5.63	114.72	111.90
32	2a	897	C	C4-C5-C6	5.63	120.22	117.40
1	1A	109	A	C5-C6-N1	5.63	120.52	117.70
1	1A	1821	C	C6-N1-C2	5.63	122.55	120.30
1	1A	2179	G	C5-C6-O6	5.63	131.98	128.60
32	1a	800	G	O5'-P-OP2	-5.63	100.63	105.70
1	2A	2040	C	O5'-P-OP1	-5.63	100.63	105.70
1	2A	2505	G	N7-C8-N9	5.63	115.92	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2282	G	C6-N1-C2	-5.63	121.72	125.10
32	1a	831	U	N3-C4-O4	5.63	123.34	119.40
1	2A	271(S)	G	N1-C6-O6	5.63	123.28	119.90
1	2A	297	C	O5'-P-OP2	-5.63	100.63	105.70
1	1A	627	G	C5'-C4'-O4'	5.63	115.86	109.10
1	1A	768	C	C2-N3-C4	-5.63	117.09	119.90
1	1A	2842	U	O5'-P-OP2	-5.63	100.64	105.70
16	1U	50	ARG	CB-CA-C	5.63	121.66	110.40
1	2A	831	G	O5'-P-OP1	-5.63	100.63	105.70
1	1A	1350	C	OP1-P-OP2	-5.63	111.16	119.60
1	1A	1833	A	N1-C6-N6	5.63	121.98	118.60
32	1a	105	G	C5-C6-O6	-5.63	125.22	128.60
1	2A	80	G	C4-C5-N7	-5.63	108.55	110.80
1	2A	2136	C	C6-N1-C2	-5.63	118.05	120.30
32	2a	388	G	C8-N9-C4	5.63	108.65	106.40
1	1A	1102	G	C8-N9-C4	5.62	108.65	106.40
1	2A	1046	A	N3-C4-C5	-5.62	122.86	126.80
32	2a	1014	A	C8-N9-C4	-5.62	103.55	105.80
1	1A	52	A	N7-C8-N9	5.62	116.61	113.80
1	1A	107	G	C4-C5-N7	-5.62	108.55	110.80
1	1A	2001	C	N1-C2-O2	-5.62	115.53	118.90
1	1A	2576	A	C4-C5-N7	5.62	113.51	110.70
32	1a	322	C	C6-N1-C2	5.62	122.55	120.30
1	2A	740	U	OP1-P-O3'	5.62	117.57	105.20
1	2A	2139	C	C6-N1-C2	-5.62	118.05	120.30
1	2A	2206	G	N7-C8-N9	-5.62	110.29	113.10
32	2a	802	A	C5-C6-N6	-5.62	119.20	123.70
1	1A	285	U	C5-C4-O4	-5.62	122.53	125.90
1	1A	833	C	N3-C4-N4	-5.62	114.07	118.00
1	1A	1861	C	C6-N1-C2	5.62	122.55	120.30
32	1a	498	U	N3-C4-O4	-5.62	115.47	119.40
1	2A	1982	C	C5-C6-N1	-5.62	118.19	121.00
32	2a	60	A	P-O3'-C3'	5.62	126.45	119.70
1	1A	1594	C	O5'-P-OP2	-5.62	100.64	105.70
1	1A	1972	G	N9-C4-C5	-5.62	103.15	105.40
1	1A	2056	U	C5-C6-N1	-5.62	119.89	122.70
1	2A	74	A	O5'-P-OP1	5.62	117.44	110.70
1	2A	2056	G	C8-N9-C1'	-5.62	119.69	127.00
2	2B	41	U	OP1-P-O3'	5.62	117.56	105.20
32	2a	1282	C	C5-C6-N1	5.62	123.81	121.00
1	1A	1091	A	O4'-C1'-N9	5.62	112.69	108.20
2	1B	55	U	N1-C2-N3	5.62	118.27	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	98	G	OP1-P-OP2	5.62	128.03	119.60
32	1a	1033	G	N9-C4-C5	-5.62	103.15	105.40
1	2A	1320	C	N3-C4-C5	5.62	124.15	121.90
32	2a	19	C	N1-C2-O2	-5.62	115.53	118.90
32	2a	414	A	OP1-P-O3'	5.62	117.56	105.20
1	1A	1608	G	C8-N9-C4	-5.62	104.15	106.40
32	1a	1497	G	C5-C6-O6	-5.62	125.23	128.60
1	2A	1148	A	N9-C4-C5	5.62	108.05	105.80
1	2A	1825	A	O5'-P-OP1	-5.62	100.64	105.70
32	2a	832	C	C6-N1-C2	-5.62	118.05	120.30
1	1A	96	C	C5-C4-N4	5.62	124.13	120.20
1	1A	1052	C	C6-N1-C2	5.62	122.55	120.30
1	1A	1211	U	C5-C4-O4	5.62	129.27	125.90
32	1a	502	G	OP1-P-OP2	-5.62	111.18	119.60
1	2A	2733	A	C8-N9-C4	-5.62	103.55	105.80
32	2a	1530	G	N7-C8-N9	-5.62	110.29	113.10
1	1A	61	C	C2-N1-C1'	-5.61	112.62	118.80
1	1A	397	G	C5-C6-N1	5.61	114.31	111.50
1	1A	598	A	C2-N3-C4	-5.61	107.79	110.60
1	2A	1970	A	O4'-C1'-N9	-5.61	103.71	108.20
1	2A	2373	G	C8-N9-C4	5.61	108.64	106.40
1	1A	2285	A	OP2-P-O3'	5.61	117.55	105.20
1	1A	2805	G	C8-N9-C4	-5.61	104.16	106.40
9	1N	25	ARG	NE-CZ-NH1	-5.61	117.49	120.30
32	1a	996	A	N7-C8-N9	5.61	116.61	113.80
32	1a	1276	G	N3-C4-C5	-5.61	125.79	128.60
1	2A	2629	A	C2-N3-C4	-5.61	107.79	110.60
1	1A	274	U	N3-C4-O4	5.61	123.33	119.40
1	1A	705	C	OP1-P-OP2	5.61	128.02	119.60
1	1A	731	G	N3-C4-N9	5.61	129.37	126.00
1	1A	740	C	N1-C2-O2	5.61	122.27	118.90
32	1a	872	A	O4'-C1'-N9	5.61	112.69	108.20
1	2A	2167	U	N1-C2-O2	5.61	126.73	122.80
1	2A	2443	C	C6-N1-C2	-5.61	118.06	120.30
1	1A	1003	U	N1-C2-N3	5.61	118.27	114.90
1	1A	1269	G	N3-C2-N2	5.61	123.83	119.90
1	1A	1427	G	C5-N7-C8	5.61	107.10	104.30
1	1A	2584	A	C2-N3-C4	5.61	113.40	110.60
1	1A	1577	C	OP2-P-O3'	5.61	117.54	105.20
1	1A	2265	G	N1-C2-N2	5.61	121.25	116.20
32	1a	253	U	OP2-P-O3'	5.61	117.54	105.20
1	1A	452	G	C5-C6-O6	-5.61	125.24	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	766	C	C2-N3-C4	-5.61	117.10	119.90
1	1A	2510	C	C5-C6-N1	-5.61	118.20	121.00
32	1a	774	G	C5-C6-N1	-5.61	108.70	111.50
32	1a	1532	U	C5-C6-N1	5.61	125.50	122.70
1	2A	2886	G	N9-C4-C5	5.61	107.64	105.40
1	1A	2792	U	C2-N3-C4	-5.60	123.64	127.00
1	2A	2444	G	C5-C6-O6	5.60	131.96	128.60
1	2A	2463	C	C6-N1-C2	5.60	122.54	120.30
1	1A	596	G	O5'-P-OP1	5.60	117.42	110.70
1	1A	659	C	O5'-P-OP2	-5.60	100.66	105.70
1	1A	907	U	O5'-P-OP1	5.60	117.42	110.70
1	1A	1314	A	C5-C6-N6	5.60	128.18	123.70
1	1A	1958	A	C6-C5-N7	-5.60	128.38	132.30
1	1A	2440	G	N7-C8-N9	5.60	115.90	113.10
1	1A	2512	U	N3-C4-O4	-5.60	115.48	119.40
1	1A	2654	G	N1-C6-O6	-5.60	116.54	119.90
32	1a	353	A	N1-C6-N6	5.60	121.96	118.60
32	1a	1209	C	N3-C4-C5	-5.60	119.66	121.90
1	2A	612	C	N1-C2-O2	-5.60	115.54	118.90
1	2A	2307	G	N1-C6-O6	5.60	123.26	119.90
1	2A	2870	C	C6-N1-C2	-5.60	118.06	120.30
32	2a	1023	G	C8-N9-C4	-5.60	104.16	106.40
32	1a	189(G)	G	N1-C6-O6	5.60	123.26	119.90
32	1a	1299	A	N9-C4-C5	5.60	108.04	105.80
1	2A	718	A	C4-C5-C6	5.60	119.80	117.00
1	1A	238	C	OP1-P-O3'	5.60	117.52	105.20
1	1A	731	G	N3-C2-N2	5.60	123.82	119.90
1	1A	1182	G	N1-C6-O6	5.60	123.26	119.90
1	1A	1274	G	N1-C6-O6	-5.60	116.54	119.90
32	1a	620	C	C6-N1-C2	5.60	122.54	120.30
32	1a	1024	G	C2-N3-C4	5.60	114.70	111.90
1	2A	1462	C	C6-N1-C2	-5.60	118.06	120.30
1	1A	73	A	C5-C6-N1	5.60	120.50	117.70
1	1A	108	G	C4-C5-N7	-5.60	108.56	110.80
1	1A	476	G	N3-C4-N9	5.60	129.36	126.00
1	1A	1122	C	O4'-C1'-N1	5.60	112.68	108.20
1	1A	1595	C	C6-N1-C2	-5.60	118.06	120.30
1	1A	1822	A	C5-C6-N6	5.60	128.18	123.70
1	1A	2006	G	OP2-P-O3'	5.60	117.52	105.20
1	1A	2876	U	N3-C2-O2	-5.60	118.28	122.20
1	1A	860	U	N1-C2-N3	5.60	118.26	114.90
1	1A	2649	U	N1-C2-N3	5.60	118.26	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2718	G	N1-C6-O6	-5.60	116.54	119.90
1	1A	2898	C	N3-C2-O2	-5.60	117.98	121.90
32	1a	200	G	C8-N9-C4	5.60	108.64	106.40
1	2A	854	G	C5-C6-O6	5.60	131.96	128.60
1	2A	1133	U	N1-C2-O2	-5.60	118.88	122.80
32	2a	711	G	OP1-P-O3'	5.60	117.51	105.20
32	1a	1134	G	N3-C4-C5	-5.59	125.80	128.60
1	2A	1688	U	O5'-P-OP2	-5.59	100.67	105.70
1	2A	2234	G	N1-C2-N2	-5.59	111.17	116.20
1	2A	2805	G	C2-N3-C4	5.59	114.70	111.90
2	2B	50	G	O5'-P-OP2	-5.59	100.66	105.70
32	2a	111	G	C5-C6-N1	-5.59	108.70	111.50
1	1A	106	U	C2-N3-C4	-5.59	123.64	127.00
1	1A	339	G	O5'-P-OP2	-5.59	100.67	105.70
1	1A	1448	C	C6-N1-C2	5.59	122.54	120.30
1	1A	2115	G	N7-C8-N9	-5.59	110.30	113.10
1	1A	2386	C	C5-C6-N1	-5.59	118.20	121.00
1	1A	2626	A	C2-N3-C4	5.59	113.40	110.60
32	1a	345	C	N1-C2-O2	5.59	122.26	118.90
32	1a	670	G	N9-C4-C5	5.59	107.64	105.40
1	2A	1690	A	C4-C5-N7	5.59	113.50	110.70
1	2A	2609	U	O5'-P-OP2	-5.59	100.67	105.70
32	2a	1134	G	C2-N3-C4	5.59	114.70	111.90
1	1A	102	U	N3-C2-O2	5.59	126.11	122.20
1	1A	167	G	C4-C5-N7	-5.59	108.56	110.80
1	1A	1050	C	C4-C5-C6	5.59	120.20	117.40
1	1A	2235	G	C8-N9-C4	5.59	108.64	106.40
1	1A	2762	A	C2-N3-C4	5.59	113.40	110.60
1	2A	2154	G	N1-C6-O6	5.59	123.25	119.90
1	1A	124	A	C6-N1-C2	5.59	121.95	118.60
1	1A	355	A	C5-C6-N6	-5.59	119.23	123.70
1	1A	1215	G	OP2-P-O3'	5.59	117.50	105.20
1	1A	1976	G	C8-N9-C4	-5.59	104.16	106.40
1	1A	2051	G	N1-C2-N2	5.59	121.23	116.20
1	1A	2233	G	O5'-P-OP1	-5.59	100.67	105.70
1	1A	2551	C	N3-C4-N4	-5.59	114.09	118.00
1	1A	2569	G	C5-C6-N1	-5.59	108.71	111.50
1	2A	463	G	C4-C5-N7	-5.59	108.56	110.80
1	2A	763	G	O4'-C1'-N9	-5.59	103.73	108.20
32	2a	1279	A	N7-C8-N9	5.59	116.59	113.80
32	2a	1412	C	O5'-P-OP1	-5.59	100.67	105.70
1	1A	828	A	N7-C8-N9	-5.59	111.01	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1268	C	C6-N1-C2	5.59	122.53	120.30
32	1a	584	G	C8-N9-C1'	-5.59	119.73	127.00
32	1a	1325	C	O5'-P-OP2	-5.59	100.67	105.70
32	1a	1382	C	C6-N1-C2	-5.59	118.06	120.30
1	2A	1909	C	N3-C2-O2	-5.59	117.99	121.90
32	2a	1057	G	C8-N9-C4	5.59	108.64	106.40
1	1A	294	C	O5'-P-OP1	5.59	117.40	110.70
1	1A	1199	C	C2-N3-C4	-5.59	117.11	119.90
1	1A	1341	C	C5-C6-N1	-5.59	118.21	121.00
1	1A	2441	G	C8-N9-C4	-5.59	104.17	106.40
1	2A	1835	G	OP2-P-O3'	5.59	117.49	105.20
1	2A	2061	G	O4'-C1'-N9	5.59	112.67	108.20
1	2A	2553	G	C5-C6-O6	-5.59	125.25	128.60
1	2A	2822	G	N7-C8-N9	-5.59	110.31	113.10
1	1A	2522	C	C6-N1-C2	-5.58	118.07	120.30
1	1A	355	A	N9-C4-C5	-5.58	103.57	105.80
1	1A	1676	G	N9-C4-C5	5.58	107.63	105.40
1	1A	1692	G	C5-C6-O6	5.58	131.95	128.60
32	1a	728	A	O5'-P-OP1	-5.58	100.67	105.70
32	1a	1504	G	C8-N9-C4	5.58	108.63	106.40
1	1A	886	U	N3-C4-O4	-5.58	115.49	119.40
1	1A	1043	G	C5-C6-O6	5.58	131.95	128.60
1	1A	2111	U	C5-C6-N1	-5.58	119.91	122.70
1	1A	2221	A	OP1-P-OP2	-5.58	111.23	119.60
1	1A	2430	A	N1-C2-N3	-5.58	126.51	129.30
1	1A	2698	G	C5-N7-C8	-5.58	101.51	104.30
32	1a	762	C	N3-C2-O2	-5.58	117.99	121.90
1	1A	2566	U	N1-C2-O2	-5.58	118.89	122.80
1	2A	673	C	C4-C5-C6	5.58	120.19	117.40
32	2a	1111	A	C8-N9-C4	-5.58	103.57	105.80
1	1A	542	C	N3-C4-C5	5.58	124.13	121.90
1	1A	616	G	O5'-P-OP2	-5.58	100.68	105.70
1	1A	665	C	N1-C2-O2	-5.58	115.55	118.90
1	1A	724	A	C4-C5-N7	-5.58	107.91	110.70
1	1A	1159	U	N3-C2-O2	5.58	126.11	122.20
1	2A	1421	G	C5-C6-N1	-5.58	108.71	111.50
32	2a	5	U	N3-C4-O4	5.58	123.31	119.40
32	2a	1530	G	C4-N9-C1'	-5.58	119.25	126.50
1	1A	173	C	N3-C2-O2	-5.58	118.00	121.90
1	1A	606	G	C5-C6-N1	5.58	114.29	111.50
1	1A	1452	U	C2-N3-C4	-5.58	123.65	127.00
1	1A	2407	C	C6-N1-C2	5.58	122.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	142	G	C8-N9-C1'	5.58	134.25	127.00
32	1a	878	G	C2-N3-C4	-5.58	109.11	111.90
32	1a	1062	U	C6-N1-C2	-5.58	117.65	121.00
1	1A	1001	G	C8-N9-C4	5.58	108.63	106.40
1	1A	1588	G	N1-C6-O6	-5.58	116.56	119.90
1	1A	1691	C	C2-N3-C4	-5.58	117.11	119.90
1	1A	1739	U	C6-N1-C2	5.58	124.34	121.00
1	1A	2250	G	C8-N9-C4	5.58	108.63	106.40
1	2A	2449	U	OP2-P-O3'	5.58	117.47	105.20
1	1A	76	C	N1-C2-O2	5.57	122.24	118.90
1	1A	2427	G	O5'-P-OP1	5.57	117.39	110.70
32	1a	78	G	C8-N9-C1'	5.57	134.25	127.00
32	1a	490	G	N1-C6-O6	-5.57	116.56	119.90
32	1a	584	G	N3-C4-N9	5.57	129.34	126.00
32	1a	1082	G	C4-C5-N7	5.57	113.03	110.80
1	2A	1045	A	N7-C8-N9	5.57	116.59	113.80
1	2A	2332	U	C5-C4-O4	5.57	129.24	125.90
32	2a	248	C	O5'-P-OP2	-5.57	100.69	105.70
1	1A	1715	A	C5-C6-N1	-5.57	114.91	117.70
32	1a	1224	G	C4-C5-N7	-5.57	108.57	110.80
1	1A	556	C	C5-C6-N1	-5.57	118.22	121.00
1	1A	1186	U	O4'-C1'-N1	5.57	112.66	108.20
1	1A	1697	G	C8-N9-C4	-5.57	104.17	106.40
1	1A	2251	G	C5-C6-O6	5.57	131.94	128.60
1	1A	2566	U	C2-N3-C4	-5.57	123.66	127.00
2	1B	9	G	OP2-P-O3'	5.57	117.46	105.20
32	1a	1030(D)	A	N7-C8-N9	5.57	116.59	113.80
1	2A	2056	G	C4-N9-C1'	5.57	133.74	126.50
1	2A	2598	A	OP2-P-O3'	5.57	117.45	105.20
32	2a	740	U	O5'-P-OP2	-5.57	100.69	105.70
49	2q	63	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	1A	1144	A	C8-N9-C4	-5.57	103.57	105.80
1	1A	1720	U	C2-N3-C4	-5.57	123.66	127.00
1	2A	2815	C	N1-C2-O2	-5.57	115.56	118.90
32	2a	649	G	C4-N9-C1'	-5.57	119.26	126.50
1	1A	1678	A	OP1-P-O3'	5.57	117.44	105.20
1	1A	2278	A	N1-C6-N6	5.57	121.94	118.60
1	1A	2877	G	C5-C6-O6	-5.57	125.26	128.60
32	1a	774	G	OP2-P-O3'	5.57	117.44	105.20
1	2A	2514	U	N1-C2-N3	-5.57	111.56	114.90
1	2A	2635	C	N3-C4-N4	5.57	121.89	118.00
1	2A	76	C	C6-N1-C2	-5.56	118.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1020	U	C2-N1-C1'	5.56	124.38	117.70
1	1A	645	G	OP1-P-O3'	5.56	117.44	105.20
1	1A	654	G	C5-C6-O6	5.56	131.94	128.60
1	1A	855	G	C5-N7-C8	5.56	107.08	104.30
1	1A	1234	A	C5-C6-N6	-5.56	119.25	123.70
1	1A	1334	U	C5-C6-N1	-5.56	119.92	122.70
1	1A	2200	C	N3-C4-C5	-5.56	119.67	121.90
2	1B	112	U	N3-C4-C5	-5.56	111.26	114.60
1	2A	2049	G	N9-C4-C5	5.56	107.62	105.40
2	2B	11	C	C6-N1-C2	-5.56	118.08	120.30
1	1A	716	G	C6-C5-N7	5.56	133.74	130.40
1	1A	1216	G	C5-N7-C8	-5.56	101.52	104.30
1	1A	2209	G	N1-C6-O6	5.56	123.23	119.90
1	1A	2348	A	O4'-C1'-N9	-5.56	103.75	108.20
1	1A	2597	U	P-O3'-C3'	5.56	126.37	119.70
1	2A	1073	A	OP1-P-OP2	5.56	127.94	119.60
1	2A	2425	A	OP1-P-OP2	-5.56	111.26	119.60
1	1A	308	U	N1-C2-O2	-5.56	118.91	122.80
1	1A	479	C	N3-C4-N4	-5.56	114.11	118.00
1	1A	893	C	N3-C4-C5	5.56	124.12	121.90
1	2A	310	A	OP1-P-O3'	5.56	117.43	105.20
1	2A	1256	G	C8-N9-C4	5.56	108.62	106.40
32	2a	1515	C	C6-N1-C2	5.56	122.52	120.30
1	2A	2331	G	C5-C6-O6	-5.56	125.27	128.60
1	2A	2439	A	O5'-P-OP2	-5.56	100.70	105.70
1	1A	616	G	OP1-P-OP2	5.55	127.93	119.60
1	1A	1628	G	OP2-P-O3'	5.55	117.42	105.20
1	1A	1882	U	O5'-P-OP1	-5.55	100.70	105.70
1	1A	2401	G	OP1-P-O3'	5.55	117.42	105.20
1	1A	2467	G	N3-C2-N2	5.55	123.79	119.90
1	1A	2596	U	O4'-C1'-N1	5.55	112.64	108.20
32	1a	427	U	OP2-P-O3'	5.55	117.42	105.20
1	2A	661	C	C2-N3-C4	-5.55	117.12	119.90
32	2a	375	U	O5'-P-OP2	5.55	117.37	110.70
32	2a	649	G	N3-C4-N9	-5.55	122.67	126.00
32	2a	700	G	OP2-P-O3'	5.55	117.42	105.20
1	1A	2453	C	N3-C4-N4	-5.55	114.11	118.00
1	1A	2512	U	OP1-P-OP2	-5.55	111.27	119.60
32	1a	625	G	C8-N9-C4	-5.55	104.18	106.40
32	1a	1192	C	O5'-P-OP2	5.55	117.36	110.70
32	1a	1316	G	C8-N9-C4	5.55	108.62	106.40
1	2A	2349	G	C5-C6-N1	5.55	114.28	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2521	C	N3-C4-C5	-5.55	119.68	121.90
1	1A	130	G	N9-C4-C5	5.55	107.62	105.40
1	1A	494	G	N7-C8-N9	-5.55	110.32	113.10
1	1A	1353	A	N9-C4-C5	-5.55	103.58	105.80
1	1A	2265	G	C4-C5-N7	-5.55	108.58	110.80
32	1a	372	C	C4-C5-C6	-5.55	114.62	117.40
1	2A	2252	G	N3-C2-N2	5.55	123.79	119.90
32	2a	860	A	C8-N9-C4	-5.55	103.58	105.80
1	1A	200	A	C2-N3-C4	5.55	113.38	110.60
1	1A	730	C	N3-C4-C5	5.55	124.12	121.90
1	1A	2255	U	C5-C6-N1	5.55	125.47	122.70
1	1A	2291	G	C5-N7-C8	-5.55	101.53	104.30
1	1A	2611	G	C6-C5-N7	5.55	133.73	130.40
32	1a	781	A	OP2-P-O3'	5.55	117.41	105.20
1	2A	250	G	C5-C6-N1	5.55	114.28	111.50
1	2A	1649	G	N3-C2-N2	5.55	123.78	119.90
1	1A	659	C	OP2-P-O3'	5.55	117.41	105.20
1	1A	2272	C	N3-C4-N4	-5.55	114.12	118.00
32	1a	730	G	C8-N9-C4	5.55	108.62	106.40
1	2A	779	U	N1-C2-O2	-5.55	118.92	122.80
32	2a	455	C	C5-C6-N1	5.55	123.77	121.00
32	2a	569	C	C4-C5-C6	5.55	120.17	117.40
32	2a	1286	A	C8-N9-C4	-5.55	103.58	105.80
1	1A	303	C	O5'-P-OP2	-5.55	100.71	105.70
1	1A	367	C	C4-C5-C6	5.55	120.17	117.40
32	1a	185	A	C8-N9-C4	-5.55	103.58	105.80
1	2A	2481	G	O5'-P-OP2	-5.55	100.71	105.70
32	2a	43	C	N1-C2-O2	-5.55	115.57	118.90
1	1A	2049	G	N1-C6-O6	-5.54	116.57	119.90
32	1a	190	U	C6-N1-C2	-5.54	117.67	121.00
32	1a	266	G	C6-C5-N7	-5.54	127.07	130.40
1	2A	453	C	O5'-P-OP2	5.54	117.35	110.70
1	2A	2049	G	N3-C4-N9	-5.54	122.67	126.00
1	1A	858	U	N1-C2-N3	5.54	118.23	114.90
1	1A	975	U	C2-N3-C4	-5.54	123.67	127.00
1	2A	249	C	N3-C2-O2	5.54	125.78	121.90
1	2A	950	G	C8-N9-C4	-5.54	104.18	106.40
1	2A	1261	C	C6-N1-C1'	5.54	127.45	120.80
32	2a	220	G	C6-C5-N7	-5.54	127.07	130.40
1	1A	167	G	N1-C2-N3	5.54	127.22	123.90
1	1A	274	U	C6-N1-C1'	-5.54	113.44	121.20
1	1A	1092	A	N7-C8-N9	5.54	116.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1666	G	C5-N7-C8	5.54	107.07	104.30
1	1A	1823	G	OP2-P-O3'	5.54	117.39	105.20
1	1A	2187	G	N1-C6-O6	-5.54	116.58	119.90
5	1F	195	ASP	CB-CA-C	-5.54	99.32	110.40
1	2A	1973	G	C5-C6-O6	5.54	131.93	128.60
1	1A	554	A	N7-C8-N9	5.54	116.57	113.80
1	1A	901	G	C4-C5-N7	-5.54	108.58	110.80
32	1a	777	A	C6-N1-C2	5.54	121.92	118.60
32	2a	869	G	O5'-P-OP1	-5.54	100.71	105.70
1	1A	1858	C	C5-C4-N4	5.54	124.08	120.20
8	1I	43	ASN	N-CA-CB	5.54	120.57	110.60
32	2a	505	G	OP1-P-O3'	5.54	117.38	105.20
32	2a	724	G	C5-C6-O6	-5.54	125.28	128.60
1	1A	329	U	O5'-P-OP1	-5.54	100.72	105.70
1	2A	2467	C	C5-C6-N1	5.54	123.77	121.00
32	2a	145	G	N3-C2-N2	-5.54	116.02	119.90
1	1A	2093	A	C6-N1-C2	-5.54	115.28	118.60
1	2A	2078	C	N1-C2-O2	-5.54	115.58	118.90
32	2a	404	U	C2-N3-C4	5.54	130.32	127.00
32	2a	945	G	N1-C6-O6	5.54	123.22	119.90
1	1A	2193	A	C6-C5-N7	-5.53	128.43	132.30
32	1a	23	C	OP1-P-OP2	-5.53	111.30	119.60
1	2A	47	C	N3-C4-C5	5.53	124.11	121.90
1	2A	702	G	O5'-P-OP2	-5.53	100.72	105.70
1	2A	1663	C	N3-C4-N4	-5.53	114.13	118.00
1	1A	1169	C	OP1-P-OP2	5.53	127.90	119.60
1	1A	1453	C	C4-C5-C6	5.53	120.17	117.40
32	1a	405	U	O5'-P-OP2	5.53	117.34	110.70
32	1a	899	C	C5-C6-N1	-5.53	118.23	121.00
1	1A	40	C	C4-C5-C6	5.53	120.17	117.40
1	1A	138	G	C4-C5-N7	-5.53	108.59	110.80
1	1A	801	C	C2-N3-C4	-5.53	117.14	119.90
1	1A	852	G	N3-C4-N9	5.53	129.32	126.00
1	1A	2086	C	N3-C4-C5	-5.53	119.69	121.90
32	1a	588	G	OP2-P-O3'	5.53	117.37	105.20
1	2A	353	G	C6-C5-N7	-5.53	127.08	130.40
1	2A	726	G	O5'-P-OP1	-5.53	100.72	105.70
1	2A	2133	G	N3-C4-C5	5.53	131.37	128.60
1	2A	2858	C	C5-C4-N4	-5.53	116.33	120.20
32	2a	900	A	O5'-P-OP2	5.53	117.34	110.70
1	1A	1331	G	N1-C2-N2	-5.53	111.22	116.20
1	1A	1804	A	N7-C8-N9	-5.53	111.04	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	940	G	N1-C6-O6	-5.53	116.58	119.90
1	1A	367	C	OP2-P-O3'	5.53	117.36	105.20
1	1A	765	A	C2-N3-C4	-5.53	107.84	110.60
1	1A	2464	C	N3-C2-O2	5.53	125.77	121.90
32	1a	1031	G	O4'-C1'-N9	5.53	112.62	108.20
32	2a	675	A	OP1-P-O3'	5.53	117.36	105.20
32	2a	918	A	C8-N9-C4	-5.53	103.59	105.80
1	1A	590	A	C4-C5-C6	-5.53	114.24	117.00
1	1A	1418	U	C2-N1-C1'	5.53	124.33	117.70
1	1A	1515	C	N1-C2-O2	-5.53	115.58	118.90
1	1A	1642	A	N1-C2-N3	5.53	132.06	129.30
1	1A	2603	C	C6-N1-C2	-5.53	118.09	120.30
32	1a	334	C	OP2-P-O3'	5.53	117.36	105.20
1	2A	2559	C	O5'-P-OP2	-5.53	100.73	105.70
2	2B	30	C	C6-N1-C2	-5.53	118.09	120.30
32	2a	577	G	OP2-P-O3'	5.53	117.36	105.20
1	1A	250	G	N1-C6-O6	5.52	123.22	119.90
1	1A	618	C	N3-C4-C5	5.52	124.11	121.90
1	1A	1708	G	C8-N9-C4	5.52	108.61	106.40
1	1A	1892	G	C4-N9-C1'	-5.52	119.32	126.50
32	2a	38	G	N3-C4-C5	5.52	131.36	128.60
32	2a	574	A	C5-C6-N6	-5.52	119.28	123.70
32	2a	811	C	N3-C2-O2	5.52	125.77	121.90
1	1A	288	U	O5'-P-OP2	-5.52	100.73	105.70
1	1A	1104	G	N1-C6-O6	5.52	123.21	119.90
1	1A	1293	A	C5-N7-C8	-5.52	101.14	103.90
32	1a	965	A	N3-C4-C5	5.52	130.67	126.80
1	2A	1913	A	N9-C4-C5	5.52	108.01	105.80
1	2A	2030	A	C4-C5-C6	-5.52	114.24	117.00
32	2a	564	C	OP2-P-O3'	5.52	117.35	105.20
1	1A	581	G	N3-C2-N2	5.52	123.77	119.90
32	1a	878	G	N1-C2-N2	-5.52	111.23	116.20
1	2A	1903	G	C8-N9-C4	-5.52	104.19	106.40
1	2A	2433	A	N9-C4-C5	-5.52	103.59	105.80
1	1A	562	C	OP1-P-OP2	-5.52	111.32	119.60
1	1A	1461	U	C5-C4-O4	5.52	129.21	125.90
1	1A	1702	A	N7-C8-N9	-5.52	111.04	113.80
1	1A	1752	G	C5-C6-O6	5.52	131.91	128.60
1	1A	2117	C	OP2-P-O3'	5.52	117.34	105.20
1	1A	2569	G	C5-C6-O6	5.52	131.91	128.60
1	1A	2807	C	C6-N1-C2	-5.52	118.09	120.30
32	1a	1406	U	C5-C6-N1	-5.52	119.94	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1071	G	C5-N7-C8	-5.52	101.54	104.30
32	2a	1030	C	C6-N1-C1'	-5.52	114.18	120.80
1	1A	198	C	N3-C2-O2	-5.52	118.04	121.90
1	1A	322	G	N3-C4-C5	-5.52	125.84	128.60
1	1A	1701	A	OP1-P-OP2	-5.52	111.32	119.60
1	1A	1952	G	N1-C6-O6	-5.52	116.59	119.90
2	1B	75	G	C5-C6-N1	5.52	114.26	111.50
32	1a	559	A	C8-N9-C4	-5.52	103.59	105.80
32	1a	885	G	C8-N9-C4	5.52	108.61	106.40
32	1a	1054	C	N1-C2-O2	5.52	122.21	118.90
32	1a	1075	C	C6-N1-C2	5.52	122.51	120.30
32	1a	1131	G	N1-C6-O6	5.52	123.21	119.90
1	1A	1317	G	N9-C4-C5	-5.52	103.19	105.40
1	1A	1934	A	O5'-P-OP2	-5.52	100.74	105.70
1	1A	1041	C	C6-N1-C2	-5.51	118.09	120.30
1	1A	1065	U	C2-N3-C4	-5.51	123.69	127.00
1	1A	1274	G	N3-C4-N9	-5.51	122.69	126.00
1	1A	1659	G	O5'-P-OP1	5.51	117.32	110.70
1	1A	1724	A	N1-C6-N6	5.51	121.91	118.60
1	1A	1813	C	N1-C2-O2	-5.51	115.59	118.90
1	1A	1870	G	C8-N9-C4	5.51	108.61	106.40
1	1A	2229	A	C6-C5-N7	-5.51	128.44	132.30
1	2A	301	G	N3-C4-N9	-5.51	122.69	126.00
1	2A	1094	U	O4'-C1'-N1	5.51	112.61	108.20
2	1B	27	C	C5-C6-N1	-5.51	118.24	121.00
2	1B	113	G	O5'-P-OP2	-5.51	100.74	105.70
1	1A	1201	A	N1-C2-N3	-5.51	126.55	129.30
1	1A	2010	C	C4-C5-C6	5.51	120.16	117.40
1	1A	2622	C	C6-N1-C2	-5.51	118.10	120.30
1	2A	602	G	N3-C2-N2	5.51	123.76	119.90
1	2A	2827	C	N3-C4-C5	5.51	124.10	121.90
1	1A	45	C	C4-C5-C6	-5.51	114.64	117.40
1	1A	201	G	C4-C5-N7	5.51	113.00	110.80
1	1A	790	G	C8-N9-C4	-5.51	104.20	106.40
1	1A	843	C	C5-C6-N1	-5.51	118.25	121.00
1	2A	1071	G	N9-C1'-C2'	-5.51	105.94	112.00
1	2A	1351	C	C6-N1-C2	-5.51	118.10	120.30
1	2A	1658	C	C2-N1-C1'	5.51	124.86	118.80
1	1A	762	G	C6-C5-N7	-5.51	127.09	130.40
15	1T	118	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	2A	231	C	C6-N1-C2	-5.51	118.10	120.30
1	2A	594	U	C5-C6-N1	-5.51	119.95	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1482	G	O5'-P-OP2	-5.51	100.74	105.70
1	2A	2447	G	OP2-P-O3'	5.51	117.32	105.20
32	2a	1421	G	O5'-P-OP2	-5.51	100.74	105.70
1	1A	824	A	N1-C2-N3	5.51	132.05	129.30
32	1a	622	A	N9-C4-C5	5.51	108.00	105.80
32	1a	965	A	C2-N3-C4	-5.51	107.85	110.60
32	1a	1162	C	C5-C6-N1	5.51	123.75	121.00
1	2A	1086	A	C2-N3-C4	5.51	113.35	110.60
1	2A	1536	C	C2-N3-C4	5.51	122.65	119.90
1	2A	2105	C	C2-N1-C1'	5.51	124.86	118.80
32	2a	424	G	OP1-P-O3'	5.51	117.31	105.20
32	2a	1132	C	N3-C4-C5	-5.51	119.70	121.90
1	1A	596	G	C5-C6-N1	5.50	114.25	111.50
1	1A	765	A	C5-C6-N1	-5.50	114.95	117.70
32	1a	890	G	O4'-C1'-N9	5.50	112.60	108.20
1	2A	271(M)	G	P-O3'-C3'	5.50	126.31	119.70
32	2a	900	A	O5'-P-OP1	-5.50	100.75	105.70
1	1A	34	C	C6-N1-C2	-5.50	118.10	120.30
1	1A	114	C	N3-C4-N4	-5.50	114.15	118.00
1	1A	713	G	O5'-P-OP2	-5.50	100.75	105.70
1	1A	1285	G	C8-N9-C4	-5.50	104.20	106.40
1	1A	1560	U	N1-C2-O2	-5.50	118.95	122.80
1	2A	214	G	C8-N9-C4	-5.50	104.20	106.40
1	2A	494	G	C4-C5-N7	-5.50	108.60	110.80
1	2A	1203	G	C5-C6-O6	-5.50	125.30	128.60
32	2a	1112	C	O5'-P-OP1	5.50	117.30	110.70
1	1A	143	C	O5'-P-OP1	-5.50	100.75	105.70
1	1A	1259	A	C4-C5-N7	-5.50	107.95	110.70
1	1A	1451	U	N3-C2-O2	-5.50	118.35	122.20
1	1A	2134	G	N7-C8-N9	5.50	115.85	113.10
1	1A	2608	U	C2-N3-C4	-5.50	123.70	127.00
1	1A	2663	C	O5'-P-OP1	5.50	117.30	110.70
32	1a	549	C	O5'-P-OP2	5.50	117.30	110.70
32	1a	799	G	C4-C5-N7	-5.50	108.60	110.80
1	2A	529	A	N7-C8-N9	5.50	116.55	113.80
1	2A	2058	A	C6-N1-C2	-5.50	115.30	118.60
1	1A	2862	G	C8-N9-C4	5.50	108.60	106.40
32	1a	1465	C	N1-C2-N3	5.50	123.05	119.20
32	2a	93	G	C8-N9-C1'	5.50	134.15	127.00
1	1A	973	G	OP1-P-O3'	5.50	117.30	105.20
1	1A	1837	C	C2-N3-C4	-5.50	117.15	119.90
1	1A	2019	G	C5'-C4'-O4'	5.50	115.70	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1091	G	O3'-P-O5'	5.50	114.45	104.00
32	2a	1394	A	C6-N1-C2	5.50	121.90	118.60
1	1A	89	U	N3-C2-O2	-5.50	118.35	122.20
1	1A	577	U	C2-N3-C4	-5.50	123.70	127.00
1	1A	839	G	O4'-C1'-N9	-5.50	103.80	108.20
1	1A	1155	C	N3-C4-C5	-5.50	119.70	121.90
1	1A	1383	G	C5-C6-N1	5.50	114.25	111.50
1	1A	2636	G	N1-C2-N2	-5.50	111.25	116.20
32	1a	1137	C	C2-N3-C4	5.50	122.65	119.90
32	1a	1495	U	N3-C4-C5	-5.50	111.30	114.60
1	2A	1275	A	N7-C8-N9	-5.50	111.05	113.80
1	2A	2158	A	P-O3'-C3'	5.50	126.30	119.70
1	1A	2034	G	O5'-P-OP2	-5.50	100.75	105.70
1	2A	473	G	N3-C2-N2	-5.50	116.05	119.90
1	2A	2137	C	C5-C6-N1	5.50	123.75	121.00
1	2A	2138	C	C2-N3-C4	5.50	122.65	119.90
1	1A	36	G	C5-C6-O6	5.49	131.90	128.60
1	1A	502	G	C8-N9-C4	5.49	108.60	106.40
1	1A	2016	C	O5'-P-OP1	5.49	117.29	110.70
32	1a	888	G	C5-N7-C8	-5.49	101.55	104.30
1	2A	789	A	C5-C6-N6	-5.49	119.31	123.70
1	2A	1810	A	N1-C6-N6	5.49	121.90	118.60
1	2A	2207	G	C8-N9-C1'	-5.49	119.86	127.00
32	2a	1034	G	N1-C6-O6	5.49	123.20	119.90
1	1A	1522	G	N3-C4-N9	-5.49	122.70	126.00
32	1a	119	A	OP1-P-O3'	5.49	117.28	105.20
1	1A	115	G	O5'-P-OP1	5.49	117.29	110.70
1	1A	633	G	N1-C6-O6	-5.49	116.61	119.90
1	1A	2358	A	OP1-P-OP2	-5.49	111.36	119.60
1	1A	2449	U	C4-C5-C6	5.49	123.00	119.70
1	2A	228	A	C4-C5-C6	-5.49	114.25	117.00
1	1A	119	G	N9-C4-C5	-5.49	103.20	105.40
1	1A	857	U	C5-C4-O4	-5.49	122.61	125.90
1	1A	905	U	N3-C2-O2	-5.49	118.36	122.20
1	1A	1305	G	C5-C6-O6	5.49	131.89	128.60
1	1A	1371	G	O4'-C1'-N9	5.49	112.59	108.20
1	1A	1391	C	N3-C4-N4	-5.49	114.16	118.00
1	1A	1981	G	OP2-P-O3'	5.49	117.27	105.20
1	1A	2006	G	C4-C5-N7	-5.49	108.61	110.80
1	1A	2234	G	N7-C8-N9	-5.49	110.36	113.10
1	1A	2390	A	C6-C5-N7	-5.49	128.46	132.30
1	2A	473	G	O5'-P-OP2	-5.49	100.76	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2382	G	C8-N9-C4	5.49	108.60	106.40
1	2A	2643	G	O5'-P-OP1	-5.49	100.76	105.70
32	2a	518	C	N3-C2-O2	-5.49	118.06	121.90
1	1A	826	U	C5-C4-O4	-5.49	122.61	125.90
1	1A	1207	C	OP2-P-O3'	5.49	117.27	105.20
32	1a	1355	G	C8-N9-C4	-5.49	104.20	106.40
1	1A	715	G	OP2-P-O3'	5.49	117.27	105.20
1	1A	1033	G	C4-C5-N7	-5.49	108.61	110.80
32	1a	911	U	N1-C2-O2	-5.49	118.96	122.80
1	2A	2504	U	OP1-P-O3'	5.49	117.27	105.20
1	2A	2507	C	C2-N3-C4	5.49	122.64	119.90
1	2A	2553	G	N9-C4-C5	-5.49	103.21	105.40
1	1A	844	C	N3-C4-C5	5.48	124.09	121.90
1	1A	1033	G	O5'-P-OP2	5.48	117.28	110.70
1	1A	1630	A	C8-N9-C4	5.48	107.99	105.80
1	1A	1674	G	N3-C4-C5	-5.48	125.86	128.60
1	1A	2802	C	C6-N1-C2	5.48	122.49	120.30
1	2A	236	C	C6-N1-C2	5.48	122.49	120.30
32	2a	323	U	N3-C2-O2	-5.48	118.36	122.20
32	2a	869	G	C2-N3-C4	-5.48	109.16	111.90
32	2a	930	C	C2-N1-C1'	-5.48	112.77	118.80
1	1A	2454	C	C6-N1-C2	5.48	122.49	120.30
1	1A	2651	A	N9-C4-C5	-5.48	103.61	105.80
32	1a	1480	G	O5'-P-OP1	-5.48	100.77	105.70
1	2A	1806	C	N1-C2-O2	-5.48	115.61	118.90
1	2A	271(X)	G	C5-C6-O6	5.48	131.89	128.60
32	2a	266	G	C8-N9-C1'	-5.48	119.88	127.00
32	2a	1217	C	C5-C6-N1	-5.48	118.26	121.00
1	1A	1027	A	C6-N1-C2	-5.48	115.31	118.60
1	1A	1383	G	C2-N3-C4	5.48	114.64	111.90
1	1A	2414	C	O5'-P-OP2	-5.48	100.77	105.70
2	1B	41	U	N1-C2-N3	5.48	118.19	114.90
32	1a	757	U	C5-C6-N1	-5.48	119.96	122.70
1	2A	205	G	OP1-P-OP2	5.48	127.82	119.60
1	1A	1956	C	OP1-P-OP2	5.48	127.81	119.60
32	1a	188	C	N1-C2-O2	5.48	122.19	118.90
1	2A	2447	G	OP1-P-O3'	-5.48	93.15	105.20
1	2A	2457	U	N3-C2-O2	-5.48	118.37	122.20
1	1A	533	G	OP1-P-O3'	5.47	117.24	105.20
1	1A	609	A	N1-C2-N3	5.47	132.04	129.30
1	1A	1832	G	O4'-C1'-N9	5.47	112.58	108.20
32	1a	948	C	C6-N1-C2	5.47	122.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1081	G	C8-N9-C4	5.47	108.59	106.40
1	2A	1689	A	C5-N7-C8	-5.47	101.16	103.90
1	2A	2616	C	N3-C2-O2	-5.47	118.07	121.90
1	2A	2738	A	O5'-P-OP1	-5.47	100.77	105.70
32	2a	557	G	O5'-P-OP2	-5.47	100.77	105.70
32	2a	664	G	C4-C5-N7	-5.47	108.61	110.80
32	2a	1072	G	C5-C6-O6	5.47	131.88	128.60
1	1A	649	C	C6-N1-C2	5.47	122.49	120.30
1	1A	2286	A	C2-N3-C4	-5.47	107.86	110.60
1	1A	2329	C	C4-C5-C6	5.47	120.14	117.40
1	1A	2361	G	OP1-P-OP2	5.47	127.81	119.60
32	1a	189(G)	G	N3-C2-N2	-5.47	116.07	119.90
32	1a	821	G	C4-C5-C6	5.47	122.08	118.80
32	1a	1331	G	O4'-C1'-N9	5.47	112.58	108.20
1	2A	271(X)	G	C2-N3-C4	-5.47	109.16	111.90
1	2A	1311	G	OP1-P-O3'	5.47	117.24	105.20
1	2A	1933	G	OP1-P-OP2	5.47	127.81	119.60
1	2A	2030	A	N3-C4-C5	5.47	130.63	126.80
1	2A	2300	G	N9-C4-C5	5.47	107.59	105.40
32	2a	438	G	N3-C4-N9	5.47	129.28	126.00
32	2a	800	G	N1-C6-O6	5.47	123.18	119.90
1	1A	1645	C	N3-C4-N4	-5.47	114.17	118.00
1	1A	1665	G	N7-C8-N9	-5.47	110.36	113.10
32	1a	1343	G	OP2-P-O3'	5.47	117.24	105.20
32	1a	1499	A	O5'-P-OP2	-5.47	100.78	105.70
32	2a	125	U	O5'-P-OP2	-5.47	100.78	105.70
1	1A	722	A	C5-N7-C8	-5.47	101.17	103.90
1	1A	1222	A	O4'-C1'-N9	5.47	112.58	108.20
1	1A	2137	G	N7-C8-N9	5.47	115.83	113.10
1	1A	2614	A	OP2-P-O3'	5.47	117.23	105.20
1	1A	2826	C	OP1-P-OP2	5.47	127.80	119.60
1	2A	2312	U	C6-N1-C2	-5.47	117.72	121.00
1	2A	2855	C	C5-C6-N1	5.47	123.73	121.00
1	2A	1846	G	C2-N3-C4	-5.47	109.17	111.90
1	1A	248	G	O5'-P-OP2	-5.47	100.78	105.70
1	1A	489	G	N1-C6-O6	-5.47	116.62	119.90
1	1A	1434	G	OP1-P-OP2	5.47	127.80	119.60
1	1A	2407	C	N3-C4-C5	5.47	124.09	121.90
1	1A	2853	G	C5-C6-O6	5.47	131.88	128.60
2	1B	1	U	C6-N1-C1'	-5.47	113.55	121.20
2	1B	24	G	C6-N1-C2	-5.47	121.82	125.10
32	1a	823	G	O5'-P-OP2	5.47	117.26	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1049	U	C5-C4-O4	-5.47	122.62	125.90
1	1A	831	A	O4'-C1'-N9	5.46	112.57	108.20
1	1A	1196	C	OP1-P-OP2	-5.46	111.40	119.60
1	1A	1371	G	C8-N9-C4	-5.46	104.21	106.40
1	1A	1455	C	C6-N1-C2	5.46	122.49	120.30
1	1A	2606	C	C2-N3-C4	-5.46	117.17	119.90
4	1E	154	LYS	CD-CE-NZ	-5.46	99.13	111.70
32	1a	104	G	O5'-P-OP1	-5.46	100.78	105.70
32	1a	906	G	OP1-P-OP2	5.46	127.80	119.60
1	2A	701	G	C6-N1-C2	5.46	128.38	125.10
1	2A	2400	G	N1-C6-O6	5.46	123.18	119.90
1	2A	2894	G	C6-C5-N7	5.46	133.68	130.40
32	2a	64	G	C2-N3-C4	-5.46	109.17	111.90
1	1A	702	A	N3-C4-C5	5.46	130.62	126.80
1	1A	1264	G	C4-C5-N7	5.46	112.98	110.80
32	1a	398	C	C6-N1-C2	5.46	122.48	120.30
32	1a	528	C	C5-C6-N1	5.46	123.73	121.00
32	1a	671	G	O5'-P-OP1	-5.46	100.78	105.70
1	2A	2377	A	C8-N9-C4	5.46	107.98	105.80
1	2A	2645	G	N9-C4-C5	5.46	107.58	105.40
1	1A	1766	G	C5-C6-O6	-5.46	125.32	128.60
1	1A	1815	A	C8-N9-C4	5.46	107.98	105.80
1	1A	2489	C	O5'-P-OP2	-5.46	100.78	105.70
32	1a	1113	C	C6-N1-C2	-5.46	118.11	120.30
32	1a	1140	C	C6-N1-C2	-5.46	118.12	120.30
32	1a	1441	G	N1-C6-O6	-5.46	116.62	119.90
1	1A	1558	G	OP1-P-O3'	5.46	117.21	105.20
1	1A	84	G	N7-C8-N9	-5.46	110.37	113.10
1	1A	188	A	C4-C5-N7	-5.46	107.97	110.70
1	1A	332	G	N3-C2-N2	-5.46	116.08	119.90
1	1A	905	U	C5-C6-N1	-5.46	119.97	122.70
1	1A	1001	G	N3-C4-C5	5.46	131.33	128.60
1	1A	1550	C	C6-N1-C2	-5.46	118.12	120.30
2	1B	51	G	O5'-P-OP1	5.46	117.25	110.70
2	1B	80	U	C5-C4-O4	5.46	129.18	125.90
10	2O	23	ARG	CB-CG-CD	5.46	125.79	111.60
1	1A	694	G	N1-C6-O6	5.46	123.17	119.90
1	1A	1196	C	N3-C4-C5	5.46	124.08	121.90
32	1a	194	C	C5-C6-N1	5.46	123.73	121.00
2	2B	101	G	N9-C4-C5	-5.46	103.22	105.40
32	2a	655	A	O5'-P-OP2	-5.46	100.79	105.70
1	1A	2275	C	N1-C2-O2	-5.46	115.63	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	24	G	C5-C6-N1	5.46	114.23	111.50
1	2A	551	G	N1-C6-O6	-5.46	116.63	119.90
1	2A	1935	G	C4-C5-N7	5.46	112.98	110.80
1	1A	643	C	C5-C6-N1	-5.45	118.27	121.00
1	1A	737	G	C2-N3-C4	5.45	114.63	111.90
1	1A	1050	C	N1-C2-N3	5.45	123.02	119.20
1	1A	1414	G	C5-C6-O6	5.45	131.87	128.60
1	1A	2207	C	C2-N3-C4	5.45	122.63	119.90
1	1A	2481	A	OP1-P-OP2	5.45	127.78	119.60
32	1a	1000	U	O4'-C1'-N1	5.45	112.56	108.20
1	2A	417	C	C5-C6-N1	5.45	123.73	121.00
1	2A	940	G	C5-C6-O6	5.45	131.87	128.60
1	1A	514	G	N1-C2-N3	5.45	127.17	123.90
32	1a	1022	G	N3-C2-N2	5.45	123.72	119.90
1	1A	315	C	N3-C2-O2	5.45	125.72	121.90
1	1A	350	G	C8-N9-C4	5.45	108.58	106.40
1	1A	395	C	C5-C6-N1	-5.45	118.28	121.00
1	1A	795	G	N1-C6-O6	-5.45	116.63	119.90
1	1A	1168	G	C2-N3-C4	5.45	114.62	111.90
1	1A	1204	C	N3-C4-C5	5.45	124.08	121.90
1	1A	1328	U	N1-C2-N3	5.45	118.17	114.90
1	1A	1857	G	C5-C6-O6	5.45	131.87	128.60
1	1A	2068	G	N1-C6-O6	-5.45	116.63	119.90
1	1A	2467	G	N3-C4-N9	5.45	129.27	126.00
1	1A	2691	A	O5'-P-OP2	-5.45	100.80	105.70
1	1A	2735	G	C5-N7-C8	5.45	107.03	104.30
1	2A	363(E)	U	N3-C4-O4	5.45	123.22	119.40
1	2A	1666	G	N3-C2-N2	5.45	123.72	119.90
1	2A	2886	G	C4-C5-N7	-5.45	108.62	110.80
1	1A	1837	C	N3-C4-C5	5.45	124.08	121.90
1	1A	2297	C	OP2-P-O3'	5.45	117.19	105.20
1	1A	2548	G	N1-C2-N3	5.45	127.17	123.90
1	2A	97	C	N3-C4-N4	-5.45	114.19	118.00
1	2A	220	G	N3-C2-N2	-5.45	116.09	119.90
1	2A	551	G	N3-C4-C5	-5.45	125.88	128.60
1	2A	1076	C	C6-N1-C1'	-5.45	114.26	120.80
1	2A	1969	A	C8-N9-C4	-5.45	103.62	105.80
1	1A	935	C	P-O3'-C3'	5.45	126.24	119.70
1	1A	1742	G	C8-N9-C4	-5.45	104.22	106.40
1	1A	2534	U	N3-C2-O2	5.45	126.01	122.20
1	2A	17	G	OP1-P-OP2	-5.45	111.43	119.60
1	2A	2699	C	C2-N3-C4	-5.45	117.18	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2B	30	C	C4-C5-C6	5.45	120.12	117.40
32	2a	572	A	C8-N9-C1'	5.45	137.50	127.70
1	1A	315	C	N1-C2-O2	-5.45	115.63	118.90
1	1A	579	G	C4-C5-N7	-5.45	108.62	110.80
1	1A	2620	G	C5-C6-N1	5.45	114.22	111.50
1	1A	2702	C	O5'-P-OP2	5.45	117.23	110.70
1	1A	2776	G	N9-C4-C5	-5.45	103.22	105.40
32	1a	1276	G	C4-N9-C1'	5.45	133.58	126.50
1	2A	575	A	O5'-P-OP1	-5.45	100.80	105.70
1	2A	1120	G	O5'-P-OP2	-5.45	100.80	105.70
1	1A	724	A	C4-C5-C6	5.44	119.72	117.00
1	1A	1037	C	O5'-P-OP1	-5.44	100.80	105.70
1	1A	1922	A	N3-C4-C5	-5.44	122.99	126.80
32	1a	1144	G	C2-N3-C4	5.44	114.62	111.90
1	2A	145	G	N1-C6-O6	5.44	123.17	119.90
1	2A	365	C	C2-N3-C4	-5.44	117.18	119.90
1	2A	1954	G	N3-C4-N9	-5.44	122.73	126.00
1	1A	1106	U	N3-C2-O2	5.44	126.01	122.20
1	1A	2250	G	N1-C2-N3	-5.44	120.63	123.90
1	1A	2289	G	C4-C5-N7	-5.44	108.62	110.80
32	1a	354	G	C4-N9-C1'	5.44	133.57	126.50
1	2A	538	G	OP2-P-O3'	5.44	117.17	105.20
1	2A	1718	G	C4-C5-N7	-5.44	108.62	110.80
1	2A	1835	G	C5'-C4'-C3'	-5.44	107.29	116.00
1	2A	1883	G	C8-N9-C4	5.44	108.58	106.40
1	2A	2718	G	C8-N9-C4	-5.44	104.22	106.40
32	2a	33	A	N1-C6-N6	-5.44	115.33	118.60
1	1A	834	U	N1-C2-N3	5.44	118.16	114.90
13	1R	114	VAL	CB-CA-C	-5.44	101.06	111.40
32	1a	173	U	O5'-P-OP1	-5.44	100.80	105.70
32	1a	825	G	C6-C5-N7	5.44	133.66	130.40
32	1a	1531	A	C4-C5-C6	-5.44	114.28	117.00
1	2A	214	G	N1-C6-O6	-5.44	116.64	119.90
1	2A	571	A	N1-C6-N6	-5.44	115.34	118.60
1	2A	2196	C	OP1-P-O3'	5.44	117.17	105.20
1	2A	2473	U	N1-C2-O2	5.44	126.61	122.80
1	2A	2789	C	N1-C2-O2	-5.44	115.64	118.90
1	1A	455	A	C5'-C4'-C3'	-5.44	107.30	116.00
1	2A	2137	C	C6-N1-C2	-5.44	118.12	120.30
1	1A	1711	A	C4-C5-C6	5.44	119.72	117.00
1	1A	1803	G	C4-C5-N7	-5.44	108.62	110.80
1	1A	2080	A	C2-N3-C4	-5.44	107.88	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2387	G	O5'-P-OP2	-5.44	100.81	105.70
1	1A	2804	C	C5-C6-N1	5.44	123.72	121.00
32	1a	533	A	C8-N9-C1'	-5.44	117.91	127.70
32	1a	1341	U	C2-N1-C1'	-5.44	111.18	117.70
1	2A	329	G	OP1-P-OP2	5.44	127.76	119.60
1	2A	1773	A	N9-C1'-C2'	-5.44	106.02	112.00
32	2a	619	U	C5-C6-N1	-5.44	119.98	122.70
32	2a	632	A	C8-N9-C4	-5.44	103.62	105.80
1	1A	252	C	N3-C4-C5	-5.44	119.73	121.90
1	1A	1316	C	OP2-P-O3'	5.44	117.16	105.20
1	1A	1921	G	C4-C5-N7	5.44	112.97	110.80
32	1a	1076	C	N1-C2-O2	-5.44	115.64	118.90
1	2A	285	C	OP2-P-O3'	5.44	117.16	105.20
1	2A	725	G	N3-C2-N2	-5.44	116.09	119.90
1	2A	1638	C	C5-C6-N1	-5.44	118.28	121.00
32	2a	1093	A	N1-C6-N6	5.44	121.86	118.60
1	1A	1959	A	C4-C5-N7	-5.43	107.98	110.70
32	1a	1105	A	C8-N9-C4	-5.43	103.63	105.80
32	1a	1417	G	N1-C6-O6	-5.43	116.64	119.90
1	2A	189	G	N3-C2-N2	-5.43	116.10	119.90
1	2A	2629	A	C5-C6-N1	-5.43	114.98	117.70
1	1A	452	G	C5-C6-N1	5.43	114.22	111.50
1	1A	1015	C	C4-C5-C6	5.43	120.12	117.40
1	1A	2401	G	C5-C6-O6	5.43	131.86	128.60
1	1A	2443	U	C4-C5-C6	5.43	122.96	119.70
1	1A	2697	G	C6-C5-N7	5.43	133.66	130.40
32	1a	779	C	OP1-P-OP2	-5.43	111.45	119.60
1	2A	1758	G	C8-N9-C4	5.43	108.57	106.40
32	2a	886	G	N1-C6-O6	5.43	123.16	119.90
1	1A	344	A	N7-C8-N9	5.43	116.52	113.80
1	1A	1925	G	OP2-P-O3'	5.43	117.15	105.20
32	1a	754	C	C5-C4-N4	5.43	124.00	120.20
1	2A	778	G	N3-C4-C5	5.43	131.31	128.60
1	1A	409	G	N3-C2-N2	5.43	123.70	119.90
1	1A	2883	A	O4'-C1'-N9	5.43	112.54	108.20
32	1a	220	G	C8-N9-C4	-5.43	104.23	106.40
32	1a	1526	G	C5-C6-N1	5.43	114.21	111.50
1	2A	103	A	C5-C6-N6	-5.43	119.36	123.70
1	2A	271(J)	C	N1-C2-N3	-5.43	115.40	119.20
1	2A	1075	C	N3-C2-O2	-5.43	118.10	121.90
1	2A	1649	G	N1-C2-N2	-5.43	111.31	116.20
1	2A	1984	G	C5-N7-C8	-5.43	101.59	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	816	A	O5'-P-OP2	-5.43	100.81	105.70
1	1A	1065	U	N1-C2-O2	-5.43	119.00	122.80
1	1A	2139	A	C2-N3-C4	5.43	113.31	110.60
1	2A	303	U	N3-C4-O4	-5.43	115.60	119.40
32	2a	1058	G	O5'-P-OP1	5.43	117.21	110.70
1	1A	614	C	C2-N3-C4	-5.42	117.19	119.90
1	1A	961	C	N3-C4-C5	5.42	124.07	121.90
1	1A	1539	C	N1-C2-O2	5.42	122.16	118.90
1	1A	1980	C	N3-C4-N4	5.42	121.80	118.00
32	1a	194	C	C2-N1-C1'	5.42	124.77	118.80
32	1a	573	A	O5'-P-OP1	5.42	117.21	110.70
32	1a	1108	G	N3-C4-C5	-5.42	125.89	128.60
1	1A	981	C	N3-C4-N4	5.42	121.80	118.00
1	1A	1220	U	P-O3'-C3'	5.42	126.21	119.70
1	1A	1494	G	N9-C4-C5	5.42	107.57	105.40
1	1A	2442	A	C5-C6-N1	5.42	120.41	117.70
1	1A	2463	A	C6-N1-C2	-5.42	115.35	118.60
32	1a	266	G	O4'-C1'-N9	-5.42	103.86	108.20
34	1b	231	GLU	C-N-CD	5.42	139.79	128.40
1	2A	1333	C	C6-N1-C2	-5.42	118.13	120.30
1	1A	692	C	N1-C2-O2	5.42	122.15	118.90
2	1B	116	G	C5-C6-O6	-5.42	125.35	128.60
32	1a	423	G	C4-C5-N7	5.42	112.97	110.80
1	2A	271(J)	C	C6-N1-C2	5.42	122.47	120.30
1	2A	461	C	N3-C4-N4	5.42	121.80	118.00
1	2A	2177	C	C2-N3-C4	5.42	122.61	119.90
1	2A	2230	G	O5'-P-OP1	-5.42	100.82	105.70
32	2a	115	G	N3-C2-N2	5.42	123.69	119.90
1	1A	10	G	C2-N3-C4	5.42	114.61	111.90
1	1A	1135	G	N9-C1'-C2'	5.42	121.05	114.00
1	1A	2102	G	O5'-P-OP1	5.42	117.20	110.70
32	1a	67	C	C5-C4-N4	5.42	123.99	120.20
1	2A	1444	G	N1-C6-O6	-5.42	116.65	119.90
1	2A	1663	C	N3-C4-C5	5.42	124.07	121.90
1	2A	2446	G	N1-C2-N2	-5.42	111.32	116.20
1	1A	2088	C	C5-C4-N4	5.42	123.99	120.20
32	1a	141	A	O4'-C1'-N9	5.42	112.53	108.20
32	1a	1471	G	OP2-P-O3'	5.42	117.12	105.20
1	2A	195	A	C8-N9-C4	-5.42	103.63	105.80
32	2a	1048	G	N9-C1'-C2'	-5.42	106.04	112.00
32	2a	1158	C	C5-C6-N1	5.42	123.71	121.00
1	1A	1346	U	C2-N3-C4	-5.42	123.75	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	467	G	N9-C1'-C2'	-5.42	106.04	112.00
1	2A	1349	A	O5'-P-OP1	-5.42	100.83	105.70
1	2A	1502	C	OP2-P-O3'	5.42	117.12	105.20
1	2A	1982	C	C2-N3-C4	-5.42	117.19	119.90
1	2A	2043	C	N3-C4-C5	5.42	124.07	121.90
32	2a	220	G	N3-C4-N9	5.42	129.25	126.00
32	2a	572	A	N3-C4-N9	-5.42	123.07	127.40
1	2A	1632	A	C8-N9-C4	5.42	107.97	105.80
32	2a	1505	G	O5'-P-OP1	5.42	117.20	110.70
1	1A	635	C	C5-C6-N1	-5.41	118.29	121.00
1	1A	824	A	OP1-P-OP2	5.41	127.72	119.60
1	1A	1383	G	N3-C4-C5	-5.41	125.89	128.60
1	1A	1578	C	C6-N1-C2	-5.41	118.13	120.30
1	1A	1826	C	C6-N1-C2	5.41	122.47	120.30
1	1A	2021	C	OP2-P-O3'	5.41	117.11	105.20
1	1A	2286	A	C4-C5-N7	-5.41	107.99	110.70
1	1A	2353	G	N7-C8-N9	5.41	115.81	113.10
1	1A	2387	G	N1-C6-O6	5.41	123.15	119.90
1	1A	2903	G	C8-N9-C1'	5.41	134.04	127.00
2	1B	1	U	N3-C4-O4	5.41	123.19	119.40
16	1U	55	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	2A	2694	G	N1-C6-O6	-5.41	116.65	119.90
2	2B	92	C	OP2-P-O3'	5.41	117.11	105.20
32	2a	1303	C	N1-C2-O2	5.41	122.15	118.90
1	1A	1175	A	O5'-P-OP2	-5.41	100.83	105.70
1	1A	1911	A	C5-C6-N1	-5.41	114.99	117.70
32	1a	895	G	N1-C6-O6	-5.41	116.65	119.90
1	1A	500	G	OP2-P-O3'	5.41	117.10	105.20
1	1A	1664	A	N7-C8-N9	-5.41	111.09	113.80
1	1A	1991	A	O5'-P-OP2	5.41	117.19	110.70
1	1A	2220	A	N7-C8-N9	-5.41	111.09	113.80
32	1a	129	U	C6-N1-C2	-5.41	117.75	121.00
32	1a	509	A	C4-C5-C6	5.41	119.71	117.00
32	2a	704	A	C8-N9-C4	-5.41	103.64	105.80
1	1A	389	G	C4-C5-N7	5.41	112.96	110.80
1	1A	1714	G	N9-C4-C5	5.41	107.56	105.40
1	1A	2092	G	N1-C2-N2	-5.41	111.33	116.20
1	1A	2559	U	C5-C6-N1	-5.41	120.00	122.70
1	2A	1046	A	N1-C6-N6	-5.41	115.36	118.60
1	2A	1320	C	C5-C6-N1	-5.41	118.30	121.00
2	2B	25	A	O5'-P-OP1	-5.41	100.83	105.70
32	2a	91	C	C6-N1-C2	5.41	122.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	530	G	C2-N3-C4	5.41	114.60	111.90
32	2a	1466	C	N1-C2-O2	-5.41	115.65	118.90
1	1A	150	C	N3-C2-O2	-5.41	118.11	121.90
1	1A	2347	A	O5'-P-OP1	-5.41	100.83	105.70
1	1A	2777	A	C5-C6-N1	-5.41	115.00	117.70
1	1A	2902	G	C8-N9-C4	5.41	108.56	106.40
1	2A	1170	G	C8-N9-C4	-5.41	104.24	106.40
32	2a	560	U	C2-N1-C1'	5.41	124.19	117.70
1	1A	1035	G	C6-N1-C2	-5.41	121.86	125.10
1	1A	1852	A	N9-C4-C5	5.41	107.96	105.80
1	1A	1875	C	N3-C4-C5	5.41	124.06	121.90
1	1A	2057	G	O4'-C1'-N9	5.41	112.52	108.20
1	1A	2193	A	C4-C5-N7	5.41	113.40	110.70
1	1A	2612	A	C4-C5-N7	-5.41	108.00	110.70
1	2A	204	A	C5-C6-N6	-5.41	119.38	123.70
1	2A	753	C	C2-N3-C4	-5.41	117.20	119.90
1	2A	1913	A	C5-C6-N1	-5.41	115.00	117.70
2	2B	54	G	N9-C4-C5	5.41	107.56	105.40
2	2B	109	C	OP1-P-OP2	5.41	127.71	119.60
1	1A	124	A	N1-C2-N3	-5.40	126.60	129.30
1	1A	1700	G	C4-N9-C1'	5.40	133.53	126.50
1	1A	1716	A	C8-N9-C4	-5.40	103.64	105.80
5	1F	176	LEU	CB-CG-CD1	-5.40	101.82	111.00
32	1a	262	A	OP1-P-O3'	5.40	117.08	105.20
32	1a	859	A	OP1-P-O3'	5.40	117.08	105.20
32	1a	892	A	OP2-P-O3'	5.40	117.09	105.20
1	2A	595	C	N3-C2-O2	5.40	125.68	121.90
1	2A	752	A	C8-N9-C4	-5.40	103.64	105.80
1	2A	1271	G	N7-C8-N9	-5.40	110.40	113.10
32	2a	830	G	C4-C5-N7	5.40	112.96	110.80
32	2a	1001	A	C4-C5-N7	-5.40	108.00	110.70
1	1A	841	G	N7-C8-N9	-5.40	110.40	113.10
1	1A	1242	G	C6-C5-N7	5.40	133.64	130.40
1	1A	2873	C	O5'-P-OP2	-5.40	100.84	105.70
32	1a	1514	C	OP2-P-O3'	5.40	117.08	105.20
1	2A	752	A	OP1-P-O3'	-5.40	93.32	105.20
1	2A	2055	C	N1-C2-O2	-5.40	115.66	118.90
1	2A	2479	G	C8-N9-C4	-5.40	104.24	106.40
1	1A	909	G	OP1-P-O3'	-5.40	93.32	105.20
1	1A	1411	A	N3-C4-N9	5.40	131.72	127.40
1	1A	2385	G	C2-N3-C4	-5.40	109.20	111.90
1	1A	2402	U	N3-C4-C5	-5.40	111.36	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2761	A	OP2-P-O3'	5.40	117.08	105.20
1	2A	90	U	N3-C2-O2	-5.40	118.42	122.20
1	2A	828	U	OP2-P-O3'	5.40	117.08	105.20
1	2A	2476	A	N1-C6-N6	-5.40	115.36	118.60
2	2B	52	A	N1-C6-N6	5.40	121.84	118.60
32	2a	760	G	O5'-P-OP2	-5.40	100.84	105.70
32	2a	1226	C	C6-N1-C2	-5.40	118.14	120.30
1	1A	480	A	C8-N9-C4	-5.40	103.64	105.80
1	1A	1149	A	O4'-C1'-N9	5.40	112.52	108.20
1	1A	2712	C	N1-C2-O2	-5.40	115.66	118.90
32	1a	474	G	O5'-P-OP1	5.40	117.18	110.70
1	2A	2366	A	O5'-P-OP2	-5.40	100.84	105.70
1	1A	722	A	C5-C6-N6	-5.40	119.38	123.70
1	1A	1309	U	C5-C6-N1	-5.40	120.00	122.70
1	1A	1769	G	N9-C4-C5	5.40	107.56	105.40
32	1a	1024	G	N3-C4-C5	-5.40	125.90	128.60
1	2A	2397	G	OP2-P-O3'	5.40	117.07	105.20
1	1A	2491	G	C5-N7-C8	5.39	107.00	104.30
1	2A	311	A	OP1-P-OP2	-5.39	111.51	119.60
32	2a	885	G	N3-C4-C5	-5.39	125.90	128.60
1	1A	2227	G	C2-N3-C4	-5.39	109.20	111.90
1	1A	2700	U	N3-C4-C5	-5.39	111.36	114.60
32	1a	181	G	N9-C4-C5	5.39	107.56	105.40
1	2A	1721	G	N3-C4-C5	-5.39	125.90	128.60
1	1A	188	A	C5-C6-N6	5.39	128.01	123.70
1	1A	1966	U	C5-C4-O4	-5.39	122.67	125.90
1	1A	2251	G	N7-C8-N9	-5.39	110.40	113.10
1	1A	608	G	OP1-P-OP2	-5.39	111.52	119.60
1	1A	1152	G	N1-C2-N3	-5.39	120.67	123.90
1	1A	1303	C	N1-C2-N3	5.39	122.97	119.20
1	1A	2874	G	C5-C6-O6	5.39	131.83	128.60
1	1A	2897	U	O5'-P-OP1	-5.39	100.85	105.70
1	2A	2832	U	C6-N1-C2	5.39	124.23	121.00
32	2a	140	A	C8-N9-C4	-5.39	103.64	105.80
32	2a	649	G	C8-N9-C4	5.39	108.56	106.40
1	1A	587	C	N1-C2-O2	-5.39	115.67	118.90
1	1A	1392	G	C4-C5-N7	-5.39	108.64	110.80
1	1A	2633	A	O5'-P-OP1	-5.39	100.85	105.70
1	2A	271(Y)	U	N3-C2-O2	-5.39	118.43	122.20
1	1A	476	G	C6-N1-C2	-5.39	121.87	125.10
1	1A	1088	G	C4-N9-C1'	5.39	133.50	126.50
1	1A	2260	C	C2-N3-C4	-5.39	117.21	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	588	G	C8-N9-C4	-5.39	104.25	106.40
32	1a	1046	A	C6-N1-C2	-5.39	115.37	118.60
1	2A	113	G	N3-C4-C5	5.39	131.29	128.60
1	2A	1696	G	C5-C6-N1	5.39	114.19	111.50
32	2a	1217	C	C4-C5-C6	5.39	120.09	117.40
1	1A	75	C	N3-C4-N4	5.38	121.77	118.00
1	1A	119	G	C5-C6-O6	-5.38	125.37	128.60
1	1A	150	C	OP2-P-O3'	5.38	117.04	105.20
1	1A	582	G	C4-C5-N7	5.38	112.95	110.80
1	1A	1486	G	N7-C8-N9	-5.38	110.41	113.10
1	1A	1649	A	N1-C6-N6	-5.38	115.37	118.60
1	1A	2426	G	O5'-P-OP1	5.38	117.16	110.70
15	1T	96	ARG	CA-CB-CG	5.38	125.25	113.40
1	2A	247	G	O5'-P-OP2	-5.38	100.85	105.70
1	1A	554	A	C4-C5-N7	5.38	113.39	110.70
30	18	57	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	2A	1678	G	N7-C8-N9	5.38	115.79	113.10
32	2a	230	G	N9-C4-C5	5.38	107.55	105.40
1	1A	654	G	N7-C8-N9	-5.38	110.41	113.10
1	1A	1523	C	N1-C2-O2	-5.38	115.67	118.90
27	15	13	LYS	CD-CE-NZ	5.38	124.08	111.70
1	2A	527	C	N3-C2-O2	5.38	125.67	121.90
1	2A	1179	C	C6-N1-C2	5.38	122.45	120.30
32	2a	1129	C	C5-C6-N1	5.38	123.69	121.00
1	1A	2702	C	N3-C2-O2	5.38	125.67	121.90
1	2A	1411	C	OP2-P-O3'	5.38	117.03	105.20
32	2a	1140	C	C6-N1-C2	-5.38	118.15	120.30
1	1A	1143	U	C6-N1-C2	-5.38	117.77	121.00
1	1A	2525	G	C5-C6-N1	-5.38	108.81	111.50
32	1a	125	U	OP2-P-O3'	5.38	117.03	105.20
32	1a	301	G	N3-C4-C5	-5.38	125.91	128.60
32	1a	728	A	O5'-P-OP2	-5.38	100.86	105.70
1	2A	1236	G	O5'-P-OP2	5.38	117.16	110.70
32	2a	360	A	C6-N1-C2	-5.38	115.37	118.60
1	1A	86	C	O5'-P-OP2	-5.38	100.86	105.70
1	1A	317	U	O5'-P-OP2	-5.38	100.86	105.70
1	2A	1751	C	OP2-P-O3'	5.38	117.03	105.20
1	2A	1964	G	N3-C2-N2	5.38	123.66	119.90
1	2A	2419	U	OP1-P-O3'	5.38	117.03	105.20
1	2A	2465	C	C6-N1-C2	-5.38	118.15	120.30
32	2a	673	G	N3-C2-N2	5.38	123.66	119.90
32	2a	977	A	C8-N9-C4	-5.38	103.65	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	722	A	C2-N3-C4	-5.38	107.91	110.60
1	2A	2406	U	O4'-C1'-N1	-5.38	103.90	108.20
1	1A	857	U	N3-C4-O4	5.37	123.16	119.40
1	1A	1105	G	N9-C1'-C2'	-5.37	106.09	112.00
1	1A	1281	G	C2-N3-C4	-5.37	109.21	111.90
1	1A	1423	G	N1-C2-N2	-5.37	111.36	116.20
1	1A	2077	C	N3-C2-O2	5.37	125.66	121.90
16	1U	19	LYS	CD-CE-NZ	-5.37	99.34	111.70
1	2A	236	C	C2-N3-C4	-5.37	117.21	119.90
1	2A	1882	C	O5'-P-OP1	-5.37	100.86	105.70
1	2A	2166	G	C8-N9-C4	-5.37	104.25	106.40
32	2a	616	G	C8-N9-C4	-5.37	104.25	106.40
32	2a	1461	G	N1-C6-O6	5.37	123.12	119.90
32	2a	1495	U	C5-C6-N1	5.37	125.39	122.70
1	1A	642	G	OP2-P-O3'	5.37	117.02	105.20
1	1A	1670	G	OP1-P-OP2	-5.37	111.54	119.60
1	1A	2521	G	N3-C2-N2	5.37	123.66	119.90
32	1a	1211	U	C2-N3-C4	-5.37	123.78	127.00
1	2A	2146	C	C2-N1-C1'	5.37	124.71	118.80
1	2A	2358	G	N3-C4-C5	5.37	131.29	128.60
32	2a	390	C	C5-C6-N1	-5.37	118.31	121.00
32	2a	818	G	O4'-C1'-N9	5.37	112.50	108.20
32	2a	993	G	C8-N9-C1'	-5.37	120.02	127.00
1	1A	1696	G	N9-C4-C5	5.37	107.55	105.40
32	1a	1145	C	C6-N1-C2	-5.37	118.15	120.30
1	2A	1779	U	O4'-C1'-N1	5.37	112.50	108.20
2	1B	1	U	N1-C2-N3	-5.37	111.68	114.90
32	1a	23	C	C6-N1-C2	-5.37	118.15	120.30
32	1a	635	G	C5-C6-O6	-5.37	125.38	128.60
1	2A	474	G	N7-C8-N9	5.37	115.78	113.10
32	2a	791	G	N1-C6-O6	5.37	123.12	119.90
1	1A	25	U	C2-N1-C1'	5.37	124.14	117.70
1	1A	1042	A	C5-N7-C8	5.37	106.58	103.90
1	1A	1494	G	O4'-C1'-N9	5.37	112.49	108.20
1	2A	2042	A	N3-C4-C5	5.37	130.56	126.80
32	2a	186	C	C6-N1-C2	-5.37	118.15	120.30
32	2a	1060	C	C6-N1-C2	-5.37	118.15	120.30
1	1A	162	G	C8-N9-C4	-5.37	104.25	106.40
1	1A	706	C	C4-C5-C6	-5.37	114.72	117.40
1	1A	2250	G	N9-C4-C5	-5.37	103.25	105.40
32	1a	308	C	N3-C2-O2	-5.37	118.14	121.90
32	1a	1175	G	N1-C6-O6	5.37	123.12	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1197	G	N9-C4-C5	-5.37	103.25	105.40
1	2A	214	G	N9-C4-C5	5.37	107.55	105.40
32	2a	345	C	N1-C2-O2	-5.37	115.68	118.90
1	1A	702	A	C8-N9-C1'	5.36	137.35	127.70
1	1A	1282	G	N3-C4-C5	5.36	131.28	128.60
1	1A	1354	A	C5-C6-N6	5.36	127.99	123.70
1	1A	1924	C	N1-C2-O2	-5.36	115.68	118.90
32	1a	346	G	C6-N1-C2	-5.36	121.88	125.10
32	1a	427	U	C5-C6-N1	5.36	125.38	122.70
1	2A	767	U	N3-C4-O4	-5.36	115.65	119.40
1	2A	1054	A	C8-N9-C4	-5.36	103.65	105.80
1	2A	2571	C	O5'-P-OP1	-5.36	100.87	105.70
1	2A	2836	U	N1-C2-O2	5.36	126.56	122.80
1	2A	2896	C	N1-C2-O2	5.36	122.12	118.90
32	2a	490	G	N1-C6-O6	-5.36	116.68	119.90
1	1A	20	C	N1-C2-N3	5.36	122.95	119.20
1	1A	149	A	C2-N3-C4	-5.36	107.92	110.60
1	1A	920	G	OP2-P-O3'	5.36	117.00	105.20
1	1A	1985	U	C2-N1-C1'	5.36	124.14	117.70
1	1A	2129	C	C5-C6-N1	5.36	123.68	121.00
27	15	15	ARG	NE-CZ-NH1	-5.36	117.62	120.30
32	1a	322	C	N3-C4-C5	5.36	124.05	121.90
32	1a	1010	G	N3-C4-C5	5.36	131.28	128.60
1	2A	1122	G	O5'-P-OP2	-5.36	100.87	105.70
1	1A	1475	G	C2-N3-C4	5.36	114.58	111.90
1	1A	1700	G	N1-C2-N2	-5.36	111.38	116.20
1	1A	1809	U	C5-C6-N1	-5.36	120.02	122.70
1	1A	2441	G	C5-C6-N1	-5.36	108.82	111.50
32	1a	28	G	N3-C2-N2	-5.36	116.15	119.90
32	1a	668	G	OP2-P-O3'	5.36	116.99	105.20
1	2A	260	G	N9-C4-C5	5.36	107.54	105.40
1	2A	602	G	N1-C2-N2	-5.36	111.38	116.20
1	1A	652	A	O5'-P-OP1	5.36	117.13	110.70
1	1A	1527	G	N3-C4-C5	5.36	131.28	128.60
1	2A	353	G	C5-C6-O6	-5.36	125.39	128.60
1	1A	1184	G	C6-N1-C2	-5.36	121.89	125.10
1	1A	1482	G	N1-C6-O6	-5.36	116.69	119.90
1	1A	2784	C	O5'-P-OP2	5.36	117.13	110.70
2	1B	82	G	N1-C6-O6	-5.36	116.69	119.90
1	1A	1613	A	C4-C5-C6	-5.36	114.32	117.00
1	1A	2387	G	C8-N9-C4	5.36	108.54	106.40
1	1A	2484	G	C6-N1-C2	-5.36	121.89	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1024	G	C8-N9-C4	-5.36	104.26	106.40
32	1a	1504	G	C5-C6-O6	-5.36	125.39	128.60
1	2A	271(M)	G	C8-N9-C4	-5.36	104.26	106.40
1	1A	1178	A	O5'-P-OP1	-5.35	100.88	105.70
1	1A	2171	G	C6-C5-N7	5.35	133.61	130.40
1	1A	1739	U	C2-N3-C4	-5.35	123.79	127.00
1	2A	227	A	C6-N1-C2	-5.35	115.39	118.60
1	2A	1602	U	C6-N1-C2	5.35	124.21	121.00
1	2A	2106	G	N3-C4-C5	-5.35	125.92	128.60
1	2A	2695	C	C6-N1-C2	5.35	122.44	120.30
2	2B	24	G	N9-C4-C5	-5.35	103.26	105.40
15	2T	53	ARG	CB-CA-C	-5.35	99.69	110.40
1	1A	2007	G	C4-C5-N7	-5.35	108.66	110.80
1	2A	871	U	C5-C4-O4	-5.35	122.69	125.90
1	2A	1858	G	O4'-C1'-N9	5.35	112.48	108.20
32	2a	795	C	N1-C2-O2	5.35	122.11	118.90
1	1A	1441	A	C8-N9-C4	5.35	107.94	105.80
1	1A	2041	A	C2-N3-C4	-5.35	107.92	110.60
1	2A	531	C	N1-C2-O2	5.35	122.11	118.90
32	2a	9	G	C5-C6-O6	-5.35	125.39	128.60
32	2a	1163	C	N1-C2-O2	5.35	122.11	118.90
32	2a	1184	G	O5'-P-OP1	-5.35	100.89	105.70
51	2s	30	LEU	CA-CB-CG	5.35	127.60	115.30
1	1A	150	C	C2-N3-C4	-5.35	117.23	119.90
1	1A	194	G	P-O3'-C3'	5.35	126.12	119.70
1	1A	201	G	C5-N7-C8	-5.35	101.63	104.30
1	1A	1273	G	C5-N7-C8	5.35	106.97	104.30
1	1A	1729	G	N1-C6-O6	-5.35	116.69	119.90
1	1A	1845	G	N1-C2-N3	5.35	127.11	123.90
32	1a	455	C	N1-C2-O2	5.35	122.11	118.90
32	2a	830	G	C6-C5-N7	-5.35	127.19	130.40
1	1A	474	U	N3-C4-O4	-5.35	115.66	119.40
1	1A	2552	C	N3-C4-C5	5.35	124.04	121.90
1	2A	655	A	C6-C5-N7	-5.35	128.56	132.30
1	2A	1533	G	N7-C8-N9	5.35	115.77	113.10
1	2A	1899	G	OP1-P-O3'	5.35	116.96	105.20
1	1A	520	G	N9-C4-C5	5.34	107.54	105.40
1	1A	1615	G	N1-C2-N2	-5.34	111.39	116.20
34	1b	178	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	1A	41	C	O5'-P-OP1	5.34	117.11	110.70
1	1A	179	A	C5-C6-N1	-5.34	115.03	117.70
1	1A	1345	G	N1-C6-O6	5.34	123.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1874	C	C6-N1-C2	5.34	122.44	120.30
1	1A	2633	A	OP2-P-O3'	5.34	116.95	105.20
1	1A	2788	A	C5-N7-C8	5.34	106.57	103.90
32	1a	183	G	C4-N9-C1'	5.34	133.44	126.50
1	2A	2747	G	N3-C2-N2	-5.34	116.16	119.90
1	1A	1630	A	N1-C6-N6	-5.34	115.39	118.60
1	1A	2641	A	O4'-C1'-N9	5.34	112.47	108.20
2	1B	48	A	C8-N9-C4	5.34	107.94	105.80
32	1a	1217	C	C2-N1-C1'	-5.34	112.92	118.80
1	2A	1256	G	OP1-P-OP2	5.34	127.61	119.60
1	2A	2499	C	N3-C2-O2	5.34	125.64	121.90
32	2a	184	G	C8-N9-C4	-5.34	104.26	106.40
1	1A	162	G	OP1-P-O3'	5.34	116.95	105.20
1	1A	1959	A	C6-N1-C2	-5.34	115.40	118.60
1	1A	2255	U	N1-C2-O2	-5.34	119.06	122.80
1	1A	2335	G	N7-C8-N9	5.34	115.77	113.10
32	1a	820	U	N3-C2-O2	-5.34	118.46	122.20
1	2A	502	A	N1-C2-N3	5.34	131.97	129.30
32	1a	134	A	N9-C4-C5	-5.34	103.67	105.80
32	1a	819	A	C6-C5-N7	-5.34	128.56	132.30
1	2A	1251	C	C5-C4-N4	-5.34	116.46	120.20
1	2A	2514	U	N3-C4-O4	5.34	123.14	119.40
32	2a	917	G	N1-C6-O6	5.34	123.10	119.90
1	1A	217	A	N3-C4-N9	-5.34	123.13	127.40
1	1A	2193	A	N3-C4-N9	5.34	131.67	127.40
1	1A	2292	G	C6-C5-N7	5.34	133.60	130.40
32	1a	884	U	OP1-P-OP2	5.34	127.60	119.60
32	1a	1026	G	N3-C4-N9	5.34	129.20	126.00
1	2A	789	A	C4-C5-N7	5.34	113.37	110.70
1	2A	1032	A	C2-N3-C4	-5.34	107.93	110.60
1	2A	1838	C	C2-N3-C4	-5.34	117.23	119.90
1	2A	2231	C	O5'-P-OP2	-5.34	100.90	105.70
32	2a	304	U	OP1-P-OP2	5.34	127.61	119.60
32	2a	549	C	N3-C4-C5	5.34	124.03	121.90
32	2a	733	A	C8-N9-C4	5.34	107.93	105.80
32	2a	1161	C	N1-C2-O2	5.34	122.10	118.90
1	1A	50	G	N1-C2-N3	5.33	127.10	123.90
1	1A	2887	G	C8-N9-C4	5.33	108.53	106.40
1	2A	2483	C	C5-C6-N1	5.33	123.67	121.00
1	1A	2024	G	C8-N9-C4	5.33	108.53	106.40
1	1A	2436	C	C2-N1-C1'	-5.33	112.93	118.80
1	1A	2792	U	N1-C2-N3	5.33	118.10	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	30	U	N3-C2-O2	-5.33	118.47	122.20
32	1a	858	G	N7-C8-N9	5.33	115.77	113.10
1	2A	746	A	O4'-C1'-N9	5.33	112.47	108.20
1	2A	2853	C	N1-C2-O2	-5.33	115.70	118.90
32	2a	1259	C	C5-C6-N1	5.33	123.67	121.00
32	2a	1510	U	N3-C4-O4	5.33	123.13	119.40
1	1A	483	A	N1-C2-N3	-5.33	126.63	129.30
1	1A	577	U	OP2-P-O3'	5.33	116.93	105.20
1	1A	1453	C	N1-C2-N3	5.33	122.93	119.20
1	1A	2065	C	C6-N1-C2	-5.33	118.17	120.30
32	1a	807	A	N9-C4-C5	5.33	107.93	105.80
1	2A	303	U	N1-C2-O2	5.33	126.53	122.80
1	2A	1919	A	N7-C8-N9	5.33	116.47	113.80
32	2a	136	C	C6-N1-C2	-5.33	118.17	120.30
32	2a	281	G	N1-C6-O6	5.33	123.10	119.90
32	2a	1279	A	C2-N3-C4	5.33	113.27	110.60
1	1A	815	G	N3-C2-N2	-5.33	116.17	119.90
1	1A	1426	G	C5-C6-O6	-5.33	125.40	128.60
1	1A	1666	G	N7-C8-N9	-5.33	110.44	113.10
1	1A	2574	U	C5-C4-O4	5.33	129.10	125.90
21	1Z	77	ASP	CB-CG-OD1	5.33	123.10	118.30
1	2A	1394	U	O5'-P-OP1	-5.33	100.90	105.70
1	2A	2433	A	C5-C6-N6	-5.33	119.44	123.70
1	2A	2827	C	C5-C6-N1	-5.33	118.33	121.00
32	2a	851	G	N7-C8-N9	5.33	115.77	113.10
1	1A	60	G	N1-C6-O6	5.33	123.10	119.90
1	1A	218	A	C8-N9-C4	-5.33	103.67	105.80
1	1A	731	G	OP1-P-OP2	5.33	127.59	119.60
1	1A	877	G	N3-C4-C5	-5.33	125.94	128.60
1	1A	1178	A	N9-C4-C5	5.33	107.93	105.80
1	1A	1524	A	O5'-P-OP2	-5.33	100.90	105.70
1	1A	1784	G	C5-N7-C8	-5.33	101.64	104.30
1	1A	2142	G	C8-N9-C4	-5.33	104.27	106.40
2	1B	38	C	N1-C2-O2	5.33	122.10	118.90
1	2A	281	G	N1-C6-O6	5.33	123.10	119.90
32	2a	644	G	N7-C8-N9	-5.33	110.44	113.10
32	2a	912	C	O5'-P-OP2	-5.33	100.91	105.70
32	2a	1081	G	C8-N9-C4	5.33	108.53	106.40
1	1A	1280	U	C5-C6-N1	-5.33	120.04	122.70
1	1A	2693	C	N1-C2-O2	-5.33	115.70	118.90
32	1a	821	G	N3-C4-N9	5.33	129.20	126.00
32	2a	1005	A	P-O3'-C3'	5.33	126.09	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	987	G	C5-C6-N1	5.33	114.16	111.50
1	1A	1398	U	O5'-P-OP1	-5.33	100.91	105.70
2	1B	90	A	C8-N9-C4	5.33	107.93	105.80
1	1A	614	C	N3-C2-O2	-5.32	118.17	121.90
1	1A	822	G	O4'-C1'-N9	5.32	112.46	108.20
1	1A	883	G	C5-N7-C8	-5.32	101.64	104.30
1	1A	2501	G	N3-C4-N9	5.32	129.19	126.00
1	2A	116	C	C6-N1-C2	-5.32	118.17	120.30
32	2a	1059	C	OP1-P-O3'	5.32	116.91	105.20
32	2a	1363	C	C6-N1-C1'	5.32	127.19	120.80
1	1A	2099	A	C8-N9-C4	5.32	107.93	105.80
1	1A	2245	U	C2-N3-C4	-5.32	123.81	127.00
32	1a	1397	C	C6-N1-C2	-5.32	118.17	120.30
32	2a	918	A	OP2-P-O3'	5.32	116.91	105.20
32	2a	1511	G	C4-C5-N7	-5.32	108.67	110.80
1	1A	500	G	N3-C2-N2	5.32	123.62	119.90
1	1A	500	G	O5'-P-OP2	-5.32	100.91	105.70
1	1A	845	G	C4-C5-N7	-5.32	108.67	110.80
1	1A	1093	G	C8-N9-C1'	-5.32	120.08	127.00
1	1A	1386	U	N1-C2-N3	5.32	118.09	114.90
1	1A	2100	C	O5'-P-OP1	-5.32	100.91	105.70
1	1A	2429	C	O5'-P-OP2	-5.32	100.91	105.70
3	1D	222	ARG	NE-CZ-NH1	-5.32	117.64	120.30
32	1a	189(D)	C	C6-N1-C1'	-5.32	114.41	120.80
32	1a	857	C	N3-C4-C5	-5.32	119.77	121.90
1	2A	858	U	N1-C2-O2	5.32	126.52	122.80
32	2a	232	G	C5-C6-O6	-5.32	125.41	128.60
32	1a	1175	G	C5-C6-O6	-5.32	125.41	128.60
32	2a	19	C	OP1-P-OP2	5.32	127.58	119.60
1	1A	36	G	N1-C6-O6	-5.32	116.71	119.90
1	1A	762	G	N3-C4-C5	-5.32	125.94	128.60
1	1A	1175	A	N1-C6-N6	-5.32	115.41	118.60
1	1A	1508	G	O5'-P-OP1	-5.32	100.91	105.70
1	1A	1946	C	O5'-P-OP2	5.32	117.08	110.70
2	1B	104	U	C6-N1-C2	5.32	124.19	121.00
18	1W	83	LYS	CD-CE-NZ	-5.32	99.47	111.70
32	1a	353	A	C5-C6-N6	-5.32	119.45	123.70
32	1a	550	G	OP1-P-OP2	5.32	127.58	119.60
1	2A	1717	G	C4-C5-N7	-5.32	108.67	110.80
1	2A	1789	A	N7-C8-N9	-5.32	111.14	113.80
1	1A	818	G	N3-C2-N2	5.32	123.62	119.90
1	1A	1392	G	C5-N7-C8	5.32	106.96	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2073	A	C4-C5-N7	-5.32	108.04	110.70
1	1A	2138	G	N7-C8-N9	5.32	115.76	113.10
1	1A	2637	G	N9-C4-C5	5.32	107.53	105.40
1	1A	2722	C	OP1-P-O3'	5.32	116.89	105.20
32	1a	487	A	N1-C6-N6	5.32	121.79	118.60
1	2A	826	U	N1-C2-N3	5.32	118.09	114.90
1	2A	1020	A	O5'-P-OP1	-5.32	100.92	105.70
1	2A	1052	C	C5-C6-N1	5.32	123.66	121.00
1	2A	2155	G	N1-C2-N2	5.32	120.98	116.20
1	1A	841	G	C8-N9-C4	5.31	108.53	106.40
1	1A	1067	A	C4-C5-C6	5.31	119.66	117.00
1	2A	614(C)	A	O5'-P-OP2	-5.31	100.92	105.70
1	2A	1791	A	C5'-C4'-C3'	-5.31	107.50	116.00
1	1A	765	A	C4-C5-C6	5.31	119.66	117.00
1	1A	1344	C	N3-C4-N4	-5.31	114.28	118.00
1	1A	1422	C	C5-C4-N4	5.31	123.92	120.20
1	1A	1812	C	C6-N1-C1'	-5.31	114.42	120.80
1	1A	2030	C	C5-C6-N1	-5.31	118.34	121.00
1	1A	2215	G	C8-N9-C4	5.31	108.53	106.40
1	1A	2360	U	C5-C4-O4	5.31	129.09	125.90
1	1A	2587	C	C6-N1-C2	5.31	122.42	120.30
18	1W	107	LEU	CA-CB-CG	5.31	127.52	115.30
32	1a	227	G	C8-N9-C4	5.31	108.53	106.40
32	1a	776	G	N1-C6-O6	5.31	123.09	119.90
1	2A	1883	G	C8-N9-C1'	-5.31	120.09	127.00
1	2A	2886	G	N3-C2-N2	-5.31	116.18	119.90
1	1A	202	A	O5'-P-OP1	5.31	117.07	110.70
1	1A	815	G	N1-C2-N3	5.31	127.09	123.90
1	1A	1107	U	N1-C2-O2	5.31	126.52	122.80
1	1A	1236	G	N7-C8-N9	-5.31	110.44	113.10
32	1a	1181	G	N1-C6-O6	5.31	123.09	119.90
1	2A	587	C	N3-C2-O2	-5.31	118.18	121.90
1	2A	1986	A	C2-N3-C4	-5.31	107.94	110.60
1	2A	2877	G	O5'-P-OP1	5.31	117.07	110.70
1	1A	17	G	C6-N1-C2	-5.31	121.92	125.10
1	1A	612	C	C5-C6-N1	-5.31	118.34	121.00
1	1A	1178	A	C8-N9-C4	-5.31	103.68	105.80
1	1A	1985	U	OP1-P-O3'	5.31	116.88	105.20
1	1A	2399	U	N1-C2-O2	-5.31	119.08	122.80
1	1A	2568	C	C5-C6-N1	-5.31	118.34	121.00
32	1a	155	C	C6-N1-C2	-5.31	118.18	120.30
32	1a	563	A	C5-N7-C8	-5.31	101.25	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2632	A	N1-C6-N6	5.31	121.78	118.60
32	2a	574	A	C4-C5-N7	5.31	113.35	110.70
1	1A	1207	C	C5-C4-N4	-5.31	116.48	120.20
1	1A	2395	G	N1-C6-O6	-5.31	116.72	119.90
1	1A	2738	A	N1-C2-N3	5.31	131.95	129.30
1	2A	1231	G	OP1-P-OP2	-5.31	111.64	119.60
1	2A	1536	C	N3-C4-N4	5.31	121.72	118.00
1	2A	1776	G	N3-C4-N9	5.31	129.18	126.00
21	2Z	155	LEU	CA-CB-CG	5.31	127.51	115.30
32	1a	1003	G	C4-N9-C1'	5.31	133.40	126.50
1	2A	1997	G	C5-C6-N1	5.31	114.15	111.50
32	2a	1486	G	C8-N9-C4	5.31	108.52	106.40
1	1A	1842	G	C8-N9-C4	-5.30	104.28	106.40
1	1A	2034	G	N9-C4-C5	5.30	107.52	105.40
1	1A	2516	U	C2-N3-C4	-5.30	123.82	127.00
1	2A	411	G	O5'-P-OP1	-5.30	100.93	105.70
1	2A	1016	G	N3-C4-C5	5.30	131.25	128.60
1	2A	1610	A	N9-C4-C5	-5.30	103.68	105.80
1	1A	1694	G	N3-C2-N2	-5.30	116.19	119.90
1	1A	1771	G	N1-C6-O6	5.30	123.08	119.90
1	1A	2265	G	O4'-C1'-N9	-5.30	103.96	108.20
32	1a	345	C	C6-N1-C1'	-5.30	114.44	120.80
32	1a	696	A	N1-C6-N6	5.30	121.78	118.60
1	2A	494	G	N9-C4-C5	5.30	107.52	105.40
1	2A	1690	A	C6-C5-N7	-5.30	128.59	132.30
1	2A	2035	G	C4-N9-C1'	-5.30	119.61	126.50
1	2A	2232	U	N3-C4-C5	5.30	117.78	114.60
1	2A	2353	G	C5-C6-O6	-5.30	125.42	128.60
1	1A	215	G	C8-N9-C1'	5.30	133.89	127.00
1	1A	555	G	C5-C6-N1	5.30	114.15	111.50
1	1A	1383	G	C5-N7-C8	5.30	106.95	104.30
1	1A	2250	G	C2-N3-C4	5.30	114.55	111.90
32	1a	176	C	C6-N1-C2	-5.30	118.18	120.30
32	1a	1022	G	N3-C4-N9	5.30	129.18	126.00
32	1a	1529	G	C8-N9-C4	-5.30	104.28	106.40
1	2A	944	G	C5-C6-O6	5.30	131.78	128.60
1	2A	2140	C	C6-N1-C2	-5.30	118.18	120.30
32	2a	906	G	C5-C6-O6	-5.30	125.42	128.60
1	1A	41	C	OP2-P-O3'	5.30	116.86	105.20
1	1A	454	U	C4-C5-C6	-5.30	116.52	119.70
1	1A	616	G	C5-N7-C8	5.30	106.95	104.30
1	1A	1110	C	C6-N1-C2	-5.30	118.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1255	A	C5-N7-C8	-5.30	101.25	103.90
1	1A	2329	C	C6-N1-C2	-5.30	118.18	120.30
1	1A	2561	G	OP2-P-O3'	5.30	116.86	105.20
32	1a	149	A	C5-C6-N1	-5.30	115.05	117.70
32	1a	644	G	N1-C6-O6	-5.30	116.72	119.90
1	2A	1264	G	C5-C6-O6	5.30	131.78	128.60
1	2A	2307	G	N3-C4-N9	5.30	129.18	126.00
1	2A	2378	A	C8-N9-C1'	-5.30	118.16	127.70
1	2A	2446	G	N3-C2-N2	5.30	123.61	119.90
32	2a	498	U	N3-C4-O4	-5.30	115.69	119.40
1	1A	10	G	O4'-C1'-N9	5.30	112.44	108.20
1	1A	387	G	N3-C4-C5	5.30	131.25	128.60
1	1A	1269	G	C5-C6-O6	5.30	131.78	128.60
1	1A	2024	G	C4-C5-N7	-5.30	108.68	110.80
1	1A	2238	C	N1-C2-O2	-5.30	115.72	118.90
32	1a	266	G	N7-C8-N9	5.30	115.75	113.10
32	1a	324	G	OP2-P-O3'	5.30	116.86	105.20
1	2A	1180	C	N1-C2-O2	5.30	122.08	118.90
1	2A	2763	G	N3-C4-C5	-5.30	125.95	128.60
32	2a	1349	A	C8-N9-C4	5.30	107.92	105.80
1	1A	1828	C	N1-C2-O2	-5.30	115.72	118.90
1	1A	2008	A	OP2-P-O3'	5.30	116.85	105.20
1	1A	2351	G	O5'-P-OP2	-5.30	100.93	105.70
1	1A	2561	G	C5'-C4'-O4'	5.30	115.45	109.10
1	1A	2653	G	C5'-C4'-C3'	-5.30	107.53	116.00
32	1a	189(D)	C	C6-N1-C2	-5.30	118.18	120.30
1	2A	1369	G	C5-C6-N1	5.30	114.15	111.50
1	2A	1933	G	N9-C4-C5	5.30	107.52	105.40
32	2a	1043	C	C5-C4-N4	5.30	123.91	120.20
1	1A	839	G	N3-C4-N9	5.29	129.18	126.00
1	1A	1179	U	OP2-P-O3'	5.29	116.85	105.20
32	1a	569	C	O5'-P-OP2	-5.29	100.94	105.70
32	1a	1066	C	C6-N1-C2	5.29	122.42	120.30
1	2A	937	U	N1-C2-O2	-5.29	119.09	122.80
1	2A	2125	G	N3-C2-N2	5.29	123.61	119.90
1	2A	2583	G	OP2-P-O3'	5.29	116.84	105.20
32	2a	302	G	OP2-P-O3'	5.29	116.85	105.20
1	1A	827	G	N3-C2-N2	-5.29	116.20	119.90
1	1A	1143	U	C5-C6-N1	5.29	125.35	122.70
1	1A	2403	G	O4'-C1'-N9	5.29	112.43	108.20
32	1a	618	C	O5'-P-OP1	-5.29	100.94	105.70
1	2A	80	G	C5-C6-O6	5.29	131.78	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	300	A	N1-C6-N6	5.29	121.78	118.60
1	2A	2083	G	O5'-P-OP1	-5.29	100.94	105.70
1	2A	2817	G	C5-C6-O6	5.29	131.78	128.60
2	2B	33	G	C2-N3-C4	-5.29	109.25	111.90
1	1A	1012	C	C2-N3-C4	-5.29	117.25	119.90
32	1a	187	C	C2-N1-C1'	5.29	124.62	118.80
32	1a	250	A	N3-C4-C5	-5.29	123.10	126.80
1	2A	2262	U	OP1-P-OP2	-5.29	111.67	119.60
1	1A	846	G	OP1-P-OP2	5.29	127.53	119.60
1	1A	2440	G	C5-C6-N1	5.29	114.14	111.50
1	1A	2616	U	N3-C2-O2	-5.29	118.50	122.20
1	1A	2619	G	N1-C6-O6	-5.29	116.73	119.90
1	1A	2668	U	N3-C2-O2	-5.29	118.50	122.20
32	1a	68	G	C4-N9-C1'	-5.29	119.62	126.50
1	2A	1473	G	N9-C4-C5	-5.29	103.28	105.40
1	2A	1574	C	C2-N3-C4	5.29	122.55	119.90
1	2A	1702	G	N1-C6-O6	-5.29	116.73	119.90
1	2A	1747(A)	G	N1-C6-O6	5.29	123.07	119.90
32	2a	316	G	C8-N9-C4	-5.29	104.28	106.40
32	2a	563	A	O4'-C1'-N9	5.29	112.43	108.20
32	2a	1287	A	C6-N1-C2	5.29	121.77	118.60
1	1A	2376	C	N3-C4-C5	5.29	124.02	121.90
1	1A	2725	A	C6-N1-C2	5.29	121.77	118.60
1	2A	718	A	C5-C6-N1	-5.29	115.06	117.70
1	1A	170	A	C5-C6-N1	5.29	120.34	117.70
1	1A	716	G	C6-N1-C2	5.29	128.27	125.10
1	1A	791	G	O5'-P-OP1	-5.29	100.94	105.70
1	1A	1026	A	C4-C5-N7	5.29	113.34	110.70
1	1A	1533	G	C8-N9-C4	-5.29	104.29	106.40
1	1A	2562	G	N3-C4-C5	-5.29	125.96	128.60
1	1A	2779	G	N1-C6-O6	-5.29	116.73	119.90
1	2A	103	A	N1-C6-N6	5.29	121.77	118.60
1	2A	189	G	C5-N7-C8	5.29	106.94	104.30
1	2A	2852	G	N3-C2-N2	5.29	123.60	119.90
32	2a	509	A	N7-C8-N9	5.29	116.44	113.80
1	1A	658	A	N7-C8-N9	5.28	116.44	113.80
1	1A	2724	U	C2-N3-C4	-5.28	123.83	127.00
4	1E	77	ILE	CG1-CB-CG2	-5.28	99.78	111.40
32	1a	451	A	OP1-P-OP2	5.28	127.53	119.60
32	1a	479	C	C2-N3-C4	5.28	122.54	119.90
1	2A	271(H)	G	O5'-P-OP2	-5.28	100.95	105.70
1	2A	1180	C	C6-N1-C2	5.28	122.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1551	C	OP2-P-O3'	5.28	116.83	105.20
15	2T	96	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	1A	2278	A	C6-N1-C2	5.28	121.77	118.60
32	1a	541	G	C8-N9-C4	5.28	108.51	106.40
1	2A	386	G	C6-N1-C2	-5.28	121.93	125.10
32	2a	671	G	OP2-P-O3'	5.28	116.82	105.20
1	1A	96	C	OP1-P-OP2	5.28	127.52	119.60
1	1A	127	C	N3-C2-O2	5.28	125.60	121.90
1	1A	781	A	C4-C5-C6	5.28	119.64	117.00
1	1A	1212	C	OP2-P-O3'	5.28	116.81	105.20
1	1A	1652	G	N1-C2-N3	5.28	127.07	123.90
13	1R	64	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	2A	531	C	C6-N1-C2	5.28	122.41	120.30
32	2a	794	A	N7-C8-N9	5.28	116.44	113.80
1	2A	1997	G	OP1-P-OP2	-5.28	111.68	119.60
32	2a	991	U	P-O3'-C3'	5.28	126.03	119.70
1	1A	415	G	N3-C2-N2	5.28	123.59	119.90
1	1A	533	G	N1-C2-N2	5.28	120.95	116.20
1	1A	854	U	OP2-P-O3'	5.28	116.81	105.20
1	1A	1230	C	OP2-P-O3'	-5.28	93.59	105.20
1	1A	1611	C	N3-C4-N4	-5.28	114.31	118.00
1	1A	2078	G	O4'-C1'-N9	-5.28	103.98	108.20
32	1a	156	G	N7-C8-N9	5.28	115.74	113.10
1	2A	94(A)	G	N3-C4-C5	-5.28	125.96	128.60
1	1A	72	A	N1-C2-N3	5.28	131.94	129.30
1	1A	835	A	N7-C8-N9	-5.28	111.16	113.80
1	1A	2632	C	C2-N1-C1'	-5.28	113.00	118.80
11	1P	41	ARG	NE-CZ-NH1	5.28	122.94	120.30
32	1a	57	G	N3-C4-C5	-5.28	125.96	128.60
1	2A	61	G	C4-C5-N7	5.28	112.91	110.80
1	2A	1649	G	C8-N9-C4	5.28	108.51	106.40
1	2A	2278	A	N1-C6-N6	-5.28	115.43	118.60
32	2a	190	U	N1-C2-N3	5.28	118.06	114.90
32	2a	1530	G	N9-C4-C5	-5.28	103.29	105.40
1	1A	255	G	N1-C6-O6	5.27	123.06	119.90
1	1A	827	G	C4-C5-C6	5.27	121.97	118.80
32	1a	142	G	O4'-C1'-N9	5.27	112.42	108.20
32	1a	736	C	C6-N1-C2	-5.27	118.19	120.30
1	2A	2629	A	C5'-C4'-O4'	5.27	115.43	109.10
1	1A	1529	G	N1-C6-O6	-5.27	116.74	119.90
32	1a	15	G	C6-C5-N7	-5.27	127.24	130.40
32	1a	427	U	C6-N1-C2	-5.27	117.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	902	G	O5'-P-OP1	5.27	117.03	110.70
32	1a	1287	A	C5-C6-N6	5.27	127.92	123.70
1	2A	551	G	C5-C6-O6	5.27	131.76	128.60
1	2A	2814	C	N1-C2-O2	-5.27	115.74	118.90
32	2a	295	C	N3-C4-C5	5.27	124.01	121.90
1	1A	645	G	O5'-P-OP1	-5.27	100.96	105.70
1	2A	206	U	N3-C2-O2	-5.27	118.51	122.20
32	2a	953	G	O5'-P-OP2	-5.27	100.96	105.70
1	1A	729	G	O5'-P-OP2	5.27	117.02	110.70
1	1A	1104	G	N3-C4-N9	5.27	129.16	126.00
1	1A	1377	A	N1-C2-N3	5.27	131.94	129.30
1	1A	1814	A	N7-C8-N9	-5.27	111.17	113.80
1	1A	2207	C	C2-N1-C1'	5.27	124.60	118.80
1	1A	2578	A	C5-C6-N1	-5.27	115.07	117.70
1	2A	975(A)	G	OP1-P-O3'	5.27	116.80	105.20
32	2a	938	A	C8-N9-C4	-5.27	103.69	105.80
32	1a	1505	G	O5'-P-OP1	5.27	117.02	110.70
1	2A	1807	G	N9-C1'-C2'	-5.27	106.21	112.00
32	2a	1373	G	O4'-C1'-N9	5.27	112.41	108.20
1	1A	1028	C	C5-C4-N4	-5.27	116.51	120.20
1	1A	1652	G	C5-C6-O6	-5.27	125.44	128.60
1	2A	1670	C	C4-C5-C6	5.27	120.03	117.40
32	2a	923	A	O5'-P-OP1	-5.27	100.96	105.70
1	1A	246	A	C8-N9-C4	-5.26	103.69	105.80
1	1A	559	U	C5-C6-N1	-5.26	120.07	122.70
1	1A	723	A	O5'-P-OP2	-5.26	100.96	105.70
1	1A	1245	C	C2-N1-C1'	-5.26	113.01	118.80
1	1A	1715	A	C2-N3-C4	-5.26	107.97	110.60
1	1A	1911	A	C8-N9-C4	5.26	107.91	105.80
1	1A	2623	U	OP1-P-O3'	5.26	116.78	105.20
1	1A	2646	G	C8-N9-C4	-5.26	104.29	106.40
1	1A	2659	U	N3-C2-O2	-5.26	118.51	122.20
32	1a	557	G	N3-C2-N2	5.26	123.58	119.90
1	2A	1005	C	OP1-P-OP2	5.26	127.50	119.60
32	2a	625	G	N9-C4-C5	5.26	107.51	105.40
32	2a	1011	G	C5-C6-O6	5.26	131.76	128.60
32	2a	1394	A	N9-C4-C5	-5.26	103.69	105.80
32	1a	576	G	N3-C2-N2	5.26	123.58	119.90
32	1a	936	C	C6-N1-C2	5.26	122.41	120.30
1	2A	2817	G	C4-C5-N7	-5.26	108.69	110.80
1	1A	200	A	OP2-P-O3'	5.26	116.78	105.20
1	1A	964	A	OP2-P-O3'	5.26	116.77	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	78	G	C4-N9-C1'	-5.26	119.66	126.50
1	2A	37	C	C2-N3-C4	-5.26	117.27	119.90
1	2A	98	G	N3-C2-N2	5.26	123.58	119.90
1	2A	465	G	C2-N3-C4	5.26	114.53	111.90
1	2A	1126	A	OP1-P-OP2	5.26	127.49	119.60
1	2A	1313	U	O4'-C1'-N1	5.26	112.41	108.20
1	2A	1903	G	N9-C4-C5	5.26	107.50	105.40
32	2a	1416	G	N1-C6-O6	5.26	123.06	119.90
1	1A	407	U	N3-C2-O2	-5.26	118.52	122.20
1	1A	618	C	C5-C6-N1	5.26	123.63	121.00
1	1A	1126	C	N1-C2-O2	5.26	122.06	118.90
1	1A	2712	C	N3-C2-O2	5.26	125.58	121.90
1	2A	666	G	C5-C6-O6	-5.26	125.44	128.60
1	2A	1740	G	C5-C6-N1	5.26	114.13	111.50
1	2A	2519	U	C5-C4-O4	-5.26	122.74	125.90
32	2a	517	G	N3-C4-C5	-5.26	125.97	128.60
32	2a	1395	C	N3-C4-C5	-5.26	119.80	121.90
2	1B	68	C	OP2-P-O3'	5.26	116.77	105.20
15	1T	53	ARG	CB-CA-C	-5.26	99.88	110.40
1	2A	2434	A	OP2-P-O3'	5.26	116.77	105.20
1	2A	2678	C	OP2-P-O3'	5.26	116.77	105.20
32	2a	1151	A	O5'-P-OP2	-5.26	100.97	105.70
1	1A	620	U	N1-C2-N3	5.26	118.05	114.90
1	1A	1646	C	O5'-P-OP2	-5.26	100.97	105.70
32	1a	356	A	N1-C2-N3	-5.26	126.67	129.30
1	2A	107	C	OP2-P-O3'	5.26	116.77	105.20
1	2A	1087	G	N9-C4-C5	5.26	107.50	105.40
32	2a	35	G	N9-C4-C5	5.26	107.50	105.40
32	2a	1391	U	N3-C2-O2	-5.26	118.52	122.20
1	1A	2596	U	N3-C2-O2	-5.25	118.52	122.20
1	1A	2700	U	C5-C4-O4	-5.25	122.75	125.90
2	1B	36	C	C6-N1-C2	5.25	122.40	120.30
1	1A	106	U	N3-C4-O4	-5.25	115.72	119.40
1	1A	773	G	OP1-P-O3'	5.25	116.76	105.20
1	1A	788	G	C4-C5-N7	-5.25	108.70	110.80
1	1A	1026	A	N1-C2-N3	-5.25	126.67	129.30
1	1A	2083	G	O4'-C1'-N9	5.25	112.40	108.20
1	1A	2548	G	C5-C6-N1	-5.25	108.87	111.50
1	1A	2635	G	N3-C4-C5	-5.25	125.97	128.60
32	1a	189(L)	G	C2-N3-C4	5.25	114.53	111.90
32	1a	560	U	P-O3'-C3'	5.25	126.00	119.70
32	1a	722	A	C5-N7-C8	-5.25	101.27	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	55	G	C8-N9-C4	-5.25	104.30	106.40
1	2A	662	G	O5'-P-OP1	-5.25	100.97	105.70
32	2a	1001	A	C5-N7-C8	5.25	106.53	103.90
1	1A	24	G	N7-C8-N9	-5.25	110.47	113.10
27	15	16	ARG	CG-CD-NE	5.25	122.83	111.80
1	2A	212	G	O5'-P-OP2	-5.25	100.97	105.70
1	1A	1869	C	N3-C2-O2	-5.25	118.22	121.90
1	1A	2902	G	N3-C2-N2	5.25	123.58	119.90
1	1A	661	G	C5-C6-N1	-5.25	108.88	111.50
1	1A	980	C	C5-C6-N1	-5.25	118.38	121.00
1	1A	1301	U	N1-C2-N3	5.25	118.05	114.90
1	1A	1425	A	O4'-C1'-N9	-5.25	104.00	108.20
1	1A	1701	A	C5-N7-C8	5.25	106.52	103.90
1	2A	741	G	N1-C6-O6	-5.25	116.75	119.90
1	2A	2237	G	C4-C5-N7	-5.25	108.70	110.80
1	2A	2788	C	OP2-P-O3'	5.25	116.75	105.20
1	1A	697	C	N1-C2-O2	5.25	122.05	118.90
1	1A	1726	U	OP1-P-OP2	5.25	127.47	119.60
1	1A	1807	G	N3-C4-C5	-5.25	125.98	128.60
1	1A	2099	A	N9-C4-C5	-5.25	103.70	105.80
1	1A	2534	U	C5-C4-O4	-5.25	122.75	125.90
1	1A	2621	U	C5-C4-O4	-5.25	122.75	125.90
18	1W	92	ARG	NE-CZ-NH1	-5.25	117.68	120.30
32	1a	186	C	OP1-P-O3'	5.25	116.74	105.20
32	2a	1125	U	C6-N1-C1'	-5.25	113.85	121.20
32	2a	1351	U	O5'-P-OP1	-5.25	100.98	105.70
1	2A	1973	G	O5'-P-OP2	-5.25	100.98	105.70
1	2A	1982	C	N3-C4-C5	5.25	124.00	121.90
32	2a	525	C	C5-C6-N1	5.25	123.62	121.00
1	1A	702	A	N9-C4-C5	5.24	107.90	105.80
1	1A	1148	C	C6-N1-C2	-5.24	118.20	120.30
1	1A	2858	G	N3-C4-N9	-5.24	122.85	126.00
1	2A	2182	G	C8-N9-C1'	5.24	133.82	127.00
1	2A	2234	G	C5-C6-O6	5.24	131.75	128.60
32	2a	230	G	C5-C6-N1	-5.24	108.88	111.50
32	2a	266	G	N1-C2-N2	-5.24	111.48	116.20
32	2a	533	A	N1-C2-N3	5.24	131.92	129.30
1	1A	2086	C	O5'-P-OP2	-5.24	100.98	105.70
1	1A	2637	G	C4-C5-N7	-5.24	108.70	110.80
32	1a	732	C	N3-C4-C5	5.24	124.00	121.90
32	1a	784	C	C5-C6-N1	-5.24	118.38	121.00
1	2A	1666	G	N1-C6-O6	-5.24	116.76	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2003	G	OP2-P-O3'	5.24	116.73	105.20
1	2A	2154	G	N9-C4-C5	-5.24	103.30	105.40
1	2A	2783	G	C6-C5-N7	5.24	133.54	130.40
1	1A	1080	G	N1-C2-N2	5.24	120.92	116.20
1	1A	1757	C	C2-N1-C1'	-5.24	113.04	118.80
1	1A	1921	G	C6-N1-C2	-5.24	121.96	125.10
1	1A	1925	G	C8-N9-C4	-5.24	104.30	106.40
1	1A	2460	A	C5-N7-C8	5.24	106.52	103.90
2	1B	104	U	OP2-P-O3'	5.24	116.72	105.20
32	1a	722	A	C5-C6-N1	-5.24	115.08	117.70
1	2A	819	A	C8-N9-C4	-5.24	103.70	105.80
1	2A	2505	G	N1-C6-O6	-5.24	116.76	119.90
1	2A	1092	C	C2-N1-C1'	5.24	124.56	118.80
32	2a	572	A	N3-C4-C5	5.24	130.47	126.80
1	1A	120	G	OP2-P-O3'	5.24	116.72	105.20
1	1A	252	C	C5-C4-N4	5.24	123.86	120.20
1	1A	422	U	C2-N1-C1'	5.24	123.98	117.70
1	1A	1106	U	N3-C4-O4	5.24	123.06	119.40
1	1A	1220	U	C2-N1-C1'	-5.24	111.42	117.70
1	1A	1361	C	N3-C4-C5	5.24	123.99	121.90
1	1A	1884	A	C5-N7-C8	5.24	106.52	103.90
1	1A	2523	U	N1-C2-O2	-5.24	119.14	122.80
32	1a	1068	G	O5'-P-OP2	-5.24	100.99	105.70
32	1a	1208	C	C6-N1-C2	-5.24	118.21	120.30
32	2a	931	C	OP2-P-O3'	5.24	116.72	105.20
1	1A	199	C	C5-C6-N1	-5.23	118.38	121.00
1	1A	1031	C	N3-C4-C5	5.23	123.99	121.90
1	1A	1342	G	N7-C8-N9	-5.23	110.48	113.10
32	1a	338	A	O5'-P-OP1	-5.23	100.99	105.70
1	2A	1102	C	C2-N3-C4	5.23	122.52	119.90
1	1A	12	U	C2-N1-C1'	5.23	123.98	117.70
1	1A	621	G	C5-C6-O6	5.23	131.74	128.60
1	1A	2072	C	N3-C2-O2	5.23	125.56	121.90
1	1A	2185	C	N1-C2-O2	5.23	122.04	118.90
1	2A	1084	A	N9-C4-C5	-5.23	103.71	105.80
1	2A	2033	A	O4'-C1'-N9	5.23	112.39	108.20
1	2A	2306	C	N3-C2-O2	-5.23	118.24	121.90
2	2B	101	G	C8-N9-C4	5.23	108.49	106.40
32	2a	1276	G	C8-N9-C4	-5.23	104.31	106.40
1	1A	807	G	C8-N9-C4	5.23	108.49	106.40
1	1A	2238	C	N3-C2-O2	5.23	125.56	121.90
1	1A	2442	A	OP1-P-OP2	5.23	127.44	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	163	C	C6-N1-C1'	5.23	127.08	120.80
1	2A	1531	C	C2-N1-C1'	5.23	124.55	118.80
1	2A	2388	A	OP1-P-OP2	-5.23	111.75	119.60
1	2A	2585	U	OP1-P-O3'	5.23	116.70	105.20
32	2a	777	A	C8-N9-C4	-5.23	103.71	105.80
1	1A	252	C	N3-C2-O2	-5.23	118.24	121.90
1	1A	385	G	C5-C6-O6	-5.23	125.46	128.60
1	1A	1208	G	C8-N9-C1'	5.23	133.80	127.00
1	1A	1718	U	C2-N3-C4	-5.23	123.86	127.00
32	1a	792	A	N1-C6-N6	-5.23	115.46	118.60
32	2a	134	A	C5-C6-N6	-5.23	119.52	123.70
32	2a	404	U	C6-N1-C2	-5.23	117.86	121.00
32	2a	633	G	O5'-P-OP2	-5.23	100.99	105.70
1	1A	367	C	C5-C6-N1	-5.23	118.39	121.00
1	1A	369	A	N3-C4-N9	5.23	131.58	127.40
1	1A	2200	C	O4'-C1'-N1	5.23	112.38	108.20
32	1a	1228	C	C5-C6-N1	5.23	123.61	121.00
1	2A	955	C	N1-C2-O2	-5.23	115.76	118.90
1	2A	1471	A	C6-C5-N7	-5.23	128.64	132.30
1	2A	2678	C	N3-C4-N4	-5.23	114.34	118.00
32	2a	814	A	OP2-P-O3'	5.23	116.70	105.20
2	1B	116	G	C4-N9-C1'	5.23	133.29	126.50
32	1a	732	C	O5'-P-OP1	-5.23	101.00	105.70
32	1a	824	C	OP2-P-O3'	5.23	116.70	105.20
1	2A	1660	C	O5'-P-OP2	-5.23	101.00	105.70
1	1A	744	C	C5-C4-N4	5.22	123.86	120.20
1	1A	791	G	OP1-P-OP2	5.22	127.44	119.60
1	1A	855	G	C5-C6-N1	5.22	114.11	111.50
1	1A	872	C	C5-C6-N1	-5.22	118.39	121.00
1	1A	1183	G	N1-C6-O6	-5.22	116.77	119.90
1	1A	1721	G	O4'-C1'-N9	-5.22	104.02	108.20
1	1A	2349	G	C5-C6-O6	-5.22	125.47	128.60
1	2A	1239	G	N1-C6-O6	5.22	123.03	119.90
1	2A	2579	C	C5-C4-N4	-5.22	116.54	120.20
32	2a	770	C	N1-C2-O2	-5.22	115.77	118.90
1	1A	191	U	N3-C4-O4	-5.22	115.74	119.40
1	1A	225	C	C2-N3-C4	-5.22	117.29	119.90
1	1A	251	A	N1-C2-N3	5.22	131.91	129.30
1	1A	594	A	N7-C8-N9	-5.22	111.19	113.80
32	1a	73	G	C6-C5-N7	5.22	133.53	130.40
32	1a	544	G	C5-C6-N1	5.22	114.11	111.50
32	1a	572	A	O5'-P-OP2	-5.22	101.00	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	801	U	C5-C6-N1	-5.22	120.09	122.70
32	1a	1174	G	C8-N9-C1'	5.22	133.79	127.00
32	1a	1441	G	O5'-P-OP2	-5.22	101.00	105.70
1	2A	856	C	N3-C4-C5	-5.22	119.81	121.90
1	2A	982	C	N3-C2-O2	5.22	125.56	121.90
1	2A	2012	G	O5'-P-OP2	-5.22	101.00	105.70
1	1A	622	G	C8-N9-C4	5.22	108.49	106.40
1	1A	1213	U	C5-C4-O4	-5.22	122.77	125.90
2	1B	50	G	C4-C5-C6	-5.22	115.67	118.80
32	1a	768	A	N1-C2-N3	-5.22	126.69	129.30
1	2A	2351	G	C5-C6-O6	-5.22	125.47	128.60
1	1A	746	A	OP2-P-O3'	5.22	116.68	105.20
1	1A	1747	A	P-O3'-C3'	5.22	125.96	119.70
1	1A	1859	G	OP2-P-O3'	5.22	116.68	105.20
1	1A	2185	C	C6-N1-C2	-5.22	118.21	120.30
32	1a	113	G	C5-C6-O6	5.22	131.73	128.60
32	1a	624	C	N3-C4-C5	-5.22	119.81	121.90
32	2a	271	C	C6-N1-C2	-5.22	118.21	120.30
32	2a	1265	G	O5'-P-OP1	-5.22	101.00	105.70
1	1A	82	G	N3-C4-N9	5.22	129.13	126.00
1	1A	1801	G	OP1-P-OP2	5.22	127.43	119.60
1	1A	2204	G	N9-C4-C5	5.22	107.49	105.40
1	1A	2697	G	N3-C2-N2	5.22	123.55	119.90
1	1A	674	G	C5-C6-O6	5.22	131.73	128.60
1	1A	949	C	C2-N3-C4	-5.22	117.29	119.90
1	1A	1093	G	N7-C8-N9	5.22	115.71	113.10
1	1A	1097	G	C6-N1-C2	5.22	128.23	125.10
1	1A	1981	G	N7-C8-N9	-5.22	110.49	113.10
1	1A	2049	G	C6-C5-N7	5.22	133.53	130.40
1	1A	2668	U	C2-N1-C1'	5.22	123.96	117.70
1	2A	807	U	N3-C4-O4	5.22	123.05	119.40
1	1A	1347	A	O5'-P-OP1	5.21	116.96	110.70
1	1A	2804	C	C2-N3-C4	5.21	122.51	119.90
32	1a	446	G	N1-C6-O6	5.21	123.03	119.90
32	1a	1169	A	N7-C8-N9	5.21	116.41	113.80
1	2A	136	G	O5'-P-OP1	-5.21	101.01	105.70
1	2A	502	A	C2-N3-C4	-5.21	107.99	110.60
1	2A	1385	G	O4'-C1'-N9	5.21	112.37	108.20
1	2A	2330	G	C4-C5-N7	-5.21	108.71	110.80
32	2a	297	G	C8-N9-C4	5.21	108.49	106.40
32	2a	665	A	OP1-P-OP2	5.21	127.42	119.60
32	2a	1412	C	O5'-P-OP2	5.21	116.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2l	88	GLY	N-CA-C	5.21	126.14	113.10
1	1A	722	A	O5'-P-OP1	-5.21	101.01	105.70
1	1A	859	C	C2-N3-C4	-5.21	117.29	119.90
1	1A	1062	G	OP2-P-O3'	5.21	116.67	105.20
1	1A	1506	G	C5-C6-O6	5.21	131.73	128.60
1	1A	2061	C	O5'-P-OP1	5.21	116.95	110.70
1	1A	2654	G	N1-C2-N2	-5.21	111.51	116.20
1	2A	787	U	C6-N1-C2	-5.21	117.87	121.00
1	2A	2287	A	O5'-P-OP2	-5.21	101.01	105.70
32	1a	563	A	C8-N9-C4	-5.21	103.72	105.80
32	1a	1003	G	N7-C8-N9	5.21	115.70	113.10
32	1a	1370	G	C4-C5-N7	5.21	112.88	110.80
1	2A	1564	C	C6-N1-C2	-5.21	118.22	120.30
1	2A	2755	C	C5-C6-N1	5.21	123.61	121.00
32	2a	22	G	C2-N3-C4	5.21	114.50	111.90
1	1A	1221	G	N3-C4-N9	-5.21	122.88	126.00
1	1A	1685	C	OP2-P-O3'	5.21	116.66	105.20
1	1A	2615	G	N1-C6-O6	5.21	123.03	119.90
1	1A	2615	G	N9-C4-C5	-5.21	103.32	105.40
1	2A	2089	U	C4-C5-C6	5.21	122.83	119.70
32	2a	709	G	N9-C4-C5	5.21	107.48	105.40
32	2a	1491	G	N9-C1'-C2'	-5.21	106.27	112.00
1	1A	195	U	C4-C5-C6	5.21	122.82	119.70
1	1A	367	C	C2-N3-C4	-5.21	117.30	119.90
1	1A	836	A	O4'-C1'-N9	-5.21	104.03	108.20
1	1A	2065	C	N3-C2-O2	5.21	125.54	121.90
1	1A	2396	G	C5-C6-O6	5.21	131.72	128.60
1	1A	2513	C	N1-C2-O2	-5.21	115.78	118.90
1	1A	2595	G	C5-N7-C8	5.21	106.90	104.30
32	1a	525	C	C5-C4-N4	-5.21	116.56	120.20
32	1a	1370	G	N9-C4-C5	-5.21	103.32	105.40
1	2A	1276	A	N9-C4-C5	-5.21	103.72	105.80
1	2A	2426	A	C4-C5-N7	5.21	113.30	110.70
32	2a	668	G	O5'-P-OP2	5.21	116.95	110.70
32	2a	1183	A	OP1-P-O3'	5.21	116.65	105.20
1	2A	743	G	C4-C5-N7	-5.21	108.72	110.80
1	2A	2591	C	N1-C2-O2	-5.21	115.78	118.90
1	1A	396	C	N3-C4-C5	5.20	123.98	121.90
1	1A	529	U	OP1-P-OP2	5.20	127.41	119.60
1	1A	794	U	C5-C4-O4	5.20	129.02	125.90
1	1A	1117	G	C2-N3-C4	5.20	114.50	111.90
1	1A	1280	U	N3-C4-O4	-5.20	115.76	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1543	U	N3-C4-O4	-5.20	115.76	119.40
1	1A	1612	C	N3-C4-C5	5.20	123.98	121.90
1	1A	1623	U	OP2-P-O3'	5.20	116.65	105.20
1	1A	2060	G	C5-C6-N1	-5.20	108.90	111.50
1	1A	2256	U	N1-C2-N3	5.20	118.02	114.90
1	1A	2312	G	O5'-P-OP1	-5.20	101.02	105.70
1	1A	2713	C	OP2-P-O3'	5.20	116.65	105.20
32	1a	1409	C	N3-C2-O2	-5.20	118.26	121.90
1	2A	340	A	O5'-P-OP2	5.20	116.94	110.70
1	2A	1084	A	C6-N1-C2	5.20	121.72	118.60
2	2B	33	G	C5-C6-N1	-5.20	108.90	111.50
32	2a	685	G	N3-C4-C5	5.20	131.20	128.60
32	2a	753	A	N1-C2-N3	5.20	131.90	129.30
32	2a	1026	G	C5-N7-C8	-5.20	101.70	104.30
1	1A	514	G	N9-C4-C5	5.20	107.48	105.40
1	1A	736	A	C6-N1-C2	-5.20	115.48	118.60
32	1a	744	C	OP2-P-O3'	5.20	116.64	105.20
1	2A	630	G	C5-C6-O6	5.20	131.72	128.60
1	2A	1813	G	N9-C4-C5	-5.20	103.32	105.40
1	1A	452	G	C6-N1-C2	-5.20	121.98	125.10
1	1A	875	U	OP2-P-O3'	5.20	116.64	105.20
32	1a	569	C	N3-C4-N4	-5.20	114.36	118.00
1	2A	378	C	C6-N1-C2	-5.20	118.22	120.30
1	2A	700	G	C5-C6-N1	5.20	114.10	111.50
1	2A	753	C	O5'-P-OP1	-5.20	101.02	105.70
1	2A	989	G	C5-C6-O6	-5.20	125.48	128.60
32	2a	691	G	C5-C6-O6	-5.20	125.48	128.60
1	1A	274	U	C2-N1-C1'	5.20	123.94	117.70
1	1A	1665	G	O4'-C1'-N9	-5.20	104.04	108.20
1	2A	453	C	N3-C4-C5	5.20	123.98	121.90
1	2A	553	G	N9-C4-C5	5.20	107.48	105.40
1	2A	871	U	N3-C4-O4	5.20	123.04	119.40
1	2A	2302	G	C8-N9-C4	-5.20	104.32	106.40
1	2A	2807	G	C5-C6-O6	5.20	131.72	128.60
32	2a	435	C	C5-C6-N1	5.20	123.60	121.00
1	1A	872	C	OP2-P-O3'	5.20	116.63	105.20
1	1A	1080	G	C5-C6-O6	-5.20	125.48	128.60
1	1A	1135	G	N3-C4-N9	5.20	129.12	126.00
1	2A	2091	U	C5-C4-O4	-5.20	122.78	125.90
32	2a	299	G	O5'-P-OP2	5.20	116.94	110.70
32	2a	910	C	C6-N1-C2	5.20	122.38	120.30
1	1A	801	C	C5-C4-N4	-5.20	116.56	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	889	G	OP2-P-O3'	5.20	116.63	105.20
1	1A	1674	G	C8-N9-C4	-5.20	104.32	106.40
1	1A	2339	A	C2-N3-C4	5.20	113.20	110.60
2	1B	38	C	N3-C2-O2	-5.20	118.26	121.90
32	1a	1247	U	C5-C4-O4	-5.20	122.78	125.90
1	2A	2673	G	N3-C4-N9	5.20	129.12	126.00
1	2A	2707	G	C2-N3-C4	-5.20	109.30	111.90
1	1A	1093	G	C8-N9-C4	-5.19	104.32	106.40
1	1A	2286	A	OP2-P-O3'	5.19	116.63	105.20
1	1A	2903	G	C4-N9-C1'	-5.19	119.75	126.50
2	1B	79	C	N1-C2-N3	5.19	122.83	119.20
32	1a	533	A	N1-C2-N3	5.19	131.90	129.30
1	2A	1655	A	OP2-P-O3'	5.19	116.63	105.20
32	2a	1003	G	N9-C4-C5	5.19	107.48	105.40
1	1A	209	G	C8-N9-C4	5.19	108.48	106.40
1	1A	1153	G	O5'-P-OP1	-5.19	101.03	105.70
1	1A	1602	G	C5-C6-N1	-5.19	108.90	111.50
32	1a	34	C	C6-N1-C2	5.19	122.38	120.30
32	1a	182	U	N3-C2-O2	-5.19	118.57	122.20
32	1a	226	G	N3-C2-N2	5.19	123.53	119.90
1	2A	213	A	C5-C6-N1	5.19	120.30	117.70
1	2A	2126	A	P-O3'-C3'	5.19	125.93	119.70
32	2a	556	C	OP1-P-OP2	5.19	127.39	119.60
32	2a	999	C	C2-N1-C1'	5.19	124.51	118.80
1	1A	747	G	O5'-P-OP2	-5.19	101.03	105.70
1	1A	837	C	N1-C2-O2	-5.19	115.79	118.90
1	1A	1031	C	C4-C5-C6	-5.19	114.81	117.40
1	1A	1052	C	N1-C2-O2	-5.19	115.79	118.90
1	1A	2250	G	OP2-P-O3'	5.19	116.62	105.20
1	1A	2251	G	C5-N7-C8	5.19	106.89	104.30
1	1A	2326	C	O5'-P-OP1	5.19	116.93	110.70
1	1A	2409	G	N3-C2-N2	-5.19	116.27	119.90
32	1a	43	C	C6-N1-C2	5.19	122.38	120.30
32	1a	816	A	O5'-P-OP2	-5.19	101.03	105.70
1	2A	701	G	N3-C4-N9	-5.19	122.89	126.00
1	2A	798	G	N1-C6-O6	-5.19	116.79	119.90
1	2A	1587	A	N3-C4-C5	-5.19	123.17	126.80
1	2A	2078	C	C4-C5-C6	5.19	120.00	117.40
1	1A	807	G	N9-C4-C5	-5.19	103.32	105.40
32	1a	888	G	N1-C2-N2	-5.19	111.53	116.20
32	1a	1525	G	C4-N9-C1'	-5.19	119.75	126.50
1	2A	1960	A	O5'-P-OP2	-5.19	101.03	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	873	U	C2-N3-C4	-5.19	123.89	127.00
1	1A	876	A	O5'-P-OP2	-5.19	101.03	105.70
1	1A	1342	G	C5-N7-C8	5.19	106.89	104.30
1	1A	2286	A	C5-C6-N6	5.19	127.85	123.70
1	1A	2790	G	N1-C6-O6	-5.19	116.79	119.90
32	1a	381	C	C6-N1-C2	-5.19	118.22	120.30
1	2A	113	G	N3-C4-N9	-5.19	122.89	126.00
1	2A	620	G	N3-C2-N2	-5.19	116.27	119.90
1	2A	1082	U	C6-N1-C1'	-5.19	113.94	121.20
1	2A	1807	G	C5-N7-C8	5.19	106.89	104.30
1	2A	2008	C	C6-N1-C2	5.19	122.38	120.30
1	2A	2372	G	O5'-P-OP1	-5.19	101.03	105.70
1	2A	2805	G	N1-C2-N2	-5.19	111.53	116.20
1	1A	24	G	N1-C6-O6	-5.19	116.79	119.90
1	1A	255	G	N9-C4-C5	-5.19	103.33	105.40
1	1A	855	G	N1-C6-O6	-5.19	116.79	119.90
1	1A	1956	C	C5-C4-N4	5.19	123.83	120.20
2	1B	8	U	N3-C4-C5	5.19	117.71	114.60
32	2a	1127	G	C8-N9-C4	5.19	108.47	106.40
1	1A	1285	G	OP2-P-O3'	5.18	116.61	105.20
1	1A	2890	C	O5'-P-OP1	-5.18	101.03	105.70
1	2A	1299	G	N3-C4-N9	-5.18	122.89	126.00
32	2a	1074	G	O5'-P-OP1	-5.18	101.03	105.70
1	1A	1406	A	N1-C6-N6	5.18	121.71	118.60
1	1A	1696	G	C5-C6-O6	5.18	131.71	128.60
1	1A	2018	C	N3-C4-C5	5.18	123.97	121.90
32	1a	926	G	C8-N9-C4	-5.18	104.33	106.40
1	2A	2371	G	C5-C6-O6	-5.18	125.49	128.60
32	2a	1484	C	C6-N1-C2	5.18	122.37	120.30
32	1a	112	G	N1-C2-N2	5.18	120.86	116.20
32	2a	396	G	C5-C6-O6	-5.18	125.49	128.60
1	1A	104	C	N3-C4-N4	-5.18	114.37	118.00
1	1A	1135	G	C4-N9-C1'	5.18	133.23	126.50
1	1A	2042	A	C5-C6-N1	5.18	120.29	117.70
1	1A	2772	G	C4-C5-N7	-5.18	108.73	110.80
32	1a	901	A	C6-C5-N7	-5.18	128.67	132.30
1	2A	878	A	O4'-C1'-N9	5.18	112.34	108.20
1	2A	1902	C	N3-C4-C5	5.18	123.97	121.90
32	2a	774	G	OP2-P-O3'	5.18	116.59	105.20
32	2a	1505	G	C8-N9-C4	-5.18	104.33	106.40
1	1A	475	A	N9-C4-C5	-5.18	103.73	105.80
1	1A	670	C	C4-C5-C6	-5.18	114.81	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1889	G	N1-C6-O6	-5.18	116.79	119.90
1	1A	2607	G	O5'-P-OP2	-5.18	101.04	105.70
1	1A	2898	C	C6-N1-C2	-5.18	118.23	120.30
1	2A	181	A	OP2-P-O3'	5.18	116.59	105.20
1	2A	1386	C	O5'-P-OP1	-5.18	101.04	105.70
1	2A	2617	C	C6-N1-C2	5.18	122.37	120.30
1	1A	119	G	N7-C8-N9	-5.18	110.51	113.10
1	1A	2560	G	N1-C6-O6	-5.18	116.79	119.90
1	1A	2833	A	C2-N3-C4	-5.18	108.01	110.60
32	1a	120	A	O4'-C1'-N9	-5.18	104.06	108.20
32	1a	355	C	N3-C2-O2	-5.18	118.28	121.90
1	2A	34	C	C6-N1-C2	-5.18	118.23	120.30
1	2A	700	G	C2-N3-C4	5.18	114.49	111.90
1	2A	896	A	C5-C6-N6	5.18	127.84	123.70
1	2A	2728	U	OP2-P-O3'	5.18	116.59	105.20
1	1A	186	A	C5-C6-N1	-5.17	115.11	117.70
1	1A	1216	G	C6-C5-N7	-5.17	127.30	130.40
1	1A	1700	G	O5'-P-OP1	-5.17	101.04	105.70
1	1A	2078	G	C8-N9-C4	5.17	108.47	106.40
1	1A	2249	G	N3-C2-N2	5.17	123.52	119.90
1	1A	2642	G	C5-C6-N1	5.17	114.09	111.50
1	1A	2863	C	OP2-P-O3'	5.17	116.58	105.20
32	1a	204	U	N3-C2-O2	-5.17	118.58	122.20
32	1a	1200	C	OP1-P-O3'	5.17	116.58	105.20
1	2A	62	C	C2-N1-C1'	-5.17	113.11	118.80
1	2A	562	U	C2-N3-C4	-5.17	123.89	127.00
1	2A	1672	C	N3-C4-C5	-5.17	119.83	121.90
1	2A	2145	C	C2-N1-C1'	5.17	124.49	118.80
1	2A	2674	G	C5-C6-O6	5.17	131.71	128.60
1	1A	2034	G	C4-C5-N7	-5.17	108.73	110.80
1	1A	2095	C	OP2-P-O3'	5.17	116.58	105.20
1	2A	686	G	C8-N9-C4	-5.17	104.33	106.40
1	2A	1079	C	N3-C2-O2	-5.17	118.28	121.90
1	2A	1958	C	C2-N3-C4	-5.17	117.31	119.90
1	1A	673	G	C5-C6-N1	-5.17	108.92	111.50
1	1A	1414	G	N3-C2-N2	5.17	123.52	119.90
1	1A	1606	G	OP1-P-O3'	5.17	116.58	105.20
1	1A	1702	A	N9-C4-C5	5.17	107.87	105.80
1	1A	2106	C	C6-N1-C2	5.17	122.37	120.30
1	1A	2608	U	N3-C2-O2	5.17	125.82	122.20
32	1a	1052	U	N1-C2-O2	5.17	126.42	122.80
32	1a	1181	G	C8-N9-C4	5.17	108.47	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1278	U	C6-N1-C2	-5.17	117.90	121.00
1	2A	271	A	C2-N3-C4	5.17	113.19	110.60
1	2A	370	G	O5'-P-OP2	5.17	116.91	110.70
1	2A	630	G	O5'-P-OP2	-5.17	101.05	105.70
1	2A	2657	A	O5'-P-OP2	5.17	116.91	110.70
32	2a	732	C	OP1-P-OP2	-5.17	111.84	119.60
1	1A	451	G	C6-N1-C2	-5.17	122.00	125.10
1	1A	2511	C	C6-N1-C2	-5.17	118.23	120.30
1	1A	2813	G	N3-C2-N2	-5.17	116.28	119.90
32	1a	308	C	C6-N1-C2	-5.17	118.23	120.30
32	1a	617	G	N3-C4-C5	-5.17	126.02	128.60
1	2A	1255	U	N3-C2-O2	-5.17	118.58	122.20
1	2A	1814	G	N1-C6-O6	5.17	123.00	119.90
1	2A	2690	C	OP1-P-O3'	5.17	116.57	105.20
1	1A	918	U	C2-N3-C4	-5.17	123.90	127.00
1	1A	1575	A	OP2-P-O3'	5.17	116.57	105.20
1	1A	1595	C	N3-C2-O2	-5.17	118.28	121.90
1	1A	1683	C	OP1-P-O3'	5.17	116.57	105.20
1	1A	1746	G	C6-N1-C2	-5.17	122.00	125.10
1	1A	1988	A	N7-C8-N9	-5.17	111.22	113.80
1	1A	2073	A	C5-C6-N1	-5.17	115.11	117.70
1	1A	2700	U	N3-C2-O2	5.17	125.82	122.20
1	1A	2843	G	C6-C5-N7	-5.17	127.30	130.40
1	2A	363(C)	G	N7-C8-N9	-5.17	110.52	113.10
1	2A	1607	C	N1-C2-O2	5.17	122.00	118.90
1	2A	2260	C	O5'-P-OP2	-5.17	101.05	105.70
32	2a	728	A	C8-N9-C4	-5.17	103.73	105.80
32	2a	899	C	OP1-P-OP2	-5.17	111.85	119.60
32	2a	1011	G	N1-C6-O6	-5.17	116.80	119.90
32	2a	1137	C	C6-N1-C2	-5.17	118.23	120.30
1	1A	523	G	OP2-P-O3'	5.17	116.57	105.20
1	1A	962	G	N9-C4-C5	-5.17	103.33	105.40
1	1A	1718	U	C6-N1-C2	5.17	124.10	121.00
1	2A	1277	G	C2-N3-C4	-5.17	109.32	111.90
32	2a	1093	A	N9-C4-C5	-5.17	103.73	105.80
1	1A	652	A	C5-C6-N6	-5.17	119.57	123.70
1	2A	2358	G	C2-N3-C4	-5.17	109.32	111.90
1	1A	852	G	C6-N1-C2	-5.16	122.00	125.10
1	1A	1137	G	C4-C5-N7	-5.16	108.73	110.80
1	1A	1394	G	C5-C6-O6	5.16	131.70	128.60
1	1A	1755	C	C5-C6-N1	-5.16	118.42	121.00
1	1A	1837	C	C6-N1-C2	5.16	122.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2163	G	C2-N3-C4	5.16	114.48	111.90
2	1B	79	C	N3-C4-N4	-5.16	114.39	118.00
32	1a	906	G	O5'-P-OP1	-5.16	101.05	105.70
32	1a	1341	U	C5-C4-O4	5.16	129.00	125.90
1	2A	1309	G	C5-C6-O6	-5.16	125.50	128.60
1	2A	1326	U	O5'-P-OP2	5.16	116.90	110.70
1	2A	2133	G	C8-N9-C4	5.16	108.47	106.40
32	2a	13	U	N1-C2-N3	-5.16	111.80	114.90
32	2a	1103	C	C5-C6-N1	5.16	123.58	121.00
1	1A	1069	U	N1-C2-O2	-5.16	119.19	122.80
1	1A	1567	G	N9-C4-C5	5.16	107.47	105.40
1	2A	1381	G	C8-N9-C4	-5.16	104.33	106.40
1	2A	1937	A	C5-C6-N6	5.16	127.83	123.70
1	2A	2320	A	C2-N3-C4	5.16	113.18	110.60
32	2a	1286	A	N7-C8-N9	5.16	116.38	113.80
1	1A	116	A	N1-C6-N6	-5.16	115.50	118.60
1	1A	501	U	C4-C5-C6	5.16	122.80	119.70
1	1A	1155	C	C6-N1-C1'	-5.16	114.61	120.80
1	1A	1951	G	OP1-P-OP2	5.16	127.34	119.60
1	1A	2012	C	N3-C4-C5	5.16	123.96	121.90
1	1A	2054	G	C5-C6-O6	5.16	131.70	128.60
1	1A	2400	A	O4'-C1'-N9	5.16	112.33	108.20
1	1A	2597	U	C4-C5-C6	5.16	122.80	119.70
32	1a	286	G	C5-C6-O6	5.16	131.70	128.60
32	2a	798	G	N9-C4-C5	5.16	107.46	105.40
1	1A	556	C	N1-C2-O2	-5.16	115.81	118.90
1	1A	1522	G	C4-C5-N7	-5.16	108.74	110.80
1	1A	1807	G	C5-N7-C8	-5.16	101.72	104.30
1	1A	2117	C	OP1-P-O3'	-5.16	93.85	105.20
1	1A	2657	G	O5'-P-OP1	-5.16	101.06	105.70
2	1B	93	G	N7-C8-N9	5.16	115.68	113.10
32	1a	782	A	N1-C2-N3	5.16	131.88	129.30
32	1a	1528	U	O5'-P-OP1	5.16	116.89	110.70
1	2A	1079	C	N3-C4-C5	-5.16	119.84	121.90
1	2A	1270	C	C5-C4-N4	5.16	123.81	120.20
1	2A	1838	C	O4'-C1'-N1	5.16	112.33	108.20
1	2A	2447	G	N3-C2-N2	-5.16	116.29	119.90
1	2A	2520	C	C2-N3-C4	-5.16	117.32	119.90
2	2B	101	G	N1-C6-O6	5.16	123.00	119.90
1	1A	94	G	OP1-P-OP2	5.16	127.33	119.60
1	1A	181	C	OP1-P-OP2	5.16	127.33	119.60
1	1A	931	C	N1-C2-N3	-5.16	115.59	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	41	U	C4-C5-C6	5.16	122.79	119.70
2	1B	90	A	N9-C4-C5	-5.16	103.74	105.80
32	1a	1421	G	C8-N9-C4	-5.16	104.34	106.40
1	2A	2093	G	C5-C6-O6	-5.16	125.51	128.60
1	2A	2205	C	C6-N1-C2	-5.16	118.24	120.30
32	2a	299	G	C6-C5-N7	-5.16	127.31	130.40
32	2a	872	A	O4'-C1'-N9	5.16	112.33	108.20
1	1A	594	A	N1-C2-N3	-5.16	126.72	129.30
1	1A	742	G	C6-C5-N7	5.16	133.49	130.40
1	1A	975	U	C6-N1-C2	5.16	124.09	121.00
1	1A	1152	G	C8-N9-C4	5.16	108.46	106.40
1	1A	1234	A	O5'-P-OP1	5.16	116.89	110.70
1	1A	1281	G	OP2-P-O3'	5.16	116.54	105.20
1	1A	2278	A	C5-C6-N1	-5.16	115.12	117.70
1	1A	2528	G	N9-C4-C5	5.16	107.46	105.40
1	1A	2591	C	N3-C4-C5	5.16	123.96	121.90
1	1A	2780	C	N1-C2-O2	5.16	121.99	118.90
32	1a	643	C	C6-N1-C2	5.16	122.36	120.30
1	2A	1573	G	N9-C4-C5	5.16	107.46	105.40
1	1A	369	A	N1-C6-N6	5.15	121.69	118.60
1	1A	505	A	C4-C5-N7	-5.15	108.12	110.70
1	1A	1627	A	C5-C6-N6	-5.15	119.58	123.70
1	1A	2230	U	C2-N1-C1'	5.15	123.89	117.70
1	2A	469	G	N1-C6-O6	5.15	122.99	119.90
1	1A	199	C	C6-N1-C2	5.15	122.36	120.30
1	1A	795	G	OP1-P-O3'	5.15	116.54	105.20
1	1A	818	G	C5-C6-O6	5.15	131.69	128.60
1	1A	1056	A	N7-C8-N9	-5.15	111.22	113.80
1	1A	1691	C	C5-C6-N1	-5.15	118.42	121.00
32	1a	1181	G	C4-N9-C1'	-5.15	119.80	126.50
32	1a	1505	G	N3-C2-N2	-5.15	116.29	119.90
1	2A	948	G	O5'-P-OP2	5.15	116.88	110.70
32	2a	1502	A	O5'-P-OP2	-5.15	101.06	105.70
1	1A	2288	G	N1-C6-O6	-5.15	116.81	119.90
32	1a	552	U	O5'-P-OP1	5.15	116.88	110.70
32	1a	1077	G	N9-C1'-C2'	-5.15	106.33	112.00
32	1a	1137	C	N1-C2-O2	5.15	121.99	118.90
1	2A	2597	G	OP2-P-O3'	5.15	116.53	105.20
32	2a	261	U	C5-C4-O4	5.15	128.99	125.90
1	1A	1263	C	O5'-P-OP2	-5.15	101.07	105.70
1	1A	1361	C	N3-C2-O2	-5.15	118.30	121.90
1	1A	1928	G	C6-C5-N7	-5.15	127.31	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2093	A	O5'-P-OP1	-5.15	101.07	105.70
15	1T	96	ARG	N-CA-CB	-5.15	101.33	110.60
32	1a	486	U	C5-C4-O4	5.15	128.99	125.90
1	2A	752	A	C2'-C3'-O3'	5.15	121.94	113.70
1	2A	2511	U	C2-N3-C4	-5.15	123.91	127.00
32	2a	1011	G	N9-C4-C5	5.15	107.46	105.40
1	1A	554	A	OP1-P-O3'	5.15	116.53	105.20
1	1A	985	G	C6-N1-C2	-5.15	122.01	125.10
2	1B	32	C	OP2-P-O3'	5.15	116.53	105.20
32	1a	550	G	N9-C4-C5	5.15	107.46	105.40
32	1a	1130	A	O5'-P-OP1	5.15	116.88	110.70
1	2A	36	G	OP2-P-O3'	5.15	116.52	105.20
1	2A	228	A	C8-N9-C1'	5.15	136.96	127.70
4	2E	13	ARG	NE-CZ-NH1	-5.15	117.73	120.30
32	2a	820	U	N3-C2-O2	5.15	125.80	122.20
32	2a	968	A	N1-C6-N6	-5.15	115.51	118.60
1	1A	1449	C	C4-C5-C6	5.15	119.97	117.40
1	1A	1874	C	N3-C2-O2	5.15	125.50	121.90
20	1Y	50	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	1A	106	U	N3-C2-O2	-5.14	118.60	122.20
1	1A	893	C	OP1-P-OP2	5.14	127.31	119.60
1	1A	1301	U	C2-N3-C4	-5.14	123.91	127.00
1	1A	1513	G	OP2-P-O3'	5.14	116.52	105.20
1	1A	1521	C	N1-C2-O2	-5.14	115.81	118.90
32	1a	1341	U	C6-N1-C1'	5.14	128.40	121.20
1	2A	143	G	N9-C4-C5	5.14	107.46	105.40
1	2A	1822	G	C8-N9-C4	5.14	108.46	106.40
32	2a	245	C	O5'-P-OP2	5.14	116.87	110.70
32	2a	858	G	C6-C5-N7	-5.14	127.31	130.40
32	2a	1465	C	N1-C2-O2	-5.14	115.81	118.90
1	1A	546	G	OP2-P-O3'	5.14	116.51	105.20
1	1A	593	G	C6-N1-C2	-5.14	122.02	125.10
1	1A	733	G	N1-C2-N2	-5.14	111.57	116.20
1	1A	1427	G	N9-C4-C5	5.14	107.46	105.40
1	1A	2525	G	N3-C2-N2	5.14	123.50	119.90
2	1B	36	C	N3-C2-O2	5.14	125.50	121.90
32	1a	264	U	C5-C4-O4	5.14	128.99	125.90
1	2A	53	A	O5'-P-OP1	-5.14	101.07	105.70
1	2A	555	U	O4'-C1'-N1	5.14	112.31	108.20
1	2A	655	A	N1-C6-N6	5.14	121.69	118.60
1	2A	875	G	O5'-P-OP1	5.14	116.87	110.70
32	2a	1020	U	C5-C6-N1	5.14	125.27	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2222	C	C5-C6-N1	-5.14	118.43	121.00
1	1A	2639	G	N3-C4-N9	5.14	129.09	126.00
1	2A	2042	A	C2-N3-C4	-5.14	108.03	110.60
32	2a	1094	G	N9-C4-C5	-5.14	103.34	105.40
1	1A	1827	U	C2-N3-C4	-5.14	123.92	127.00
1	1A	2181	G	N3-C4-N9	5.14	129.08	126.00
1	1A	2331	G	N1-C2-N3	5.14	126.98	123.90
32	1a	503	C	O5'-P-OP1	-5.14	101.08	105.70
1	2A	100	G	N7-C8-N9	-5.14	110.53	113.10
1	1A	398	A	C5-C6-N6	-5.14	119.59	123.70
1	1A	436	C	C5-C6-N1	-5.14	118.43	121.00
1	1A	986	A	C8-N9-C4	-5.14	103.75	105.80
1	1A	2556	G	N9-C4-C5	5.14	107.45	105.40
1	2A	1696	G	N1-C2-N3	-5.14	120.82	123.90
2	2B	71	C	C6-N1-C2	5.14	122.36	120.30
1	1A	787	U	C5-C6-N1	-5.14	120.13	122.70
1	1A	1067	A	OP2-P-O3'	5.14	116.50	105.20
1	1A	2748	G	N1-C6-O6	-5.14	116.82	119.90
32	1a	607	A	C6-C5-N7	-5.14	128.71	132.30
1	2A	1052	C	N3-C4-C5	-5.14	119.85	121.90
1	2A	2686	G	O5'-P-OP2	-5.14	101.08	105.70
1	2A	2744	G	OP2-P-O3'	5.14	116.50	105.20
4	2E	51	PHE	N-CA-C	-5.14	97.13	111.00
32	2a	450	G	N1-C6-O6	5.14	122.98	119.90
1	1A	178	G	OP2-P-O3'	5.13	116.50	105.20
1	1A	1263	C	OP2-P-O3'	5.13	116.50	105.20
1	1A	2331	G	N9-C4-C5	5.13	107.45	105.40
1	1A	2419	G	O4'-C1'-N9	-5.13	104.09	108.20
14	1S	59	LYS	N-CA-C	5.13	124.86	111.00
32	1a	858	G	C4-N9-C1'	5.13	133.18	126.50
1	2A	1283	G	N3-C2-N2	5.13	123.49	119.90
1	2A	2177	C	N1-C2-O2	5.13	121.98	118.90
1	2A	2727	G	C8-N9-C4	-5.13	104.35	106.40
32	2a	1029	C	C5-C6-N1	5.13	123.57	121.00
1	1A	499	G	C5-C6-O6	5.13	131.68	128.60
1	1A	639	G	C4-N9-C1'	-5.13	119.83	126.50
1	1A	2045	G	O5'-P-OP2	5.13	116.86	110.70
1	1A	2684	G	OP2-P-O3'	5.13	116.49	105.20
32	1a	279	A	O5'-P-OP2	-5.13	101.08	105.70
32	1a	933	G	N1-C6-O6	5.13	122.98	119.90
1	2A	192	C	C6-N1-C2	-5.13	118.25	120.30
32	2a	1530	G	N1-C6-O6	5.13	122.98	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	176	G	C8-N9-C4	-5.13	104.35	106.40
1	1A	958	C	N1-C2-O2	5.13	121.98	118.90
1	1A	1375	U	C5-C4-O4	5.13	128.98	125.90
1	1A	1543	U	O5'-P-OP1	-5.13	101.08	105.70
1	1A	1707	C	C6-N1-C2	-5.13	118.25	120.30
1	1A	2265	G	N7-C8-N9	-5.13	110.53	113.10
1	2A	553	G	C8-N9-C4	-5.13	104.35	106.40
1	2A	1075	C	C2-N1-C1'	5.13	124.44	118.80
1	2A	2427	C	O5'-P-OP2	5.13	116.86	110.70
32	2a	603	U	N3-C4-O4	5.13	122.99	119.40
32	2a	852	G	N3-C4-N9	-5.13	122.92	126.00
1	1A	1106	U	C5-C4-O4	-5.13	122.82	125.90
32	1a	863	U	O4'-C1'-N1	5.13	112.30	108.20
1	2A	2885	C	OP2-P-O3'	5.13	116.49	105.20
32	2a	111	G	N1-C6-O6	5.13	122.98	119.90
32	2a	1030	C	N3-C2-O2	-5.13	118.31	121.90
1	1A	68	C	C5-C6-N1	-5.13	118.44	121.00
1	1A	366	G	C4-C5-N7	-5.13	108.75	110.80
1	1A	989	G	C8-N9-C1'	-5.13	120.33	127.00
1	1A	1166	G	C5-C6-O6	5.13	131.68	128.60
1	1A	2255	U	C5-C4-O4	-5.13	122.82	125.90
1	1A	2623	U	N3-C4-C5	-5.13	111.52	114.60
32	1a	1046	A	N1-C6-N6	5.13	121.68	118.60
32	1a	1153	C	O5'-P-OP2	-5.13	101.08	105.70
1	2A	383	U	O4'-C1'-N1	5.13	112.30	108.20
1	2A	787	U	C5-C4-O4	5.13	128.98	125.90
1	2A	1204	A	N7-C8-N9	-5.13	111.24	113.80
1	2A	1956	U	N3-C4-C5	5.13	117.68	114.60
1	2A	2296	U	O5'-P-OP1	-5.13	101.08	105.70
1	1A	333	G	O5'-P-OP1	-5.13	101.09	105.70
1	1A	462	C	OP1-P-OP2	5.13	127.29	119.60
1	1A	569	G	N3-C4-N9	-5.13	122.92	126.00
1	1A	994	C	O5'-P-OP2	-5.13	101.09	105.70
1	1A	1716	A	O4'-C1'-N9	5.13	112.30	108.20
1	1A	1789	G	C5-C6-O6	-5.13	125.52	128.60
1	1A	2294	G	O4'-C1'-N9	5.13	112.30	108.20
1	1A	2557	G	N7-C8-N9	-5.13	110.54	113.10
32	1a	96	U	C5-C4-O4	-5.13	122.82	125.90
32	1a	485	G	C8-N9-C4	5.13	108.45	106.40
32	1a	514	C	N3-C4-N4	5.13	121.59	118.00
1	2A	1687	G	OP2-P-O3'	5.13	116.48	105.20
1	2A	1900	A	C2-N3-C4	5.13	113.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	761	G	N3-C2-N2	-5.13	116.31	119.90
32	2a	1100	C	C6-N1-C1'	5.13	126.95	120.80
2	1B	88	C	O4'-C1'-N1	5.12	112.30	108.20
1	2A	1605	C	N3-C4-C5	-5.12	119.85	121.90
32	2a	1442	G	P-O3'-C3'	5.12	125.85	119.70
1	1A	150	C	C5-C6-N1	-5.12	118.44	121.00
1	1A	604	C	N1-C2-N3	5.12	122.79	119.20
1	1A	839	G	N3-C2-N2	5.12	123.49	119.90
1	1A	1186	U	OP1-P-OP2	-5.12	111.91	119.60
1	1A	2509	A	N1-C6-N6	-5.12	115.53	118.60
2	1B	93	G	C5-N7-C8	-5.12	101.74	104.30
1	2A	390	A	N9-C4-C5	-5.12	103.75	105.80
1	2A	581	C	O5'-P-OP1	5.12	116.85	110.70
1	2A	856	C	C2'-C3'-O3'	5.12	121.90	113.70
1	2A	1925	C	C2-N1-C1'	-5.12	113.16	118.80
32	2a	453	A	OP1-P-OP2	5.12	127.28	119.60
32	2a	1002	G	C8-N9-C4	-5.12	104.35	106.40
1	1A	117	A	OP1-P-O3'	5.12	116.47	105.20
1	1A	251	A	OP1-P-OP2	5.12	127.28	119.60
1	1A	276	C	OP2-P-O3'	5.12	116.47	105.20
1	1A	720	C	C5-C4-N4	-5.12	116.61	120.20
1	1A	874	U	N1-C2-N3	5.12	117.97	114.90
1	1A	1000	C	N3-C2-O2	-5.12	118.31	121.90
1	1A	1171	G	N1-C6-O6	5.12	122.97	119.90
1	1A	1518	A	N3-C4-C5	-5.12	123.22	126.80
1	1A	1801	G	C5-C6-N1	-5.12	108.94	111.50
1	1A	2579	G	C5-C6-O6	5.12	131.67	128.60
1	1A	2734	A	C6-N1-C2	5.12	121.67	118.60
1	2A	1835	G	N3-C4-N9	5.12	129.07	126.00
1	2A	2586	C	N3-C2-O2	5.12	125.48	121.90
32	2a	473	G	C5-C6-O6	5.12	131.67	128.60
32	2a	656	C	OP1-P-OP2	-5.12	111.92	119.60
43	2k	118	GLY	N-CA-C	5.12	125.90	113.10
1	2A	1586	A	O5'-P-OP1	-5.12	101.09	105.70
1	1A	522	A	N1-C2-N3	-5.12	126.74	129.30
1	1A	966	G	N1-C2-N3	5.12	126.97	123.90
1	1A	1071	G	C5-C6-N1	-5.12	108.94	111.50
1	1A	2005	C	C5-C6-N1	-5.12	118.44	121.00
2	1B	77	U	N1-C2-O2	-5.12	119.22	122.80
32	1a	73	G	C4-N9-C1'	-5.12	119.85	126.50
32	1a	355	C	N1-C2-N3	5.12	122.78	119.20
32	1a	804	U	C5-C6-N1	-5.12	120.14	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	271(L)	U	C5-C6-N1	5.12	125.26	122.70
1	2A	1573	G	N1-C2-N2	5.12	120.81	116.20
1	2A	2428	G	C5-C6-O6	5.12	131.67	128.60
1	2A	2721	A	C8-N9-C4	-5.12	103.75	105.80
32	2a	1259	C	C6-N1-C2	-5.12	118.25	120.30
1	1A	1117	G	C4-C5-N7	-5.12	108.75	110.80
1	1A	2139	A	N1-C6-N6	-5.12	115.53	118.60
1	1A	2450	U	N3-C4-C5	5.12	117.67	114.60
1	1A	1110	C	C2-N1-C1'	5.12	124.43	118.80
1	1A	1142	A	OP2-P-O3'	5.12	116.45	105.20
1	1A	1729	G	C6-N1-C2	-5.12	122.03	125.10
1	1A	2071	G	C2-N3-C4	5.12	114.46	111.90
1	1A	2446	A	OP2-P-O3'	5.12	116.45	105.20
1	1A	2577	A	N1-C6-N6	-5.12	115.53	118.60
32	1a	740	U	C5-C4-O4	5.12	128.97	125.90
32	1a	797	C	C6-N1-C2	-5.12	118.25	120.30
1	2A	928	G	C8-N9-C4	-5.12	104.35	106.40
1	2A	1213	A	N1-C6-N6	5.12	121.67	118.60
1	1A	499	G	N3-C2-N2	5.11	123.48	119.90
1	1A	618	C	OP1-P-OP2	5.11	127.27	119.60
1	1A	623	G	O5'-P-OP2	-5.11	101.10	105.70
1	1A	1210	G	C6-C5-N7	5.11	133.47	130.40
1	1A	1371	G	N3-C4-C5	-5.11	126.04	128.60
1	1A	1375	U	N1-C2-N3	5.11	117.97	114.90
1	1A	1847	G	C8-N9-C1'	5.11	133.65	127.00
1	2A	1935	G	O5'-P-OP1	5.11	116.84	110.70
1	2A	2474	C	C6-N1-C1'	-5.11	114.67	120.80
1	1A	1332	A	O5'-P-OP2	-5.11	101.10	105.70
1	1A	2843	G	N3-C4-N9	5.11	129.07	126.00
1	2A	1509(A)	A	C8-N9-C4	-5.11	103.75	105.80
8	2I	75	LEU	CA-CB-CG	5.11	127.06	115.30
32	2a	740	U	C5-C4-O4	5.11	128.97	125.90
1	1A	712	C	C6-N1-C2	5.11	122.34	120.30
32	1a	1326	C	N3-C4-N4	-5.11	114.42	118.00
1	2A	258	G	N1-C6-O6	-5.11	116.83	119.90
1	2A	670	A	N3-C4-C5	-5.11	123.22	126.80
1	2A	992	C	C5-C6-N1	5.11	123.56	121.00
1	2A	1060	U	N1-C2-O2	5.11	126.38	122.80
32	2a	1006	C	N3-C4-C5	-5.11	119.86	121.90
1	1A	1958	A	N1-C6-N6	5.11	121.67	118.60
1	1A	1978	U	N1-C2-O2	-5.11	119.22	122.80
1	1A	2026	G	C5-N7-C8	5.11	106.85	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2826	C	O5'-P-OP1	-5.11	101.10	105.70
32	1a	740	U	OP1-P-OP2	5.11	127.26	119.60
1	2A	380	U	C5-C6-N1	5.11	125.25	122.70
1	2A	855	G	C8-N9-C4	-5.11	104.36	106.40
1	2A	2794	C	C6-N1-C2	-5.11	118.26	120.30
1	1A	262	C	C2-N3-C4	-5.11	117.35	119.90
1	1A	514	G	C4-C5-N7	-5.11	108.76	110.80
1	1A	1259	A	C8-N9-C4	5.11	107.84	105.80
16	1U	10	ARG	NE-CZ-NH2	-5.11	117.75	120.30
32	1a	150	C	N3-C4-C5	-5.11	119.86	121.90
32	1a	444	C	C5-C6-N1	-5.11	118.45	121.00
1	2A	778	G	C5-C6-O6	5.11	131.66	128.60
1	2A	790	C	N1-C2-O2	-5.11	115.84	118.90
1	2A	1316	U	C4-C5-C6	5.11	122.76	119.70
1	2A	2633	G	C8-N9-C4	-5.11	104.36	106.40
1	1A	1035	G	N3-C4-C5	-5.11	126.05	128.60
1	1A	1094	A	N1-C6-N6	-5.11	115.54	118.60
1	1A	1345	G	O5'-P-OP1	-5.11	101.11	105.70
1	1A	1401	G	C5-C6-O6	5.11	131.66	128.60
1	1A	2605	U	C5-C6-N1	-5.11	120.15	122.70
1	1A	2750	G	N9-C4-C5	5.11	107.44	105.40
1	1A	2881	C	C6-N1-C2	5.11	122.34	120.30
32	1a	1152	A	N1-C6-N6	-5.11	115.54	118.60
1	2A	667	U	N1-C2-O2	-5.11	119.23	122.80
1	2A	2053	G	C4-C5-N7	-5.11	108.76	110.80
32	2a	60	A	O4'-C1'-N9	-5.11	104.11	108.20
32	2a	555	C	N3-C4-N4	5.11	121.57	118.00
32	2a	991	U	C2-N1-C1'	5.11	123.83	117.70
32	2a	1229	A	OP1-P-O3'	5.11	116.43	105.20
32	2a	1442	G	C2-N3-C4	5.11	114.45	111.90
1	1A	197	C	C5-C6-N1	-5.10	118.45	121.00
1	1A	1525	G	O5'-P-OP1	-5.10	101.11	105.70
32	2a	52	G	O5'-P-OP1	5.10	116.83	110.70
1	1A	411	U	N3-C2-O2	5.10	125.77	122.20
1	1A	1094	A	N9-C4-C5	5.10	107.84	105.80
1	1A	1110	C	N3-C2-O2	-5.10	118.33	121.90
1	1A	1802	C	O5'-P-OP2	-5.10	101.11	105.70
1	1A	1833	A	O4'-C1'-N9	-5.10	104.12	108.20
1	1A	1970	G	N1-C6-O6	-5.10	116.84	119.90
1	1A	2803	A	C2-N3-C4	5.10	113.15	110.60
1	1A	2855	G	N3-C4-C5	-5.10	126.05	128.60
32	1a	1026	G	C4-N9-C1'	5.10	133.13	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1790	C	OP1-P-O3'	5.10	116.42	105.20
2	2B	87	G	C5-C6-N1	5.10	114.05	111.50
1	1A	1453	C	O5'-P-OP2	-5.10	101.11	105.70
1	1A	1621	C	C2-N3-C4	-5.10	117.35	119.90
32	1a	781	A	OP1-P-O3'	-5.10	93.98	105.20
32	1a	869	G	C8-N9-C4	5.10	108.44	106.40
1	2A	390	A	C8-N9-C4	5.10	107.84	105.80
1	1A	1245	C	N1-C2-N3	5.10	122.77	119.20
1	1A	1270	C	OP1-P-O3'	5.10	116.42	105.20
1	1A	1447	G	C4-C5-N7	-5.10	108.76	110.80
1	1A	1474	C	C6-N1-C1'	5.10	126.92	120.80
1	1A	1614	A	N1-C6-N6	-5.10	115.54	118.60
32	1a	172	A	C5-N7-C8	-5.10	101.35	103.90
1	2A	975(A)	G	C8-N9-C4	-5.10	104.36	106.40
1	2A	1046	A	N9-C4-C5	5.10	107.84	105.80
1	2A	1844	C	C2-N3-C4	-5.10	117.35	119.90
18	2W	23	LEU	CA-CB-CG	5.10	127.03	115.30
32	2a	1093	A	C4-C5-N7	5.10	113.25	110.70
32	2a	1348	U	N3-C2-O2	-5.10	118.63	122.20
1	1A	1117	G	N9-C4-C5	5.10	107.44	105.40
1	1A	1842	G	OP2-P-O3'	5.10	116.42	105.20
1	1A	2187	G	N3-C4-C5	-5.10	126.05	128.60
1	1A	2556	G	N3-C4-N9	-5.10	122.94	126.00
16	1U	10	ARG	NE-CZ-NH1	5.10	122.85	120.30
31	19	27	CYS	CA-CB-SG	5.10	123.18	114.00
1	2A	482	A	O5'-P-OP1	5.10	116.82	110.70
1	2A	2056	G	C6-C5-N7	-5.10	127.34	130.40
32	2a	1499	A	N9-C4-C5	-5.10	103.76	105.80
1	1A	1131	A	O4'-C1'-N9	5.10	112.28	108.20
1	1A	1290	G	N1-C6-O6	-5.10	116.84	119.90
1	1A	1665	G	O5'-P-OP2	-5.10	101.11	105.70
1	1A	2066	C	C2-N3-C4	-5.10	117.35	119.90
1	1A	2900	G	N1-C6-O6	5.10	122.96	119.90
32	1a	1442	G	C3'-C2'-C1'	5.10	105.58	101.50
1	1A	85	C	C2-N3-C4	-5.09	117.35	119.90
1	1A	1112	U	C6-N1-C2	-5.09	117.94	121.00
1	1A	1264	G	N3-C4-C5	5.09	131.15	128.60
1	1A	1578	C	N3-C2-O2	-5.09	118.33	121.90
1	1A	2842	U	C5-C6-N1	-5.09	120.15	122.70
32	1a	810	C	O5'-P-OP2	-5.09	101.11	105.70
32	1a	838	G	O5'-P-OP1	5.09	116.81	110.70
1	2A	154	G	N9-C4-C5	-5.09	103.36	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1203	G	N3-C4-N9	5.09	129.06	126.00
32	2a	27	G	C5-N7-C8	-5.09	101.75	104.30
32	2a	1471	G	N1-C6-O6	-5.09	116.84	119.90
1	1A	954	C	OP2-P-O3'	5.09	116.40	105.20
1	1A	2107	C	N3-C4-C5	5.09	123.94	121.90
1	2A	114	U	O5'-P-OP1	5.09	116.81	110.70
1	2A	778	G	C2-N3-C4	-5.09	109.35	111.90
1	2A	1314	C	N1-C2-O2	5.09	121.96	118.90
32	2a	785	G	O5'-P-OP2	-5.09	101.12	105.70
1	1A	577	U	N1-C2-N3	5.09	117.95	114.90
1	1A	844	C	N3-C2-O2	5.09	125.47	121.90
1	1A	2093	A	C4-C5-C6	5.09	119.55	117.00
1	1A	2222	C	C6-N1-C2	5.09	122.34	120.30
1	1A	2724	U	N3-C4-O4	5.09	122.96	119.40
32	1a	280	C	C6-N1-C2	5.09	122.34	120.30
32	1a	436	C	O5'-P-OP1	-5.09	101.12	105.70
32	1a	669	U	OP2-P-O3'	5.09	116.40	105.20
32	1a	814	A	C2-N3-C4	-5.09	108.05	110.60
32	1a	1457	G	N7-C8-N9	-5.09	110.55	113.10
1	2A	217	G	C5-N7-C8	5.09	106.84	104.30
1	2A	448	U	O5'-P-OP1	-5.09	101.12	105.70
1	2A	554	U	N3-C2-O2	-5.09	118.64	122.20
1	2A	1218	C	C2-N1-C1'	-5.09	113.20	118.80
1	2A	1638	C	C6-N1-C2	5.09	122.34	120.30
1	2A	1798	U	O5'-P-OP2	-5.09	101.12	105.70
32	2a	114	U	C5-C6-N1	-5.09	120.16	122.70
1	1A	1109	G	C2-N3-C4	5.09	114.44	111.90
1	1A	1409	C	OP1-P-O3'	-5.09	94.00	105.20
1	1A	1473	A	N7-C8-N9	-5.09	111.25	113.80
1	1A	1474	C	C5-C6-N1	-5.09	118.46	121.00
1	1A	2065	C	N3-C4-N4	5.09	121.56	118.00
31	19	22	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	2A	2570	G	N1-C6-O6	-5.09	116.85	119.90
1	2A	2837	G	C8-N9-C4	5.09	108.44	106.40
19	2X	8	ILE	CB-CA-C	-5.09	101.42	111.60
32	2a	315	A	N7-C8-N9	5.09	116.34	113.80
32	2a	622	A	OP2-P-O3'	5.09	116.39	105.20
32	2a	1139	G	C5-C6-N1	-5.09	108.95	111.50
1	1A	86	C	C6-N1-C2	5.09	122.33	120.30
1	1A	696	C	C2-N3-C4	5.09	122.44	119.90
1	1A	780	G	C5-C6-O6	5.09	131.65	128.60
1	1A	1296	G	C5-C6-N1	5.09	114.04	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1485	A	C2-N3-C4	-5.09	108.06	110.60
2	1B	99	G	C8-N9-C4	5.09	108.44	106.40
1	2A	399	G	N3-C4-C5	5.09	131.14	128.60
1	2A	710	G	O5'-P-OP1	5.09	116.81	110.70
1	1A	513	C	C4-C5-C6	5.09	119.94	117.40
1	1A	954	C	C5-C6-N1	-5.09	118.46	121.00
1	1A	2459	G	O4'-C1'-N9	5.09	112.27	108.20
1	1A	2599	A	C5-C6-N1	-5.09	115.16	117.70
17	1V	82	ARG	NE-CZ-NH2	-5.09	117.76	120.30
32	1a	694	A	O5'-P-OP2	5.09	116.81	110.70
32	1a	1201	A	P-O3'-C3'	5.09	125.80	119.70
1	2A	1302	A	C2-N3-C4	-5.09	108.06	110.60
1	2A	2554	U	C2-N1-C1'	-5.09	111.60	117.70
32	2a	831	U	C6-N1-C2	-5.09	117.95	121.00
1	1A	1747	A	C4-C5-C6	-5.08	114.46	117.00
1	1A	1836	U	N1-C2-O2	-5.08	119.24	122.80
1	1A	2585	C	C5-C4-N4	-5.08	116.64	120.20
1	1A	2587	C	OP2-P-O3'	5.08	116.39	105.20
1	1A	2780	C	C2-N1-C1'	5.08	124.39	118.80
1	2A	261	G	N3-C2-N2	-5.08	116.34	119.90
1	2A	739	G	OP1-P-O3'	5.08	116.39	105.20
1	2A	1858	G	N1-C6-O6	-5.08	116.85	119.90
1	1A	198	C	N3-C4-N4	-5.08	114.44	118.00
1	1A	534	C	C6-N1-C2	5.08	122.33	120.30
1	1A	935	C	N1-C2-O2	5.08	121.95	118.90
1	1A	1014	U	N3-C4-C5	5.08	117.65	114.60
1	1A	2060	G	C5-C6-O6	5.08	131.65	128.60
1	1A	2082	A	C6-C5-N7	5.08	135.86	132.30
1	2A	951	C	OP1-P-OP2	-5.08	111.98	119.60
1	2A	1319	G	O5'-P-OP1	-5.08	101.12	105.70
1	2A	2286	A	N1-C6-N6	-5.08	115.55	118.60
1	1A	407	U	N3-C4-O4	-5.08	115.84	119.40
1	1A	1027	A	C8-N9-C4	5.08	107.83	105.80
1	1A	1599	G	O5'-P-OP2	-5.08	101.13	105.70
1	1A	1869	C	OP1-P-OP2	5.08	127.22	119.60
1	1A	2125	C	C5-C6-N1	5.08	123.54	121.00
32	1a	766	A	N1-C6-N6	5.08	121.65	118.60
1	2A	9	U	C6-N1-C2	-5.08	117.95	121.00
1	2A	41	C	O5'-P-OP2	-5.08	101.13	105.70
1	2A	526	A	N1-C6-N6	-5.08	115.55	118.60
1	2A	662	G	OP2-P-O3'	5.08	116.38	105.20
1	2A	1379	A	OP1-P-O3'	5.08	116.38	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	200	G	C8-N9-C4	5.08	108.43	106.40
1	1A	1660	A	C5-N7-C8	5.08	106.44	103.90
1	1A	2466	G	O5'-P-OP2	-5.08	101.13	105.70
1	1A	2588	G	N9-C4-C5	5.08	107.43	105.40
1	2A	1560	G	N7-C8-N9	-5.08	110.56	113.10
32	2a	761	G	OP2-P-O3'	5.08	116.38	105.20
1	1A	39	C	C5-C6-N1	-5.08	118.46	121.00
1	1A	964	A	C6-N1-C2	5.08	121.65	118.60
1	1A	1088	G	OP2-P-O3'	5.08	116.37	105.20
1	1A	1480	A	OP2-P-O3'	5.08	116.37	105.20
1	1A	1925	G	N7-C8-N9	5.08	115.64	113.10
1	1A	2750	G	C5-C6-O6	5.08	131.65	128.60
1	1A	2846	U	N3-C2-O2	-5.08	118.64	122.20
1	2A	847	U	N3-C2-O2	-5.08	118.64	122.20
1	2A	2140	C	N1-C2-O2	5.08	121.95	118.90
1	1A	1065	U	OP1-P-OP2	5.08	127.22	119.60
1	1A	2137	G	C2-N3-C4	5.08	114.44	111.90
1	1A	2421	G	N3-C4-N9	5.08	129.05	126.00
1	1A	2589	A	C5-C6-N6	5.08	127.76	123.70
1	1A	2718	G	C8-N9-C4	5.08	108.43	106.40
32	1a	38	G	N1-C6-O6	5.08	122.95	119.90
1	2A	2319	G	C8-N9-C4	-5.08	104.37	106.40
32	2a	145	G	OP1-P-OP2	-5.08	111.98	119.60
32	2a	1201	A	C6-N1-C2	-5.08	115.55	118.60
1	1A	41	C	C5-C4-N4	5.08	123.75	120.20
1	1A	218	A	N7-C8-N9	5.08	116.34	113.80
1	1A	498	A	OP2-P-O3'	5.08	116.37	105.20
1	1A	1046	A	N1-C2-N3	-5.08	126.76	129.30
1	1A	1353	A	C8-N9-C4	5.08	107.83	105.80
1	1A	1868	C	O5'-P-OP1	-5.08	101.13	105.70
1	1A	2380	C	N3-C2-O2	-5.08	118.35	121.90
1	1A	2878	A	N1-C6-N6	5.08	121.64	118.60
1	2A	178	G	O5'-P-OP2	-5.08	101.13	105.70
1	2A	455	C	C4-C5-C6	5.08	119.94	117.40
1	2A	907	U	C5-C6-N1	5.08	125.24	122.70
1	2A	2694	G	C5-C6-O6	5.08	131.65	128.60
1	2A	2807	G	N9-C4-C5	5.08	107.43	105.40
1	1A	1200	G	N1-C2-N2	-5.07	111.63	116.20
1	2A	1085	A	O5'-P-OP1	-5.07	101.14	105.70
1	2A	2127	G	O5'-P-OP2	5.07	116.79	110.70
1	2A	2182	G	C4-C5-N7	-5.07	108.77	110.80
1	2A	2344	U	OP1-P-O3'	5.07	116.36	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	122	G	C5-C6-N1	5.07	114.04	111.50
32	2a	390	C	N3-C4-N4	-5.07	114.45	118.00
32	2a	664	G	C8-N9-C4	-5.07	104.37	106.40
1	1A	1735	U	O5'-P-OP2	-5.07	101.14	105.70
1	2A	192	C	C5-C4-N4	-5.07	116.65	120.20
1	2A	655	A	O4'-C1'-N9	5.07	112.26	108.20
1	2A	799	G	N1-C6-O6	-5.07	116.86	119.90
1	2A	1373	A	C8-N9-C4	5.07	107.83	105.80
1	2A	2198	A	O4'-C1'-N9	5.07	112.26	108.20
32	2a	17	U	N3-C2-O2	-5.07	118.65	122.20
32	2a	851	G	C5-N7-C8	-5.07	101.76	104.30
1	1A	38	A	N7-C8-N9	-5.07	111.27	113.80
1	1A	152	G	N1-C6-O6	5.07	122.94	119.90
1	1A	553	A	O5'-P-OP2	-5.07	101.14	105.70
1	1A	1365	G	N1-C2-N3	5.07	126.94	123.90
1	1A	1441	A	N7-C8-N9	-5.07	111.27	113.80
1	1A	1606	G	C4-N9-C1'	-5.07	119.91	126.50
1	1A	2133	C	C2-N3-C4	5.07	122.44	119.90
1	1A	2346	G	C6-C5-N7	-5.07	127.36	130.40
1	1A	2383	G	C8-N9-C4	5.07	108.43	106.40
1	1A	2893	A	C2-N3-C4	5.07	113.14	110.60
32	1a	148	G	C2-N3-C4	5.07	114.44	111.90
32	1a	615	C	C5-C6-N1	5.07	123.53	121.00
1	2A	2640	G	C4-C5-N7	-5.07	108.77	110.80
1	2A	2764	A	C2-N3-C4	-5.07	108.06	110.60
32	2a	353	A	OP2-P-O3'	5.07	116.36	105.20
1	1A	2429	C	C5-C4-N4	5.07	123.75	120.20
1	2A	1638	C	C2-N3-C4	-5.07	117.37	119.90
1	2A	2768	C	O5'-P-OP2	-5.07	101.14	105.70
32	2a	644	G	C8-N9-C4	5.07	108.43	106.40
32	2a	1301	U	C6-N1-C2	5.07	124.04	121.00
1	1A	176	G	N1-C2-N3	5.07	126.94	123.90
1	1A	582	G	C6-C5-N7	-5.07	127.36	130.40
1	1A	716	G	OP1-P-OP2	-5.07	112.00	119.60
1	1A	779	C	N3-C2-O2	-5.07	118.35	121.90
1	1A	1988	A	O4'-C1'-N9	-5.07	104.15	108.20
1	1A	2573	A	N9-C4-C5	5.07	107.83	105.80
46	1n	3	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	2A	763	G	C5-C6-O6	5.07	131.64	128.60
1	2A	840	C	N3-C4-C5	-5.07	119.87	121.90
1	2A	1410	G	OP2-P-O3'	5.07	116.35	105.20
1	2A	1904	G	N1-C6-O6	-5.07	116.86	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	446	G	N1-C2-N2	5.07	120.76	116.20
32	2a	678	U	N1-C2-O2	-5.07	119.25	122.80
32	2a	1243	C	C2-N3-C4	5.07	122.43	119.90
1	1A	931	C	C5-C6-N1	5.07	123.53	121.00
1	1A	2155	G	C8-N9-C1'	5.07	133.59	127.00
1	1A	2528	G	C4-C5-N7	-5.07	108.77	110.80
32	1a	1273	G	N9-C4-C5	-5.07	103.37	105.40
25	23	28	LEU	CA-CB-CG	-5.07	103.65	115.30
32	2a	500	G	C6-C5-N7	-5.07	127.36	130.40
32	2a	999	C	C5-C6-N1	5.07	123.53	121.00
1	1A	1664	A	C8-N9-C4	5.06	107.83	105.80
1	1A	2443	U	C6-N1-C2	5.06	124.04	121.00
1	1A	2619	G	N9-C4-C5	5.06	107.43	105.40
32	1a	644	G	C5-C6-O6	5.06	131.64	128.60
32	1a	1367	C	C6-N1-C2	-5.06	118.27	120.30
1	2A	9	U	P-O3'-C3'	5.06	125.78	119.70
1	2A	695	G	N1-C6-O6	-5.06	116.86	119.90
32	2a	9	G	O5'-P-OP2	-5.06	101.14	105.70
32	2a	1432	G	C5-C6-O6	5.06	131.64	128.60
1	1A	925	A	C2-N3-C4	-5.06	108.07	110.60
1	1A	938	G	C8-N9-C4	5.06	108.42	106.40
1	1A	1233	U	N3-C4-C5	5.06	117.64	114.60
1	1A	1457	C	N3-C4-C5	5.06	123.92	121.90
1	1A	2341	G	N1-C6-O6	5.06	122.94	119.90
1	1A	2381	A	O5'-P-OP2	-5.06	101.14	105.70
32	1a	613	C	O5'-P-OP1	5.06	116.78	110.70
32	2a	1054	C	N1-C2-O2	5.06	121.94	118.90
1	1A	748	G	OP1-P-OP2	5.06	127.19	119.60
32	1a	1233	G	N3-C2-N2	5.06	123.44	119.90
1	2A	2755	C	C2-N3-C4	5.06	122.43	119.90
32	2a	898	G	N9-C4-C5	-5.06	103.38	105.40
32	2a	912	C	N3-C2-O2	5.06	125.44	121.90
32	2a	1154	G	N9-C4-C5	-5.06	103.38	105.40
1	1A	1233	U	N3-C4-O4	-5.06	115.86	119.40
1	1A	1347	A	OP1-P-OP2	-5.06	112.01	119.60
1	1A	1630	A	N7-C8-N9	-5.06	111.27	113.80
1	1A	1986	G	N7-C8-N9	-5.06	110.57	113.10
1	1A	2080	A	C4-C5-C6	5.06	119.53	117.00
1	1A	2242	G	N1-C2-N2	5.06	120.75	116.20
1	1A	2769	U	OP1-P-O3'	5.06	116.33	105.20
2	1B	41	U	N3-C4-O4	-5.06	115.86	119.40
2	1B	48	A	C6-N1-C2	5.06	121.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	423	G	C5-C6-O6	-5.06	125.56	128.60
32	1a	509	A	N7-C8-N9	5.06	116.33	113.80
1	2A	190	A	OP1-P-OP2	5.06	127.19	119.60
1	2A	1077	A	O5'-P-OP1	-5.06	101.15	105.70
1	2A	1580	A	OP2-P-O3'	5.06	116.33	105.20
1	2A	2143	C	C6-N1-C2	-5.06	118.28	120.30
1	2A	2825	C	N1-C1'-C2'	-5.06	106.44	112.00
1	1A	385	G	N1-C6-O6	5.06	122.94	119.90
1	1A	1505	C	C6-N1-C2	-5.06	118.28	120.30
1	1A	1862	G	C6-N1-C2	5.06	128.13	125.10
1	1A	2088	C	N1-C2-N3	5.06	122.74	119.20
1	1A	2896	G	N3-C2-N2	-5.06	116.36	119.90
1	2A	960	A	N9-C4-C5	-5.06	103.78	105.80
1	2A	1635	G	N7-C8-N9	-5.06	110.57	113.10
1	2A	2516	G	C8-N9-C4	-5.06	104.38	106.40
32	2a	64	G	N3-C4-C5	5.06	131.13	128.60
32	2a	663	A	C2-N3-C4	-5.06	108.07	110.60
32	2a	860	A	N9-C4-C5	5.06	107.82	105.80
1	1A	541	C	N1-C2-O2	-5.06	115.87	118.90
1	1A	2176	G	N3-C4-N9	-5.06	122.97	126.00
32	1a	136	C	O5'-P-OP2	-5.06	101.15	105.70
32	1a	895	G	N9-C4-C5	5.06	107.42	105.40
1	2A	1108	U	C5-C6-N1	5.06	125.23	122.70
1	2A	1776	G	N1-C2-N2	-5.06	111.65	116.20
32	2a	555	C	N3-C4-C5	-5.06	119.88	121.90
32	2a	872	A	N7-C8-N9	5.06	116.33	113.80
1	1A	125	A	C6-N1-C2	-5.05	115.57	118.60
1	1A	2294	G	N1-C2-N3	-5.05	120.87	123.90
1	1A	2826	C	C5-C6-N1	-5.05	118.47	121.00
13	1R	33	ARG	NE-CZ-NH2	-5.05	117.77	120.30
32	1a	438	G	O5'-P-OP2	-5.05	101.15	105.70
32	1a	802	A	C4-C5-N7	5.05	113.23	110.70
32	1a	903	G	OP2-P-O3'	5.05	116.32	105.20
32	1a	1197	G	N3-C2-N2	5.05	123.44	119.90
1	2A	2821	A	C2-N3-C4	-5.05	108.07	110.60
32	2a	913	A	C2-N3-C4	5.05	113.13	110.60
1	1A	748	G	C5-C6-O6	5.05	131.63	128.60
1	1A	1977	U	N1-C2-N3	5.05	117.93	114.90
1	1A	2038	U	N1-C2-O2	5.05	126.34	122.80
1	1A	2874	G	N1-C6-O6	-5.05	116.87	119.90
1	2A	2102	U	N1-C2-O2	5.05	126.34	122.80
1	2A	2595	G	N1-C2-N3	5.05	126.93	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	36	G	C5-N7-C8	5.05	106.83	104.30
1	1A	762	G	C5-C6-O6	-5.05	125.57	128.60
1	1A	1047	A	C2-N3-C4	5.05	113.13	110.60
1	1A	2038	U	N3-C2-O2	-5.05	118.66	122.20
1	2A	1607	C	O5'-P-OP1	-5.05	101.16	105.70
32	2a	1146	A	N9-C4-C5	-5.05	103.78	105.80
1	1A	837	C	N3-C4-N4	5.05	121.53	118.00
1	1A	1079	U	C2-N3-C4	-5.05	123.97	127.00
1	1A	2229	A	C4-N9-C1'	5.05	135.39	126.30
1	1A	2312	G	OP1-P-OP2	-5.05	112.03	119.60
1	1A	2897	U	OP1-P-OP2	5.05	127.17	119.60
32	1a	484	G	N1-C6-O6	-5.05	116.87	119.90
32	1a	1516	G	O5'-P-OP1	-5.05	101.16	105.70
1	2A	1904	G	C4-C5-N7	-5.05	108.78	110.80
2	2B	55	U	N1-C2-O2	-5.05	119.27	122.80
32	2a	273	A	C8-N9-C4	5.05	107.82	105.80
32	2a	677	U	N3-C4-C5	-5.05	111.57	114.60
32	2a	749	C	O5'-P-OP2	5.05	116.76	110.70
1	1A	462	C	C5-C4-N4	-5.05	116.67	120.20
27	15	15	ARG	CA-CB-CG	-5.05	102.29	113.40
32	1a	908	A	C8-N9-C4	-5.05	103.78	105.80
1	2A	495	G	N1-C6-O6	-5.05	116.87	119.90
32	2a	1163	C	C6-N1-C2	-5.05	118.28	120.30
1	1A	581	G	N9-C4-C5	5.05	107.42	105.40
1	1A	1033	G	N3-C2-N2	-5.05	116.37	119.90
1	1A	1514	C	OP1-P-OP2	-5.05	112.03	119.60
1	1A	1631	C	O4'-C1'-N1	5.05	112.24	108.20
32	1a	1255	G	C8-N9-C4	5.05	108.42	106.40
1	2A	1052	C	C2-N1-C1'	5.05	124.35	118.80
1	2A	1450	G	OP1-P-OP2	5.05	127.17	119.60
1	2A	2042	A	C8-N9-C4	5.05	107.82	105.80
1	2A	2163	C	N3-C4-N4	5.05	121.53	118.00
1	2A	2378	A	C8-N9-C4	5.05	107.82	105.80
1	1A	1190	G	N1-C6-O6	-5.04	116.87	119.90
1	1A	1706	U	C2-N3-C4	-5.04	123.97	127.00
1	1A	1845	G	C4-C5-N7	5.04	112.82	110.80
32	1a	880	C	N3-C4-C5	5.04	123.92	121.90
1	2A	1440	G	N1-C6-O6	-5.04	116.87	119.90
1	2A	2146	C	O4'-C1'-N1	-5.04	104.16	108.20
1	2A	1903	G	N3-C4-N9	-5.04	122.97	126.00
1	2A	2489	G	OP2-P-O3'	5.04	116.30	105.20
1	1A	101	A	C8-N9-C1'	-5.04	118.62	127.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	150	C	N3-C4-C5	5.04	123.92	121.90
1	1A	153	C	OP2-P-O3'	5.04	116.29	105.20
1	1A	192	C	C5-C6-N1	-5.04	118.48	121.00
1	1A	499	G	N1-C2-N2	-5.04	111.66	116.20
1	1A	814	U	C4-C5-C6	5.04	122.72	119.70
1	1A	1953	U	N1-C2-O2	5.04	126.33	122.80
1	1A	2022	G	O5'-P-OP2	-5.04	101.16	105.70
1	2A	1760	A	C8-N9-C4	5.04	107.82	105.80
1	2A	1799	G	C5-N7-C8	5.04	106.82	104.30
32	2a	346	G	N3-C4-N9	5.04	129.03	126.00
1	2A	12	U	N1-C2-O2	5.04	126.33	122.80
1	2A	1241	A	O5'-P-OP2	5.04	116.75	110.70
1	2A	1919	A	C8-N9-C4	-5.04	103.78	105.80
1	2A	2623	G	N1-C6-O6	5.04	122.92	119.90
32	2a	1072	G	N1-C6-O6	-5.04	116.88	119.90
1	1A	376	G	OP2-P-O3'	5.04	116.28	105.20
1	1A	1305	G	N1-C6-O6	-5.04	116.88	119.90
1	1A	1835	C	C6-N1-C2	5.04	122.31	120.30
1	1A	2046	G	OP2-P-O3'	5.04	116.28	105.20
1	1A	2101	U	C6-N1-C2	-5.04	117.98	121.00
1	1A	2678	C	N1-C2-O2	5.04	121.92	118.90
1	1A	2830	A	N7-C8-N9	5.04	116.32	113.80
32	1a	158	G	C8-N9-C4	-5.04	104.38	106.40
32	1a	949	A	C8-N9-C4	-5.04	103.78	105.80
1	2A	2017	U	C4-C5-C6	5.04	122.72	119.70
1	2A	2123	G	N3-C2-N2	5.04	123.43	119.90
1	2A	2244	U	C5-C6-N1	-5.04	120.18	122.70
1	2A	2516	G	N1-C2-N3	5.04	126.92	123.90
1	2A	2705	A	C2-N3-C4	-5.04	108.08	110.60
1	1A	760	G	C6-C5-N7	-5.04	127.38	130.40
1	1A	1481	G	N1-C6-O6	-5.04	116.88	119.90
1	1A	2393	C	N1-C2-O2	-5.04	115.88	118.90
32	1a	119	A	O5'-P-OP2	-5.04	101.17	105.70
1	2A	1799	G	N7-C8-N9	-5.04	110.58	113.10
1	1A	466	G	OP1-P-OP2	-5.04	112.05	119.60
1	1A	507	G	O4'-C1'-N9	5.04	112.23	108.20
1	1A	1598	C	C5-C6-N1	-5.04	118.48	121.00
1	1A	2289	G	C5-N7-C8	5.04	106.82	104.30
2	1B	52	A	N9-C4-C5	-5.04	103.79	105.80
32	1a	557	G	N1-C2-N2	-5.04	111.67	116.20
32	1a	619	U	C5-C4-O4	5.04	128.92	125.90
32	1a	1131	G	C5-C6-O6	-5.04	125.58	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	188	G	C4-C5-N7	5.04	112.81	110.80
1	2A	1000	A	OP1-P-OP2	-5.04	112.05	119.60
1	2A	1404	C	OP2-P-O3'	5.04	116.28	105.20
1	2A	2228	G	C5-C6-O6	5.04	131.62	128.60
1	2A	2837	G	C5-C6-O6	-5.04	125.58	128.60
32	2a	299	G	C5-N7-C8	-5.04	101.78	104.30
32	2a	435	C	C2-N3-C4	5.04	122.42	119.90
1	1A	136	G	OP1-P-OP2	5.03	127.15	119.60
1	1A	805	C	C2-N3-C4	-5.03	117.38	119.90
1	1A	1295	U	C5-C6-N1	-5.03	120.18	122.70
1	1A	1664	A	N1-C6-N6	-5.03	115.58	118.60
1	1A	1717	C	C4-C5-C6	5.03	119.92	117.40
1	1A	1982	A	C4-C5-C6	-5.03	114.48	117.00
1	1A	2053	A	C5-C6-N6	5.03	127.73	123.70
1	1A	2290	A	C4-C5-N7	-5.03	108.18	110.70
1	1A	2495	C	N3-C4-C5	-5.03	119.89	121.90
1	1A	2735	G	C5-C6-O6	-5.03	125.58	128.60
32	1a	175	C	N3-C4-C5	-5.03	119.89	121.90
32	1a	504	C	N1-C2-O2	5.03	121.92	118.90
32	1a	620	C	OP1-P-O3'	5.03	116.27	105.20
32	1a	819	A	N3-C4-N9	5.03	131.43	127.40
32	1a	836	G	N9-C4-C5	-5.03	103.39	105.40
1	2A	109	G	C6-N1-C2	-5.03	122.08	125.10
1	2A	350	U	N3-C2-O2	-5.03	118.68	122.20
1	2A	885	C	C6-N1-C2	-5.03	118.29	120.30
1	2A	2816	C	O5'-P-OP2	-5.03	101.17	105.70
1	1A	1364	C	O5'-P-OP1	-5.03	101.17	105.70
1	1A	2230	U	C6-N1-C1'	-5.03	114.16	121.20
1	2A	82	G	C8-N9-C4	5.03	108.41	106.40
1	2A	2063	C	OP2-P-O3'	5.03	116.27	105.20
1	1A	355	A	C8-N9-C4	5.03	107.81	105.80
1	1A	2249	G	N1-C6-O6	-5.03	116.88	119.90
1	1A	2274	U	C5-C4-O4	-5.03	122.88	125.90
1	1A	2586	G	C6-C5-N7	5.03	133.42	130.40
2	1B	93	G	C4-C5-C6	-5.03	115.78	118.80
32	1a	809	G	C2-N3-C4	-5.03	109.39	111.90
32	1a	1134	G	N7-C8-N9	5.03	115.61	113.10
50	1r	26	LEU	CA-CB-CG	5.03	126.87	115.30
1	2A	1164	G	C5-C6-O6	5.03	131.62	128.60
1	2A	2743	C	N1-C2-O2	-5.03	115.88	118.90
32	2a	887	G	C4-C5-N7	5.03	112.81	110.80
32	2a	1356	G	N1-C6-O6	5.03	122.92	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	74	G	C5-C6-N1	5.03	114.01	111.50
1	1A	1258	A	N1-C2-N3	5.03	131.81	129.30
32	1a	689	C	O5'-P-OP1	-5.03	101.17	105.70
32	2a	616	G	N9-C4-C5	5.03	107.41	105.40
1	1A	34	C	C6-N1-C1'	5.03	126.83	120.80
1	1A	742	G	C4-C5-C6	-5.03	115.78	118.80
1	1A	1539	C	C5-C6-N1	-5.03	118.49	121.00
1	1A	2394	G	N7-C8-N9	5.03	115.61	113.10
1	1A	2442	A	C4-C5-C6	-5.03	114.49	117.00
1	1A	2828	G	N3-C2-N2	5.03	123.42	119.90
32	1a	189(C)	C	C6-N1-C2	-5.03	118.29	120.30
32	1a	1446	U	O4'-C1'-N1	5.03	112.22	108.20
1	2A	769	G	N3-C2-N2	-5.03	116.38	119.90
1	2A	866	A	C8-N9-C1'	-5.03	118.65	127.70
1	2A	1297	C	C4-C5-C6	5.03	119.91	117.40
1	2A	1740	G	N9-C4-C5	-5.03	103.39	105.40
1	2A	1863	G	C2-N3-C4	-5.03	109.39	111.90
32	2a	1145	C	O5'-P-OP2	-5.03	101.17	105.70
1	1A	215	G	C8-N9-C4	-5.03	104.39	106.40
1	1A	1613	A	C8-N9-C4	5.03	107.81	105.80
1	1A	1874	C	C5-C4-N4	-5.03	116.68	120.20
1	1A	2055	A	C6-N1-C2	-5.03	115.58	118.60
1	1A	2450	U	OP2-P-O3'	5.03	116.26	105.20
32	1a	419	C	OP1-P-O3'	5.03	116.25	105.20
1	1A	1322	A	O4'-C1'-N9	-5.02	104.18	108.20
1	2A	174	C	N3-C4-C5	-5.02	119.89	121.90
32	2a	306	G	N1-C2-N2	5.02	120.72	116.20
1	1A	548	C	OP2-P-O3'	5.02	116.25	105.20
1	1A	783	C	O5'-P-OP1	-5.02	101.18	105.70
1	1A	877	G	OP1-P-OP2	-5.02	112.07	119.60
1	1A	1676	G	N3-C4-N9	-5.02	122.99	126.00
1	1A	2384	G	N1-C6-O6	5.02	122.91	119.90
1	1A	2565	G	N3-C4-C5	-5.02	126.09	128.60
1	1A	2844	G	C6-C5-N7	5.02	133.41	130.40
32	1a	73	G	O4'-C1'-N9	5.02	112.22	108.20
32	1a	641	U	N3-C4-O4	5.02	122.92	119.40
1	2A	2582	G	N3-C2-N2	5.02	123.42	119.90
32	2a	902	G	C5-C6-N1	5.02	114.01	111.50
32	2a	1495	U	N3-C4-C5	-5.02	111.59	114.60
1	1A	385	G	C4-C5-N7	5.02	112.81	110.80
1	1A	1155	C	C5-C4-N4	-5.02	116.69	120.20
1	1A	1659	G	C2-N3-C4	-5.02	109.39	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2204	G	C8-N9-C1'	5.02	133.53	127.00
1	1A	2498	G	C8-N9-C1'	-5.02	120.47	127.00
1	2A	525	U	C5-C4-O4	5.02	128.91	125.90
32	2a	1335	C	C6-N1-C1'	-5.02	114.78	120.80
1	1A	484	G	OP1-P-OP2	5.02	127.13	119.60
1	1A	822	G	O5'-P-OP1	-5.02	101.18	105.70
1	1A	1976	G	N3-C2-N2	-5.02	116.39	119.90
1	1A	2134	G	C6-N1-C2	-5.02	122.09	125.10
1	1A	2270	C	C6-N1-C2	-5.02	118.29	120.30
1	1A	2348	A	C4-C5-N7	5.02	113.21	110.70
1	1A	2702	C	OP1-P-O3'	5.02	116.24	105.20
1	1A	2748	G	C5-C6-O6	5.02	131.61	128.60
32	1a	792	A	C4-N9-C1'	-5.02	117.26	126.30
32	1a	1286	A	O5'-P-OP2	5.02	116.72	110.70
1	2A	114	U	C2-N1-C1'	5.02	123.72	117.70
1	2A	1041	C	N3-C2-O2	-5.02	118.39	121.90
1	2A	1084	A	N3-C4-C5	5.02	130.31	126.80
1	2A	2816	C	OP1-P-OP2	5.02	127.13	119.60
32	2a	108	G	C5-C6-O6	-5.02	125.59	128.60
1	1A	555	G	N9-C4-C5	-5.02	103.39	105.40
1	1A	613	A	OP1-P-OP2	-5.02	112.08	119.60
1	1A	1708	G	C4-C5-N7	-5.02	108.79	110.80
1	1A	2233	G	N9-C4-C5	5.02	107.41	105.40
1	1A	2450	U	C2-N3-C4	-5.02	123.99	127.00
32	1a	330	C	C6-N1-C2	-5.02	118.29	120.30
1	2A	882	G	N1-C2-N2	5.02	120.72	116.20
1	2A	989	G	C4-C5-N7	5.02	112.81	110.80
1	2A	1292	U	O5'-P-OP2	-5.02	101.18	105.70
1	2A	1913	A	C4-N9-C1'	5.02	135.33	126.30
1	2A	2302	G	C5-C6-O6	5.02	131.61	128.60
32	2a	604	G	C8-N9-C4	5.02	108.41	106.40
32	2a	1487	G	OP1-P-OP2	-5.02	112.07	119.60
1	1A	236	G	C5-N7-C8	-5.02	101.79	104.30
1	1A	874	U	C3'-C2'-C1'	5.02	105.51	101.50
1	1A	1873	G	C4-C5-N7	5.02	112.81	110.80
1	2A	666	G	N9-C4-C5	-5.02	103.39	105.40
32	2a	1469	G	N3-C2-N2	-5.02	116.39	119.90
1	1A	799	A	N1-C2-N3	5.01	131.81	129.30
1	1A	839	G	N1-C6-O6	-5.01	116.89	119.90
1	1A	1051	C	N3-C4-N4	-5.01	114.49	118.00
1	1A	1918	G	N1-C6-O6	-5.01	116.89	119.90
1	1A	2085	C	OP2-P-O3'	5.01	116.23	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2261	U	N3-C4-C5	5.01	117.61	114.60
1	1A	2609	G	C2-N3-C4	-5.01	109.39	111.90
32	1a	120	A	O5'-P-OP2	5.01	116.72	110.70
32	1a	595	G	N3-C4-N9	5.01	129.01	126.00
32	1a	1285	A	P-O3'-C3'	5.01	125.72	119.70
1	2A	277	C	P-O3'-C3'	5.01	125.72	119.70
1	2A	958	U	C4-C5-C6	5.01	122.71	119.70
32	2a	663	A	O5'-P-OP1	-5.01	101.19	105.70
1	1A	1504	A	N1-C6-N6	5.01	121.61	118.60
1	1A	2480	G	O4'-C1'-N9	5.01	112.21	108.20
1	1A	2762	A	N1-C6-N6	-5.01	115.59	118.60
32	1a	361	G	C4-C5-N7	5.01	112.81	110.80
1	2A	1844	C	C5-C6-N1	-5.01	118.49	121.00
32	2a	189(E)	U	N1-C2-O2	5.01	126.31	122.80
1	1A	425	G	C5-C6-N1	-5.01	109.00	111.50
1	1A	1340	U	N1-C2-N3	5.01	117.91	114.90
1	1A	1439	A	C5-C6-N6	5.01	127.71	123.70
1	1A	1694	G	O4'-C1'-N9	-5.01	104.19	108.20
1	1A	2261	U	OP1-P-OP2	-5.01	112.08	119.60
1	1A	2357	G	N1-C2-N2	-5.01	111.69	116.20
1	2A	209	C	N1-C2-O2	5.01	121.91	118.90
1	2A	1966	A	N9-C4-C5	5.01	107.81	105.80
32	2a	1086	U	N3-C2-O2	-5.01	118.69	122.20
32	2a	1370	G	C4-C5-N7	5.01	112.81	110.80
1	1A	25	U	C5-C6-N1	5.01	125.20	122.70
1	1A	1768	U	C5-C6-N1	5.01	125.20	122.70
1	1A	2348	A	N7-C8-N9	-5.01	111.30	113.80
1	1A	2459	G	C6-N1-C2	-5.01	122.09	125.10
1	1A	2625	U	O5'-P-OP2	-5.01	101.19	105.70
1	1A	2844	G	N1-C6-O6	-5.01	116.89	119.90
32	1a	183	G	N3-C4-C5	-5.01	126.09	128.60
32	1a	802	A	N1-C6-N6	5.01	121.61	118.60
32	1a	1158	C	N3-C4-C5	-5.01	119.90	121.90
1	2A	882	G	C6-C5-N7	5.01	133.41	130.40
1	2A	1128	A	N7-C8-N9	-5.01	111.30	113.80
1	2A	2058	A	N3-C4-N9	5.01	131.41	127.40
1	2A	2877	G	C8-N9-C4	5.01	108.40	106.40
32	2a	22	G	C5-C6-N1	5.01	114.00	111.50
1	1A	2476	C	C5-C4-N4	-5.01	116.69	120.20
2	1B	77	U	N3-C4-O4	5.01	122.91	119.40
27	15	20	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	2A	65	C	C6-N1-C2	-5.01	118.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1122	G	C5-C6-O6	-5.01	125.59	128.60
1	2A	1508	A	N9-C4-C5	-5.01	103.80	105.80
32	2a	563	A	C2-N3-C4	-5.01	108.10	110.60
1	1A	23	G	N1-C2-N2	5.01	120.71	116.20
1	1A	330	U	C6-N1-C2	-5.01	118.00	121.00
1	1A	741	U	C4-C5-C6	5.01	122.70	119.70
1	1A	950	C	N3-C4-C5	5.01	123.90	121.90
1	1A	1042	A	O5'-P-OP2	5.01	116.71	110.70
1	1A	2644	A	OP1-P-OP2	5.01	127.11	119.60
32	1a	157	G	N9-C4-C5	5.01	107.40	105.40
32	1a	557	G	C8-N9-C1'	-5.01	120.49	127.00
32	1a	766	A	C5-C6-N6	-5.01	119.69	123.70
1	2A	764	A	O4'-C1'-N9	5.01	112.21	108.20
1	2A	909	A	N1-C6-N6	-5.01	115.60	118.60
1	2A	1682	G	C5-C6-O6	5.01	131.60	128.60
32	2a	1079	G	C8-N9-C4	-5.01	104.40	106.40
1	1A	2723	A	C5-N7-C8	-5.00	101.40	103.90
32	1a	821	G	O5'-P-OP2	5.00	116.71	110.70
1	2A	1563	G	N1-C2-N2	-5.00	111.70	116.20
1	1A	1006	C	OP1-P-O3'	5.00	116.21	105.20
9	1N	35	ARG	CA-CB-CG	5.00	124.41	113.40
32	1a	896	C	C5-C6-N1	-5.00	118.50	121.00
32	1a	905	U	C5-C6-N1	-5.00	120.20	122.70
1	2A	1001	A	N1-C6-N6	5.00	121.60	118.60
1	2A	1353	A	N7-C8-N9	-5.00	111.30	113.80
1	2A	1547	C	C4-C5-C6	5.00	119.90	117.40
1	2A	1774	C	C2-N3-C4	5.00	122.40	119.90
32	2a	578	C	C5-C4-N4	5.00	123.70	120.20
1	1A	200	A	N7-C8-N9	-5.00	111.30	113.80
1	1A	524	U	C2-N3-C4	-5.00	124.00	127.00
1	1A	1090	G	O5'-P-OP2	-5.00	101.20	105.70
3	1D	242	ARG	CG-CD-NE	5.00	122.31	111.80
32	1a	204	U	C6-N1-C1'	-5.00	114.20	121.20
1	2A	139(A)	G	N3-C4-N9	5.00	129.00	126.00
1	2A	452	G	C5-C6-O6	-5.00	125.60	128.60
1	2A	1844	C	N3-C4-C5	5.00	123.90	121.90
1	2A	2371	G	C8-N9-C4	5.00	108.40	106.40
1	2A	2783	G	OP2-P-O3'	5.00	116.20	105.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	18	13	ARG	Peptide
19	1X	93	GLU	Peptide
19	2X	93	GLU	Peptide
44	2l	86	ARG	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/275 (99%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/275 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/204 (99%)	194 (96%)	7 (4%)	1 (0%)	29	61
4	2E	202/204 (99%)	192 (95%)	9 (4%)	1 (0%)	29	61
5	1F	201/203 (99%)	194 (96%)	6 (3%)	1 (0%)	29	61
5	2F	201/203 (99%)	195 (97%)	4 (2%)	2 (1%)	15	44
6	1G	179/181 (99%)	164 (92%)	12 (7%)	3 (2%)	9	29
6	2G	179/181 (99%)	163 (91%)	14 (8%)	2 (1%)	14	41
7	1H	172/174 (99%)	162 (94%)	10 (6%)	0	100	100
7	2H	171/174 (98%)	160 (94%)	11 (6%)	0	100	100
8	1I	145/147 (99%)	128 (88%)	15 (10%)	2 (1%)	11	34
8	2I	144/147 (98%)	125 (87%)	18 (12%)	1 (1%)	22	53
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	49
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
11	2P	147/149 (99%)	140 (95%)	6 (4%)	1 (1%)	22	53
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	53
12	2Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22	53
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	17	46
14	2S	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	17	46
15	1T	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
15	2T	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
16	1U	114/116 (98%)	114 (100%)	0	0	100	100
16	2U	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	44
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	44
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%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
21	1Z	201/203 (99%)	190 (94%)	10 (5%)	1 (0%)	29	61
21	2Z	199/203 (98%)	187 (94%)	12 (6%)	0	100	100
22	10	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
22	20	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
23	11	95/97 (98%)	94 (99%)	0	1 (1%)	14	41
23	21	95/97 (98%)	92 (97%)	2 (2%)	1 (1%)	14	41
24	12	68/70 (97%)	67 (98%)	1 (2%)	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%)	53 (93%)	4 (7%)	0	100	100
26	14	67/69 (97%)	55 (82%)	9 (13%)	3 (4%)	2	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/69 (97%)	54 (81%)	6 (9%)	7 (10%)	0	1
27	15	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
27	25	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
28	16	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
28	26	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
29	17	46/48 (96%)	46 (100%)	0	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%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1x	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
33	2x	94/97 (97%)	92 (98%)	2 (2%)	0	100	100
34	1b	229/231 (99%)	193 (84%)	27 (12%)	9 (4%)	3	10
34	2b	229/231 (99%)	194 (85%)	28 (12%)	7 (3%)	4	14
35	1c	204/206 (99%)	177 (87%)	26 (13%)	1 (0%)	29	61
35	2c	204/206 (99%)	177 (87%)	23 (11%)	4 (2%)	7	24
36	1d	206/208 (99%)	187 (91%)	16 (8%)	3 (2%)	10	33
36	2d	206/208 (99%)	187 (91%)	16 (8%)	3 (2%)	10	33
37	1e	146/148 (99%)	136 (93%)	9 (6%)	1 (1%)	22	53
37	2e	146/148 (99%)	135 (92%)	11 (8%)	0	100	100
38	1f	98/100 (98%)	87 (89%)	11 (11%)	0	100	100
38	2f	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
39	1g	153/155 (99%)	146 (95%)	7 (5%)	0	100	100
39	2g	153/155 (99%)	146 (95%)	4 (3%)	3 (2%)	7	24
40	1h	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
40	2h	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
41	1i	125/127 (98%)	109 (87%)	14 (11%)	2 (2%)	9	31
41	2i	124/127 (98%)	106 (86%)	14 (11%)	4 (3%)	4	13
42	1j	95/97 (98%)	79 (83%)	13 (14%)	3 (3%)	4	13
42	2j	94/97 (97%)	79 (84%)	12 (13%)	3 (3%)	4	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1k	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	17	46
43	2k	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
44	1l	119/122 (98%)	112 (94%)	6 (5%)	1 (1%)	19	49
44	2l	119/122 (98%)	108 (91%)	9 (8%)	2 (2%)	9	29
45	1m	114/116 (98%)	103 (90%)	9 (8%)	2 (2%)	8	28
45	2m	112/116 (97%)	102 (91%)	8 (7%)	2 (2%)	8	28
46	1n	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
46	2n	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
47	1o	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
47	2o	86/88 (98%)	80 (93%)	5 (6%)	1 (1%)	13	39
48	1p	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
48	2p	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
49	1q	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15	44
49	2q	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
50	1r	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
50	2r	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
51	1s	81/83 (98%)	71 (88%)	8 (10%)	2 (2%)	5	19
51	2s	81/83 (98%)	72 (89%)	6 (7%)	3 (4%)	3	11
52	1t	94/98 (96%)	88 (94%)	3 (3%)	3 (3%)	4	13
52	2t	96/98 (98%)	87 (91%)	6 (6%)	3 (3%)	4	14
53	1u	21/23 (91%)	19 (90%)	1 (5%)	1 (5%)	2	7
53	2u	21/23 (91%)	19 (90%)	1 (5%)	1 (5%)	2	7
54	1y	14/16 (88%)	14 (100%)	0	0	100	100
54	2y	14/16 (88%)	14 (100%)	0	0	100	100
All	All	11657/11874 (98%)	10874 (93%)	682 (6%)	101 (1%)	17	46

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	52	LEU
6	1G	49	ASP
6	1G	51	ARG
8	1I	73	GLU
14	1S	59	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	1V	79	VAL
23	11	3	LYS
34	1b	17	PHE
34	1b	22	LYS
34	1b	125	PRO
34	1b	231	GLU
42	1j	79	ARG
51	1s	12	ASP
52	1t	95	ALA
5	2F	21	ALA
5	2F	130	ALA
6	2G	81	LYS
8	2I	10	GLU
23	21	3	LYS
26	24	45	GLY
26	24	47	GLN
26	24	60	GLN
26	24	65	ASP
41	2i	44	VAL
41	2i	54	ASP
42	2j	79	ARG
45	2m	67	GLU
51	2s	28	LYS
52	2t	95	ALA
5	1F	130	ALA
26	14	45	GLY
26	14	49	PHE
34	1b	37	ASN
34	1b	127	ILE
36	1d	171	GLY
41	1i	44	VAL
42	1j	32	ALA
53	1u	3	LYS
6	2G	78	SER
10	2O	5	GLN
17	2V	79	VAL
34	2b	17	PHE
34	2b	123	ALA
34	2b	125	PRO
34	2b	127	ILE
34	2b	228	GLY
35	2c	61	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	2d	171	GLY
41	2i	11	LYS
44	2l	87	GLY
44	2l	88	GLY
8	1I	105	HIS
10	1O	5	GLN
12	1Q	59	ARG
26	14	55	ARG
4	2E	51	PHE
12	2Q	59	ARG
26	24	49	PHE
26	24	62	ARG
34	2b	232	PRO
39	2g	6	ARG
39	2g	7	ALA
45	2m	5	ALA
52	2t	100	ILE
52	2t	102	GLY
6	1G	78	SER
43	1k	117	ASN
45	1m	67	GLU
51	1s	27	GLU
42	2j	32	ALA
51	2s	27	GLU
53	2u	7	ARG
34	1b	83	MET
35	1c	144	SER
41	1i	109	VAL
45	1m	46	LYS
49	1q	49	GLU
52	1t	10	LEU
11	2P	29	LYS
14	2S	89	ARG
34	2b	120	ALA
35	2c	108	ASN
35	2c	144	SER
35	2c	156	ARG
47	2o	88	ARG
51	2s	29	ARG
36	1d	136	PRO
37	1e	147	ASP
44	1l	91	LYS

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Mol	Chain	Res	Type
26	24	55	ARG
36	2d	136	PRO
41	2i	109	VAL
52	1t	100	ILE
36	1d	5	ILE
42	1j	82	ILE
42	2j	77	PRO
21	1Z	158	PRO
34	1b	202	PRO
36	2d	5	ILE
39	2g	55	GLY
34	1b	124	SER

### 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%)	194 (91%)	20 (9%)	9 26
3	2D	215/217 (99%)	189 (88%)	26 (12%)	5 15
4	1E	164/165 (99%)	148 (90%)	16 (10%)	8 24
4	2E	164/165 (99%)	147 (90%)	17 (10%)	7 21
5	1F	160/161 (99%)	137 (86%)	23 (14%)	3 10
5	2F	159/161 (99%)	142 (89%)	17 (11%)	6 20
6	1G	144/155 (93%)	132 (92%)	12 (8%)	11 32
6	2G	142/155 (92%)	132 (93%)	10 (7%)	15 40
7	1H	144/145 (99%)	132 (92%)	12 (8%)	11 32
7	2H	143/145 (99%)	130 (91%)	13 (9%)	9 27
8	1I	111/123 (90%)	96 (86%)	15 (14%)	4 11
8	2I	108/123 (88%)	95 (88%)	13 (12%)	5 15
9	1N	119/119 (100%)	106 (89%)	13 (11%)	6 19
9	2N	118/119 (99%)	104 (88%)	14 (12%)	5 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1O	100/100 (100%)	92 (92%)	8 (8%)	12	34
10	2O	100/100 (100%)	94 (94%)	6 (6%)	19	48
11	1P	115/116 (99%)	108 (94%)	7 (6%)	18	48
11	2P	115/116 (99%)	105 (91%)	10 (9%)	10	30
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	14	38
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	33
13	1R	101/101 (100%)	89 (88%)	12 (12%)	5	16
13	2R	101/101 (100%)	87 (86%)	14 (14%)	3	11
14	1S	87/87 (100%)	76 (87%)	11 (13%)	4	14
14	2S	85/87 (98%)	76 (89%)	9 (11%)	6	20
15	1T	115/115 (100%)	107 (93%)	8 (7%)	15	40
15	2T	113/115 (98%)	107 (95%)	6 (5%)	22	54
16	1U	93/93 (100%)	82 (88%)	11 (12%)	5	16
16	2U	93/93 (100%)	87 (94%)	6 (6%)	17	44
17	1V	81/82 (99%)	71 (88%)	10 (12%)	4	15
17	2V	80/82 (98%)	71 (89%)	9 (11%)	6	18
18	1W	90/91 (99%)	81 (90%)	9 (10%)	7	22
18	2W	90/91 (99%)	82 (91%)	8 (9%)	9	28
19	1X	77/77 (100%)	73 (95%)	4 (5%)	23	55
19	2X	77/77 (100%)	73 (95%)	4 (5%)	23	55
20	1Y	86/88 (98%)	81 (94%)	5 (6%)	20	50
20	2Y	86/88 (98%)	81 (94%)	5 (6%)	20	50
21	1Z	169/176 (96%)	152 (90%)	17 (10%)	7	22
21	2Z	165/176 (94%)	149 (90%)	16 (10%)	8	24
22	10	61/62 (98%)	54 (88%)	7 (12%)	5	17
22	20	61/62 (98%)	56 (92%)	5 (8%)	11	33
23	11	79/82 (96%)	75 (95%)	4 (5%)	24	55
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%)	65 (98%)	1 (2%)	65	89
25	13	51/51 (100%)	48 (94%)	3 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	23	50/51 (98%)	47 (94%)	3 (6%)	19	48
26	14	58/62 (94%)	49 (84%)	9 (16%)	2	8
26	24	54/62 (87%)	48 (89%)	6 (11%)	6	19
27	15	51/51 (100%)	49 (96%)	2 (4%)	32	66
27	25	50/51 (98%)	47 (94%)	3 (6%)	19	48
28	16	51/51 (100%)	44 (86%)	7 (14%)	3	11
28	26	50/51 (98%)	46 (92%)	4 (8%)	12	34
29	17	41/41 (100%)	37 (90%)	4 (10%)	8	24
29	27	41/41 (100%)	39 (95%)	2 (5%)	25	57
30	18	54/54 (100%)	48 (89%)	6 (11%)	6	19
30	28	54/54 (100%)	49 (91%)	5 (9%)	9	26
31	19	34/34 (100%)	32 (94%)	2 (6%)	19	49
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1x	82/83 (99%)	77 (94%)	5 (6%)	18	48
33	2x	79/83 (95%)	69 (87%)	10 (13%)	4	14
34	1b	191/199 (96%)	162 (85%)	29 (15%)	3	8
34	2b	187/199 (94%)	164 (88%)	23 (12%)	4	15
35	1c	144/160 (90%)	141 (98%)	3 (2%)	53	84
35	2c	140/160 (88%)	126 (90%)	14 (10%)	7	22
36	1d	171/180 (95%)	155 (91%)	16 (9%)	8	26
36	2d	172/180 (96%)	157 (91%)	15 (9%)	10	30
37	1e	114/114 (100%)	104 (91%)	10 (9%)	10	29
37	2e	114/114 (100%)	105 (92%)	9 (8%)	12	34
38	1f	85/90 (94%)	81 (95%)	4 (5%)	26	59
38	2f	85/90 (94%)	79 (93%)	6 (7%)	14	39
39	1g	120/126 (95%)	113 (94%)	7 (6%)	20	50
39	2g	119/126 (94%)	112 (94%)	7 (6%)	19	49
40	1h	116/118 (98%)	108 (93%)	8 (7%)	15	41
40	2h	114/118 (97%)	108 (95%)	6 (5%)	22	54
41	1i	91/98 (93%)	83 (91%)	8 (9%)	10	29
41	2i	88/98 (90%)	80 (91%)	8 (9%)	9	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	1j	68/87 (78%)	62 (91%)	6 (9%)	10	29
42	2j	68/87 (78%)	64 (94%)	4 (6%)	19	49
43	1k	83/86 (96%)	80 (96%)	3 (4%)	35	69
43	2k	83/86 (96%)	74 (89%)	9 (11%)	6	19
44	1l	96/102 (94%)	92 (96%)	4 (4%)	30	63
44	2l	96/102 (94%)	89 (93%)	7 (7%)	14	38
45	1m	90/94 (96%)	81 (90%)	9 (10%)	7	22
45	2m	87/94 (93%)	77 (88%)	10 (12%)	5	17
46	1n	49/49 (100%)	43 (88%)	6 (12%)	5	15
46	2n	49/49 (100%)	46 (94%)	3 (6%)	18	48
47	1o	78/79 (99%)	72 (92%)	6 (8%)	13	35
47	2o	78/79 (99%)	73 (94%)	5 (6%)	17	45
48	1p	69/71 (97%)	60 (87%)	9 (13%)	4	13
48	2p	68/71 (96%)	57 (84%)	11 (16%)	2	7
49	1q	94/94 (100%)	91 (97%)	3 (3%)	39	73
49	2q	94/94 (100%)	87 (93%)	7 (7%)	13	37
50	1r	59/59 (100%)	54 (92%)	5 (8%)	10	31
50	2r	59/59 (100%)	55 (93%)	4 (7%)	16	42
51	1s	68/72 (94%)	60 (88%)	8 (12%)	5	16
51	2s	67/72 (93%)	62 (92%)	5 (8%)	13	37
52	1t	71/76 (93%)	65 (92%)	6 (8%)	10	31
52	2t	70/76 (92%)	62 (89%)	8 (11%)	5	18
53	1u	18/18 (100%)	16 (89%)	2 (11%)	6	19
53	2u	18/18 (100%)	18 (100%)	0	100	100
54	1y	14/15 (93%)	13 (93%)	1 (7%)	14	39
54	2y	14/15 (93%)	12 (86%)	2 (14%)	3	10
All	All	9552/9892 (97%)	8702 (91%)	850 (9%)	9	28

All (850) 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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	1D	37	LEU
3	1D	61	LEU
3	1D	69	ARG
3	1D	89	SER
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	141	VAL
3	1D	142	VAL
3	1D	155	LEU
3	1D	211	ARG
3	1D	217	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	1	MET
4	1E	7	VAL
4	1E	9	VAL
4	1E	34	VAL
4	1E	49	LEU
4	1E	73	GLU
4	1E	75	VAL
4	1E	78	LEU
4	1E	89	ASP
4	1E	113	PHE
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	154	LYS
4	1E	175	VAL
4	1E	181	LEU
5	1F	12	LEU
5	1F	18	ARG
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	60	SER
5	1F	74	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	1F	94	PRO
5	1F	110	LEU
5	1F	125	LEU
5	1F	127	GLU
5	1F	132	VAL
5	1F	137	LYS
5	1F	140	LEU
5	1F	158	THR
5	1F	162	LEU
5	1F	170	LEU
5	1F	191	ARG
5	1F	192	LEU
5	1F	197	ASP
5	1F	200	GLU
5	1F	201	VAL
6	1G	5	VAL
6	1G	7	LEU
6	1G	28	VAL
6	1G	43	LEU
6	1G	78	SER
6	1G	79	ASN
6	1G	126	ASP
6	1G	140	ILE
6	1G	148	MET
6	1G	153	ARG
6	1G	165	THR
6	1G	170	ARG
7	1H	2	SER
7	1H	6	ARG
7	1H	13	LYS
7	1H	44	VAL
7	1H	45	VAL
7	1H	71	LEU
7	1H	85	LYS
7	1H	105	LEU
7	1H	119	GLU
7	1H	134	SER
7	1H	139	GLN
7	1H	153	LYS
8	1I	5	LEU
8	1I	9	LEU
8	1I	10	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	1I	15	VAL
8	1I	38	LEU
8	1I	50	ARG
8	1I	64	GLU
8	1I	69	LYS
8	1I	78	THR
8	1I	85	GLU
8	1I	92	VAL
8	1I	101	LEU
8	1I	104	GLN
8	1I	109	ILE
8	1I	140	LEU
9	1N	1	MET
9	1N	9	VAL
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
10	1O	8	LEU
10	1O	10	VAL
10	1O	20	MET
10	1O	64	ARG
10	1O	94	ARG
10	1O	107	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	99	LEU
11	1P	112	LEU
11	1P	125	VAL
12	1Q	2	LEU
12	1Q	6	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	1Q	7	MET
12	1Q	18	LYS
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	130	LYS
12	1Q	133	ARG
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	75	LEU
13	1R	86	ARG
13	1R	96	ARG
13	1R	111	LEU
13	1R	114	VAL
13	1R	117	VAL
14	1S	14	VAL
14	1S	17	ARG
14	1S	21	THR
14	1S	25	ARG
14	1S	36	TYR
14	1S	49	VAL
14	1S	50	SER
14	1S	52	SER
14	1S	59	LYS
14	1S	68	GLN
14	1S	69	VAL
15	1T	13	ARG
15	1T	28	VAL
15	1T	34	VAL
15	1T	39	ARG
15	1T	59	THR
15	1T	78	LEU
15	1T	96	ARG
15	1T	108	ARG
16	1U	5	LYS
16	1U	8	VAL
16	1U	31	SER
16	1U	50	ARG
16	1U	52	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
16	1U	59	ARG
16	1U	74	LEU
16	1U	83	LEU
16	1U	95	LEU
16	1U	104	GLN
16	1U	117	GLN
17	1V	28	GLU
17	1V	35	LEU
17	1V	46	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	82	ARG
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	27	LYS
18	1W	67	ASP
18	1W	100	THR
18	1W	107	LEU
19	1X	45	THR
19	1X	57	LEU
19	1X	66	LEU
19	1X	88	LYS
20	1Y	6	HIS
20	1Y	7	VAL
20	1Y	43	ASN
20	1Y	90	LEU
20	1Y	92	ASN
21	1Z	11	GLU
21	1Z	31	ARG
21	1Z	33	LEU
21	1Z	42	VAL
21	1Z	61	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	93	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	1Z	94	GLU
21	1Z	102	LEU
21	1Z	126	VAL
21	1Z	135	GLU
21	1Z	150	LEU
21	1Z	161	VAL
21	1Z	162	GLU
21	1Z	170	THR
21	1Z	203	GLU
22	10	10	THR
22	10	11	ARG
22	10	14	ARG
22	10	39	ARG
22	10	55	ARG
22	10	59	LEU
22	10	82	ARG
23	11	21	ARG
23	11	30	VAL
23	11	59	THR
23	11	95	LEU
24	12	3	LEU
24	12	8	LYS
24	12	53	LEU
24	12	70	GLN
25	13	8	LEU
25	13	23	LEU
25	13	54	VAL
26	14	13	ARG
26	14	23	GLU
26	14	30	GLU
26	14	49	PHE
26	14	56	VAL
26	14	57	GLU
26	14	59	PHE
26	14	65	ASP
26	14	69	LYS
27	15	16	ARG
27	15	29	THR
28	16	6	ARG
28	16	14	THR
28	16	19	ARG
28	16	28	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
28	16	40	CYS
28	16	48	VAL
28	16	52	VAL
29	17	1	MET
29	17	10	ARG
29	17	24	THR
29	17	43	THR
30	18	14	VAL
30	18	23	VAL
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
30	18	52	LYS
31	19	27	CYS
31	19	35	ARG
33	2x	3	MET
33	2x	9	GLN
33	2x	11	GLU
33	2x	13	THR
33	2x	24	LEU
33	2x	32	THR
33	2x	41	LEU
33	2x	60	VAL
33	2x	62	VAL
33	2x	96	ARG
34	1b	9	GLU
34	1b	17	PHE
34	1b	19	HIS
34	1b	21	ARG
34	1b	22	LYS
34	1b	24	TRP
34	1b	28	PHE
34	1b	35	GLU
34	1b	44	LEU
34	1b	45	GLN
34	1b	67	THR
34	1b	71	VAL
34	1b	73	THR
34	1b	76	GLN
34	1b	82	ARG
34	1b	111	ARG
34	1b	122	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	1b	128	GLU
34	1b	130	ARG
34	1b	136	VAL
34	1b	157	ARG
34	1b	160	ASP
34	1b	178	ARG
34	1b	185	ILE
34	1b	187	LEU
34	1b	200	ILE
34	1b	201	ILE
34	1b	208	ILE
34	1b	226	ARG
35	1c	36	ASP
35	1c	38	ARG
35	1c	104	GLN
36	1d	8	VAL
36	1d	25	ARG
36	1d	28	SER
36	1d	31	CYS
36	1d	58	LEU
36	1d	59	ARG
36	1d	86	LYS
36	1d	107	ARG
36	1d	110	PHE
36	1d	127	THR
36	1d	135	LEU
36	1d	168	ARG
36	1d	173	TRP
36	1d	182	LYS
36	1d	194	LEU
36	1d	196	LEU
37	1e	9	LYS
37	1e	20	GLN
37	1e	24	ARG
37	1e	31	LEU
37	1e	34	VAL
37	1e	41	VAL
37	1e	75	THR
37	1e	91	LEU
37	1e	116	THR
37	1e	120	THR
38	1f	17	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	1f	40	VAL
38	1f	57	GLN
38	1f	73	ASN
39	1g	9	VAL
39	1g	15	ASP
39	1g	21	VAL
39	1g	97	GLN
39	1g	110	GLN
39	1g	115	ARG
39	1g	144	MET
40	1h	39	LEU
40	1h	52	ASP
40	1h	63	LEU
40	1h	68	ARG
40	1h	97	VAL
40	1h	104	ARG
40	1h	112	LEU
40	1h	120	THR
41	1i	42	ARG
41	1i	50	LEU
41	1i	53	VAL
41	1i	60	ASP
41	1i	81	ILE
41	1i	92	TYR
41	1i	103	THR
41	1i	125	TYR
42	1j	5	ARG
42	1j	42	THR
42	1j	56	HIS
42	1j	67	THR
42	1j	84	GLN
42	1j	100	THR
43	1k	31	THR
43	1k	70	LYS
43	1k	109	VAL
44	1l	18	VAL
44	1l	27	LEU
44	1l	33	ARG
44	1l	60	LEU
45	1m	8	GLU
45	1m	12	ASN
45	1m	19	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1m	49	THR
45	1m	55	ARG
45	1m	56	LEU
45	1m	70	LEU
45	1m	80	ARG
45	1m	102	ARG
46	1n	3	ARG
46	1n	12	ARG
46	1n	18	VAL
46	1n	32	SER
46	1n	33	VAL
46	1n	44	LEU
47	1o	3	ILE
47	1o	5	LYS
47	1o	28	GLN
47	1o	39	LEU
47	1o	66	LEU
47	1o	88	ARG
48	1p	2	VAL
48	1p	5	ARG
48	1p	8	ARG
48	1p	42	ARG
48	1p	45	THR
48	1p	54	GLU
48	1p	62	VAL
48	1p	67	THR
48	1p	69	THR
49	1q	9	VAL
49	1q	63	ARG
49	1q	70	ARG
50	1r	31	LEU
50	1r	37	VAL
50	1r	47	THR
50	1r	76	LEU
50	1r	85	LEU
51	1s	4	SER
51	1s	16	LEU
51	1s	28	LYS
51	1s	37	ARG
51	1s	40	ILE
51	1s	41	VAL
51	1s	77	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	1s	79	THR
52	1t	9	ASN
52	1t	10	LEU
52	1t	34	LYS
52	1t	58	LYS
52	1t	62	LEU
52	1t	84	LEU
53	1u	9	ARG
53	1u	24	ARG
33	1x	3	MET
33	1x	23	ARG
33	1x	24	LEU
33	1x	46	GLN
33	1x	87	LYS
54	1y	6	TYR
3	2D	3	VAL
3	2D	37	LEU
3	2D	38	LYS
3	2D	61	LEU
3	2D	89	SER
3	2D	94	LEU
3	2D	99	ASP
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	141	VAL
3	2D	142	VAL
3	2D	155	LEU
3	2D	169	GLU
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	274	ARG
3	2D	275	LYS
3	2D	276	LYS
4	2E	7	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	2E	24	THR
4	2E	33	VAL
4	2E	34	VAL
4	2E	49	LEU
4	2E	75	VAL
4	2E	78	LEU
4	2E	87	GLU
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	24	LEU
5	2F	33	LEU
5	2F	53	THR
5	2F	57	VAL
5	2F	60	SER
5	2F	74	ARG
5	2F	88	VAL
5	2F	125	LEU
5	2F	132	VAL
5	2F	140	LEU
5	2F	144	LYS
5	2F	170	LEU
5	2F	175	THR
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	28	VAL
6	2G	49	ASP
6	2G	60	LEU
6	2G	71	THR
6	2G	79	ASN
6	2G	126	ASP
6	2G	159	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	2G	165	THR
7	2H	6	ARG
7	2H	13	LYS
7	2H	15	VAL
7	2H	23	ARG
7	2H	33	LEU
7	2H	47	GLU
7	2H	85	LYS
7	2H	88	LEU
7	2H	105	LEU
7	2H	122	THR
7	2H	134	SER
7	2H	136	ILE
7	2H	139	GLN
8	2I	5	LEU
8	2I	9	LEU
8	2I	15	VAL
8	2I	38	LEU
8	2I	44	LEU
8	2I	69	LYS
8	2I	75	LEU
8	2I	87	LYS
8	2I	99	GLU
8	2I	116	LEU
8	2I	121	LYS
8	2I	123	LEU
8	2I	140	LEU
9	2N	12	ARG
9	2N	28	THR
9	2N	33	LEU
9	2N	34	LEU
9	2N	46	VAL
9	2N	48	MET
9	2N	59	LYS
9	2N	62	VAL
9	2N	67	LEU
9	2N	68	GLU
9	2N	73	THR
9	2N	87	LEU
9	2N	97	ARG
9	2N	99	LEU
10	2O	10	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	2O	24	VAL
10	2O	66	LYS
10	2O	90	GLN
10	2O	98	VAL
10	2O	108	GLU
11	2P	2	LYS
11	2P	3	LEU
11	2P	30	THR
11	2P	32	THR
11	2P	59	LEU
11	2P	76	LYS
11	2P	83	VAL
11	2P	99	LEU
11	2P	112	LEU
11	2P	125	VAL
12	2Q	2	LEU
12	2Q	7	MET
12	2Q	16	ARG
12	2Q	18	LYS
12	2Q	21	THR
12	2Q	22	LYS
12	2Q	59	ARG
12	2Q	75	THR
12	2Q	106	VAL
13	2R	18	LEU
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	86	ARG
13	2R	96	ARG
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
13	2R	117	VAL
14	2S	14	VAL
14	2S	17	ARG
14	2S	21	THR
14	2S	36	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	2S	50	SER
14	2S	52	SER
14	2S	68	GLN
14	2S	75	GLU
14	2S	85	VAL
15	2T	28	VAL
15	2T	39	ARG
15	2T	49	VAL
15	2T	65	LYS
15	2T	74	ARG
15	2T	96	ARG
16	2U	5	LYS
16	2U	31	SER
16	2U	59	ARG
16	2U	74	LEU
16	2U	83	LEU
16	2U	89	GLU
17	2V	35	LEU
17	2V	46	VAL
17	2V	51	VAL
17	2V	52	VAL
17	2V	53	GLU
17	2V	72	VAL
17	2V	79	VAL
17	2V	82	ARG
17	2V	98	GLU
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	27	LYS
18	2W	100	THR
18	2W	107	LEU
19	2X	57	LEU
19	2X	66	LEU
19	2X	88	LYS
19	2X	92	LEU
20	2Y	6	HIS
20	2Y	7	VAL
20	2Y	57	GLN
20	2Y	73	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
20	2Y	88	LYS
21	2Z	18	LEU
21	2Z	33	LEU
21	2Z	41	LEU
21	2Z	42	VAL
21	2Z	46	LYS
21	2Z	61	LEU
21	2Z	72	ARG
21	2Z	86	VAL
21	2Z	107	THR
21	2Z	131	ARG
21	2Z	136	PHE
21	2Z	150	LEU
21	2Z	161	VAL
21	2Z	170	THR
21	2Z	182	LYS
21	2Z	193	GLU
22	20	9	SER
22	20	10	THR
22	20	14	ARG
22	20	39	ARG
22	20	55	ARG
23	21	3	LYS
23	21	4	VAL
23	21	21	ARG
23	21	30	VAL
23	21	59	THR
23	21	62	VAL
23	21	75	GLU
23	21	85	LEU
23	21	95	LEU
24	22	53	LEU
25	23	23	LEU
25	23	31	LEU
25	23	54	VAL
26	24	13	ARG
26	24	53	GLU
26	24	56	VAL
26	24	61	ARG
26	24	63	TYR
26	24	69	LYS
27	25	15	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	25	16	ARG
27	25	29	THR
28	26	6	ARG
28	26	14	THR
28	26	19	ARG
28	26	48	VAL
29	27	1	MET
29	27	43	THR
30	28	14	VAL
30	28	23	VAL
30	28	31	HIS
30	28	34	TRP
30	28	46	ARG
34	2b	10	LEU
34	2b	17	PHE
34	2b	23	ARG
34	2b	24	TRP
34	2b	28	PHE
34	2b	45	GLN
34	2b	82	ARG
34	2b	94	ASN
34	2b	111	ARG
34	2b	114	ARG
34	2b	126	GLU
34	2b	128	GLU
34	2b	135	GLN
34	2b	154	LEU
34	2b	157	ARG
34	2b	158	LEU
34	2b	175	ARG
34	2b	200	ILE
34	2b	208	ILE
34	2b	222	ILE
34	2b	224	GLN
34	2b	226	ARG
34	2b	230	VAL
35	2c	3	ASN
35	2c	15	THR
35	2c	16	ARG
35	2c	32	LEU
35	2c	44	GLU
35	2c	45	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	2c	82	GLU
35	2c	105	GLU
35	2c	115	LEU
35	2c	127	ARG
35	2c	131	ARG
35	2c	152	ILE
35	2c	162	GLN
35	2c	192	THR
36	2d	8	VAL
36	2d	13	ARG
36	2d	28	SER
36	2d	31	CYS
36	2d	34	GLU
36	2d	58	LEU
36	2d	59	ARG
36	2d	65	ARG
36	2d	107	ARG
36	2d	108	LEU
36	2d	127	THR
36	2d	135	LEU
36	2d	150	GLU
36	2d	178	VAL
36	2d	194	LEU
37	2e	24	ARG
37	2e	31	LEU
37	2e	34	VAL
37	2e	40	ARG
37	2e	41	VAL
37	2e	69	VAL
37	2e	72	GLN
37	2e	91	LEU
37	2e	150	ARG
38	2f	17	SER
38	2f	40	VAL
38	2f	63	TYR
38	2f	72	VAL
38	2f	73	ASN
38	2f	94	GLN
39	2g	13	GLN
39	2g	15	ASP
39	2g	50	ILE
39	2g	104	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	2g	113	GLU
39	2g	115	ARG
39	2g	138	LYS
40	2h	54	ASP
40	2h	63	LEU
40	2h	91	ARG
40	2h	97	VAL
40	2h	104	ARG
40	2h	112	LEU
41	2i	7	THR
41	2i	64	THR
41	2i	65	VAL
41	2i	66	ARG
41	2i	87	GLN
41	2i	103	THR
41	2i	125	TYR
41	2i	127	LYS
42	2j	25	GLU
42	2j	38	ILE
42	2j	45	ARG
42	2j	92	THR
43	2k	14	VAL
43	2k	18	ARG
43	2k	28	THR
43	2k	48	ILE
43	2k	84	VAL
43	2k	103	LEU
43	2k	109	VAL
43	2k	112	THR
43	2k	114	VAL
44	2l	18	VAL
44	2l	33	ARG
44	2l	52	LEU
44	2l	60	LEU
44	2l	89	ARG
44	2l	116	SER
44	2l	117	ARG
45	2m	3	ARG
45	2m	4	ILE
45	2m	12	ASN
45	2m	14	ARG
45	2m	19	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	2m	63	THR
45	2m	65	LYS
45	2m	70	LEU
45	2m	88	ARG
45	2m	110	ARG
46	2n	12	ARG
46	2n	32	SER
46	2n	44	LEU
47	2o	5	LYS
47	2o	10	LYS
47	2o	39	LEU
47	2o	64	ARG
47	2o	66	LEU
48	2p	2	VAL
48	2p	8	ARG
48	2p	25	ARG
48	2p	42	ARG
48	2p	45	THR
48	2p	54	GLU
48	2p	62	VAL
48	2p	67	THR
48	2p	69	THR
48	2p	72	ARG
48	2p	76	GLN
49	2q	6	LEU
49	2q	9	VAL
49	2q	16	GLN
49	2q	63	ARG
49	2q	70	ARG
49	2q	74	LEU
49	2q	87	LYS
50	2r	25	THR
50	2r	76	LEU
50	2r	85	LEU
50	2r	86	VAL
51	2s	13	ASP
51	2s	27	GLU
51	2s	56	GLN
51	2s	77	THR
51	2s	79	THR
52	2t	15	ARG
52	2t	24	LEU

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Mol	Chain	Res	Type
52	2t	38	LYS
52	2t	45	GLN
52	2t	62	LEU
52	2t	74	LYS
52	2t	84	LEU
52	2t	89	ARG
54	2y	5	SER
54	2y	6	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) 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	69	HIS
5	1F	75	HIS
5	1F	203	GLN
6	1G	108	ASN
7	1H	139	GLN
8	1I	105	HIS
10	1O	3	GLN
10	1O	5	GLN
14	1S	95	HIS
15	1T	58	ASN
16	1U	104	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	34	ASN
21	1Z	73	GLN
21	1Z	151	HIS
24	12	9	GLN
25	13	32	GLN
26	14	60	GLN
33	2x	33	HIS
33	2x	79	ASN
35	1c	6	HIS
35	1c	102	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	1c	104	GLN
36	1d	77	ASN
36	1d	119	GLN
36	1d	123	HIS
36	1d	125	HIS
36	1d	129	ASN
38	1f	73	ASN
38	1f	100	ASN
39	1g	28	ASN
39	1g	110	GLN
40	1h	82	HIS
41	1i	3	GLN
41	1i	58	HIS
41	1i	73	GLN
42	1j	56	HIS
42	1j	84	GLN
44	1l	99	HIS
47	1o	28	GLN
48	1p	13	HIS
49	1q	16	GLN
49	1q	26	GLN
51	1s	69	HIS
51	1s	83	HIS
52	1t	18	GLN
33	1x	38	HIS
3	2D	87	ASN
3	2D	126	GLN
3	2D	253	GLN
5	2F	69	HIS
5	2F	75	HIS
6	2G	26	GLN
9	2N	8	GLN
12	2Q	12	GLN
12	2Q	123	HIS
15	2T	58	ASN
16	2U	104	GLN
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	34	ASN
21	2Z	73	GLN

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Mol	Chain	Res	Type
22	20	50	ASN
22	20	70	GLN
25	23	32	GLN
26	24	46	GLN
34	2b	19	HIS
34	2b	78	GLN
35	2c	6	HIS
35	2c	162	GLN
36	2d	77	ASN
36	2d	116	GLN
36	2d	119	GLN
36	2d	123	HIS
36	2d	125	HIS
36	2d	161	ASN
37	2e	72	GLN
38	2f	94	GLN
38	2f	100	ASN
39	2g	28	ASN
39	2g	86	GLN
41	2i	3	GLN
41	2i	58	HIS
41	2i	117	HIS
42	2j	69	ASN
43	2k	117	ASN
44	2l	99	HIS
47	2o	28	GLN
48	2p	16	HIS
49	2q	26	GLN
51	2s	14	HIS
51	2s	65	ASN

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	396 (13%)	51 (1%)
1	2A	2856/2915 (97%)	414 (14%)	49 (1%)
2	1B	119/120 (99%)	5 (4%)	0
2	2B	118/120 (98%)	5 (4%)	0
32	1a	1494/1521 (98%)	319 (21%)	0
32	2a	1498/1521 (98%)	305 (20%)	0
All	All	8950/9112 (98%)	1444 (16%)	100 (1%)

All (1444) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
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	185	A
1	1A	188	A
1	1A	189	U
1	1A	194	G
1	1A	202	A
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	255	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	304	C
1	1A	335	A
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	455	A
1	1A	474	U
1	1A	480	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	482	C
1	1A	483	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
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	609	A
1	1A	615	G
1	1A	618	C
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	633	G
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	693	G
1	1A	697	C
1	1A	698	G
1	1A	715	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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	831	A
1	1A	832	G
1	1A	836	A
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	934	A
1	1A	936	C
1	1A	937	A
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	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	1089	C
1	1A	1090	G
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1106	U
1	1A	1107	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1108	G
1	1A	1109	G
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	1121	C
1	1A	1122	C
1	1A	1123	A
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	1137	G
1	1A	1139	G
1	1A	1142	A
1	1A	1143	U
1	1A	1154	U
1	1A	1155	C
1	1A	1156	G
1	1A	1158	G
1	1A	1162	C
1	1A	1174	A
1	1A	1180	C
1	1A	1181	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	1232	G
1	1A	1256	U
1	1A	1263	C
1	1A	1265	A
1	1A	1299	A
1	1A	1302	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	1406	A
1	1A	1411	A
1	1A	1430	A
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	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1571	G
1	1A	1578	C
1	1A	1589	A
1	1A	1590	C
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	1787	G
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	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1918	G
1	1A	1922	A
1	1A	1927	C
1	1A	1928	G
1	1A	1935	A
1	1A	1936	C
1	1A	1937	5MU
1	1A	1942	OMC
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C
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	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	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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2180	A
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2194	U
1	1A	2195	A
1	1A	2206	G
1	1A	2208	G
1	1A	2209	G
1	1A	2211	U
1	1A	2212	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
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	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	2332	A
1	1A	2333	G
1	1A	2334	A
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	2405	A
1	1A	2418	U
1	1A	2426	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2532	C
1	1A	2541	G
1	1A	2561	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	2614	A
1	1A	2615	G
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2642	G
1	1A	2666	A
1	1A	2675	G
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2746	A
1	1A	2770	A
1	1A	2771	A
1	1A	2774	G
1	1A	2777	A
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	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2903	G
2	1B	45	A
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	32	A
32	1a	33	A
32	1a	39	G
32	1a	44	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
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	110	C
32	1a	115	G
32	1a	116	A
32	1a	121	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	131	C
32	1a	135	C
32	1a	143	A
32	1a	163	C
32	1a	164	U
32	1a	166	G
32	1a	173	U
32	1a	174	C
32	1a	179	A
32	1a	181	G
32	1a	182	U
32	1a	189(D)	C
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	218	C
32	1a	219	C
32	1a	222	U
32	1a	227	G
32	1a	231	G
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	270	A
32	1a	289	G
32	1a	298	A
32	1a	301	G
32	1a	309	G
32	1a	321	A
32	1a	328	C
32	1a	331	G
32	1a	332	G
32	1a	346	G
32	1a	348	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	385	C
32	1a	388	G
32	1a	398	C
32	1a	406	G
32	1a	410	G
32	1a	411	A
32	1a	412	A
32	1a	413	G
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	436	C
32	1a	439	A
32	1a	452	A
32	1a	454	C
32	1a	455	C
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	475	G
32	1a	480	U
32	1a	485	G
32	1a	487	A
32	1a	490	G
32	1a	495	A
32	1a	496	A
32	1a	498	U
32	1a	499	A
32	1a	500	G
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	561	U
32	1a	563	A
32	1a	570	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	590	C
32	1a	592	G
32	1a	618	C
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	633	G
32	1a	634	C
32	1a	639	G
32	1a	653	A
32	1a	659	U
32	1a	660	G
32	1a	661	G
32	1a	665	A
32	1a	666	G
32	1a	671	G
32	1a	672	U
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	692	U
32	1a	722	A
32	1a	723	U
32	1a	733	A
32	1a	755	G
32	1a	759	A
32	1a	765	G
32	1a	774	G
32	1a	777	A
32	1a	793	U
32	1a	794	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	802	A
32	1a	805	C
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	853	G
32	1a	863	U
32	1a	872	A
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	931	C
32	1a	933	G
32	1a	934	C
32	1a	935	A
32	1a	937	A
32	1a	938	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	966	M2G
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	984	C
32	1a	990	C
32	1a	992	U
32	1a	993	G
32	1a	998	G
32	1a	1006	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1009	G
32	1a	1012	U
32	1a	1017	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1031	G
32	1a	1032	G
32	1a	1033	G
32	1a	1034	G
32	1a	1037	C
32	1a	1042	G
32	1a	1044	A
32	1a	1046	A
32	1a	1053	G
32	1a	1056	U
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	1086	U
32	1a	1094	G
32	1a	1101	A
32	1a	1117	G
32	1a	1120	G
32	1a	1123	A
32	1a	1125	U
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1135	U
32	1a	1136	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1145	C
32	1a	1146	A
32	1a	1150	U
32	1a	1152	A
32	1a	1155	G
32	1a	1157	A
32	1a	1159	U
32	1a	1168	A
32	1a	1176	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	1202	G
32	1a	1204	A
32	1a	1208	C
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1218	C
32	1a	1223	C
32	1a	1224	G
32	1a	1227	A
32	1a	1232	U
32	1a	1238	A
32	1a	1240	U
32	1a	1241	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1269	A
32	1a	1270	C
32	1a	1272	G
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1303	C
32	1a	1305	G
32	1a	1317	C
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	1361	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1368	G
32	1a	1370	G
32	1a	1377	A
32	1a	1378	C
32	1a	1383	C
32	1a	1397	C
32	1a	1409	C
32	1a	1418	A
32	1a	1419	G
32	1a	1441	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1452	C
32	1a	1456	G
32	1a	1464	G
32	1a	1479	C
32	1a	1487	G
32	1a	1491	G
32	1a	1493	A
32	1a	1497	G
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1507	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1517	G
32	1a	1520	G
32	1a	1523	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	10	G
1	2A	11	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	196	A
1	2A	199	A
1	2A	200	U
1	2A	205	G
1	2A	213	A
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
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	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	280	C
1	2A	311	A
1	2A	327	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	405	U
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	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	595	C
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	610	G
1	2A	614(B)	G
1	2A	615	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	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	857	C
1	2A	859	G
1	2A	866	A
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	896	A
1	2A	900	A
1	2A	901	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
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1033	U
1	2A	1042	G
1	2A	1043	C
1	2A	1044	G
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	1080	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
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1093	G
1	2A	1094	U
1	2A	1095	A
1	2A	1096	A
1	2A	1097	U
1	2A	1108	U
1	2A	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1128	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1171	G
1	2A	1187	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	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1525	G
1	2A	1531	C
1	2A	1542	A
1	2A	1543	C
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	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	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1722	A
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1839	G
1	2A	1847	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	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2039	C
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	2101	G
1	2A	2103	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2110	G
1	2A	2112	G
1	2A	2115	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	2144	U
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	2161	C
1	2A	2162	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
1	2A	2190	G
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2225	A
1	2A	2239	G
1	2A	2268	A
1	2A	2269	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	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	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
1	2A	2474	C
1	2A	2476	A
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2529	G
1	2A	2549	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	2601	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	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2820	A
1	2A	2821	A
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2B	45	A
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	13	U
32	2a	25	C
32	2a	26	A
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	59	A
32	2a	60	A
32	2a	61	G
32	2a	65	U
32	2a	66	G
32	2a	80	G
32	2a	89	C
32	2a	91	C
32	2a	98	G
32	2a	105	G
32	2a	112	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	143	A
32	2a	144	G
32	2a	146	G
32	2a	151	A
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	195	A
32	2a	197	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	240	C
32	2a	245	C
32	2a	247	G
32	2a	251	G
32	2a	257	G
32	2a	258	G
32	2a	262	A
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	298	A
32	2a	309	G
32	2a	320	C
32	2a	321	A
32	2a	328	C
32	2a	332	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	388	G
32	2a	393	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	410	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	445	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	450	G
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	473	G
32	2a	474	G
32	2a	476	G
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	500	G
32	2a	502	G
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	532	A
32	2a	533	A
32	2a	536	C
32	2a	547	A
32	2a	558	G
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C
32	2a	570	G
32	2a	571	U
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	587	G
32	2a	596	C
32	2a	597	G
32	2a	606	G
32	2a	608	A
32	2a	616	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	618	C
32	2a	630	G
32	2a	632	A
32	2a	633	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	693	G
32	2a	702	A
32	2a	718	G
32	2a	723	U
32	2a	724	G
32	2a	728	A
32	2a	731	G
32	2a	737	A
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	777	A
32	2a	782	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	819	A
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	829	G
32	2a	830	G
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	870	U
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	934	C
32	2a	935	A
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
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	978	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	1001(A)	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1009	G
32	2a	1011	G
32	2a	1012	U
32	2a	1020	U
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	1041	A
32	2a	1044	A
32	2a	1052	U
32	2a	1054	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1063	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1079	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1115	C
32	2a	1117	G
32	2a	1123	A
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1147	C
32	2a	1152	A
32	2a	1154	G
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1162	C
32	2a	1165	C
32	2a	1170	A
32	2a	1171	G
32	2a	1183	A
32	2a	1184	G
32	2a	1189	C
32	2a	1196	U
32	2a	1197	G
32	2a	1213	A
32	2a	1217	C
32	2a	1224	G
32	2a	1227	A
32	2a	1238	A
32	2a	1250	A
32	2a	1256	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1261	A
32	2a	1267	C
32	2a	1270	C
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A
32	2a	1290	G
32	2a	1293	G
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1312	G
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1368	G
32	2a	1370	G
32	2a	1378	C
32	2a	1381	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1445	C
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1487	G
32	2a	1489	G
32	2a	1492	A
32	2a	1493	A
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	1528	U
32	2a	1529	G
32	2a	1530	G
32	2a	1532	U

All (100) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	793	A
1	1A	811	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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1099	C
1	1A	1115	A
1	1A	1116	A
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	1346	U
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	2227	G
1	1A	2347	A
1	1A	2418	U
1	1A	2434	A
1	1A	2442	A
1	1A	2451	A
1	1A	2613	C
1	1A	2623	U
1	1A	2701	U
1	1A	2769	U
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	573	G
1	2A	685	A
1	2A	746	A
1	2A	752	A
1	2A	764	A

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Mol	Chain	Res	Type
1	2A	776	G
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	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	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	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1608	A
1	2A	1992	G
1	2A	1997	G
1	2A	2126	A
1	2A	2158	A
1	2A	2172	U
1	2A	2308	G
1	2A	2335	A
1	2A	2406	U
1	2A	2422	A
1	2A	2439	A
1	2A	2601	C
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	5MC	2A	1962	55,1	18,22,23	1.16	4 (22%)	26,32,35	1.49	4 (15%)
32	5MC	2a	1400	32	18,22,23	0.90	0	26,32,35	1.36	5 (19%)
32	MA6	2a	1519	32	19,26,27	1.13	2 (10%)	18,38,41	4.93	3 (16%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	22,30,33	1.71	5 (22%)
1	OMU	1A	2564	55,1	19,22,23	6.38	9 (47%)	26,31,34	2.90	11 (42%)
32	4OC	2a	1402	32	20,23,24	2.61	7 (35%)	26,32,35	1.13	2 (7%)
32	5MC	1a	1404	32	18,22,23	1.23	3 (16%)	26,32,35	1.41	3 (11%)
32	G7M	1a	527	55,32	20,26,27	2.89	4 (20%)	17,39,42	0.81	1 (5%)
1	PSU	2A	1911	1	18,21,22	1.42	3 (16%)	22,30,33	1.38	2 (9%)
32	M2G	1a	966	32	20,27,28	2.87	5 (25%)	22,40,43	1.46	6 (27%)
1	OMG	1A	2263	55,1	18,26,27	1.77	6 (33%)	19,38,41	1.51	5 (26%)
1	OMU	2A	2552	55,1	19,22,23	6.64	10 (52%)	26,31,34	2.69	8 (30%)
1	5MC	1A	1964	1	18,22,23	0.99	1 (5%)	26,32,35	1.16	3 (11%)
32	UR3	1a	1498	32	19,22,23	1.89	4 (21%)	26,32,35	1.40	3 (11%)
1	5MC	2A	1942	1	18,22,23	1.02	1 (5%)	26,32,35	1.14	3 (11%)
1	2MA	1A	2515	55,1	17,25,26	1.58	5 (29%)	17,37,40	1.93	3 (17%)
1	PSU	1A	1933	1	18,21,22	1.41	3 (16%)	22,30,33	1.47	3 (13%)
32	5MC	1a	967	32	18,22,23	1.04	2 (11%)	26,32,35	1.33	4 (15%)
32	5MC	2a	1404	32	18,22,23	1.06	2 (11%)	26,32,35	1.44	4 (15%)
1	PSU	1A	2617	1	18,21,22	1.64	4 (22%)	22,30,33	1.78	5 (22%)
32	MA6	1a	1518	32	19,26,27	1.05	1 (5%)	18,38,41	4.70	3 (16%)
32	PSU	1a	516	32	18,21,22	1.43	3 (16%)	22,30,33	2.05	4 (18%)
32	2MG	1a	1207	55,32	18,26,27	1.97	4 (22%)	16,38,41	1.83	5 (31%)
1	5MU	2A	1915	1	19,22,23	1.75	3 (15%)	28,32,35	1.59	5 (17%)
1	OMC	2A	1920	1	19,22,23	2.43	7 (36%)	26,31,34	1.01	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.34	2 (11%)	22,30,33	1.72	5 (22%)
32	G7M	2a	527	32	20,26,27	3.15	6 (30%)	17,39,42	0.97	2 (11%)
32	5MC	2a	1407	32	18,22,23	1.24	1 (5%)	26,32,35	1.42	3 (11%)
1	5MU	1A	1961	55,1	19,22,23	1.00	2 (10%)	28,32,35	1.48	4 (14%)
44	0TD	1l	92	44	7,9,10	2.06	2 (28%)	6,11,13	4.14	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	4OC	1a	1402	32	20,23,24	2.41	7 (35%)	26,32,35	0.78	0
32	5MC	2a	967	32	18,22,23	0.97	1 (5%)	26,32,35	1.66	4 (15%)
1	OMG	2A	2251	55,1	18,26,27	1.73	3 (16%)	19,38,41	1.64	5 (26%)
32	PSU	2a	516	32	18,21,22	1.84	3 (16%)	22,30,33	2.03	5 (22%)
1	OMC	1A	1942	55,1	19,22,23	2.18	6 (31%)	26,31,34	1.01	3 (11%)
1	PSU	1A	1939	55,1	18,21,22	1.35	2 (11%)	22,30,33	1.75	5 (22%)
32	MA6	2a	1518	32	19,26,27	1.05	1 (5%)	18,38,41	4.81	3 (16%)
32	2MG	2a	1207	32	18,26,27	1.92	4 (22%)	16,38,41	1.12	2 (12%)
1	5MU	2A	1939	55,1	19,22,23	0.91	1 (5%)	28,32,35	1.37	4 (14%)
1	5MC	1A	1984	1	18,22,23	1.11	2 (11%)	26,32,35	1.68	5 (19%)
32	5MC	1a	1400	32	18,22,23	1.03	1 (5%)	26,32,35	1.61	6 (23%)
32	5MC	1a	1407	32	18,22,23	1.37	1 (5%)	26,32,35	1.51	5 (19%)
32	MA6	1a	1519	32	19,26,27	1.03	2 (10%)	18,38,41	4.46	3 (16%)
1	5MU	1A	1937	1	19,22,23	1.43	2 (10%)	28,32,35	1.58	6 (21%)
32	M2G	2a	966	32	20,27,28	3.02	7 (35%)	22,40,43	1.37	3 (13%)
44	0TD	2l	92	44	7,9,10	2.21	1 (14%)	6,11,13	2.99	4 (66%)
32	UR3	2a	1498	32	19,22,23	1.89	4 (21%)	26,32,35	1.48	4 (15%)
1	2MA	2A	2503	55,1	17,25,26	1.54	2 (11%)	17,37,40	1.11	2 (11%)

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	5MC	2A	1962	55,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	2/7/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2564	55,1	-	0/9/27/28	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	55,32	-	1/3/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	OMG	1A	2263	55,1	-	0/5/27/28	0/3/3/3
1	OMU	2A	2552	55,1	-	0/9/27/28	0/2/2/2
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	55,1	-	1/3/25/26	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	PSU	1a	516	32	-	2/7/25/26	0/2/2/2
32	2MG	1a	1207	55,32	-	0/5/27/28	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	1/3/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	55,1	-	0/7/25/26	0/2/2/2
44	0TD	1l	92	44	-	4/7/12/14	-
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
32	PSU	2a	516	32	-	3/7/25/26	0/2/2/2
1	OMC	1A	1942	55,1	-	3/9/27/28	0/2/2/2
1	PSU	1A	1939	55,1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	5MU	2A	1939	55,1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	1	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	5/7/29/30	0/3/3/3
1	5MU	1A	1937	1	-	4/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
44	0TD	2l	92	44	-	2/7/12/14	-
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	55,1	-	1/3/25/26	0/3/3/3

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	C4-N3	-15.09	1.11	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2564	OMU	C4-N3	-14.97	1.11	1.38
1	2A	2552	OMU	C5-C4	14.92	1.76	1.43
1	1A	2564	OMU	C5-C4	13.65	1.73	1.43
1	1A	2564	OMU	C6-C5	-11.10	1.09	1.35
1	2A	2552	OMU	C6-C5	-10.45	1.10	1.35
32	2a	966	M2G	C2-N3	10.42	1.43	1.30
32	1a	966	M2G	C2-N3	10.26	1.43	1.30
32	2a	527	G7M	C8-N9	8.77	1.49	1.33
32	1a	527	G7M	C8-N9	8.59	1.48	1.33
1	2A	2552	OMU	C3'-C2'	-8.50	1.34	1.52
32	2a	527	G7M	C8-N7	8.13	1.48	1.33
1	2A	2552	OMU	C6-N1	8.05	1.57	1.38
1	1A	2564	OMU	C6-N1	7.45	1.56	1.38
1	1A	2564	OMU	C3'-C2'	-7.40	1.36	1.52
32	1a	527	G7M	C8-N7	7.27	1.46	1.33
1	2A	2552	OMU	O4'-C4'	-6.78	1.29	1.45
1	1A	2564	OMU	O4'-C4'	-6.33	1.30	1.45
1	2A	2552	OMU	O4'-C1'	6.14	1.56	1.42
1	1A	2564	OMU	O4'-C1'	6.04	1.56	1.42
32	2a	1402	4OC	C4-N4	5.91	1.48	1.35
32	2a	516	PSU	C2-N1	5.79	1.44	1.36
32	1a	1402	4OC	C4-N4	5.76	1.47	1.35
1	2A	1915	5MU	C2-N1	5.75	1.47	1.38
1	1A	2564	OMU	C1'-N1	-5.74	1.31	1.47
1	2A	1920	OMC	C4-N4	5.68	1.47	1.33
1	2A	2552	OMU	C1'-N1	-5.40	1.32	1.47
1	1A	1942	OMC	C4-N4	5.19	1.46	1.33
32	2a	1498	UR3	C6-C5	5.12	1.46	1.35
32	2a	1402	4OC	C2-N3	4.99	1.46	1.36
32	2a	966	M2G	C2-N2	4.89	1.44	1.35
1	1A	1937	5MU	C2-N1	4.82	1.46	1.38
1	2A	1920	OMC	C6-C5	4.75	1.46	1.35
32	1a	1498	UR3	C6-C5	4.74	1.46	1.35
44	2l	92	0TD	CB-SB	-4.73	1.77	1.82
32	1a	1207	2MG	C2-N1	4.72	1.44	1.36
32	2a	1207	2MG	C2-N1	4.66	1.44	1.36
32	2a	1402	4OC	C6-C5	4.65	1.45	1.35
32	1a	1407	5MC	C2-N1	4.60	1.50	1.40
32	1a	1207	2MG	C2-N2	4.52	1.43	1.33
32	1a	966	M2G	C2-N2	4.44	1.43	1.35
1	2A	1920	OMC	C2-N3	4.41	1.45	1.36
32	2a	1207	2MG	C2-N2	4.38	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	527	G7M	C2-N3	4.37	1.43	1.33
1	2A	1917	PSU	C2-N1	4.30	1.42	1.36
1	1A	1942	OMC	C6-C5	4.14	1.44	1.35
32	1a	1498	UR3	C2-N1	4.09	1.44	1.38
44	1l	92	0TD	CB-SB	-4.09	1.78	1.82
32	2a	1402	4OC	C4-N3	4.07	1.39	1.32
32	2a	1498	UR3	C2-N3	4.06	1.46	1.39
32	1a	1402	4OC	C4-N3	4.02	1.39	1.32
1	2A	2251	OMG	C2-N3	3.95	1.42	1.33
1	1A	1942	OMC	C2-N3	3.89	1.44	1.36
1	2A	2503	2MA	C2-N3	3.84	1.39	1.31
32	1a	1402	4OC	C6-C5	3.80	1.43	1.35
32	1a	527	G7M	C2-N3	3.80	1.42	1.33
1	2A	2552	OMU	C3'-C4'	3.79	1.62	1.53
32	2a	1407	5MC	C2-N1	3.79	1.48	1.40
1	2A	1911	PSU	C2-N1	3.77	1.41	1.36
1	1A	1939	PSU	C2-N1	3.75	1.41	1.36
32	1a	1498	UR3	C2-N3	3.69	1.46	1.39
32	1a	1402	4OC	O2-C2	-3.67	1.16	1.23
1	2A	1920	OMC	C2-N1	3.61	1.47	1.40
32	1a	1402	4OC	C5-C4	3.61	1.48	1.40
32	1a	1402	4OC	C2-N3	3.61	1.43	1.36
32	2a	1402	4OC	C5-C4	3.59	1.48	1.40
1	1A	1933	PSU	C4-N3	3.57	1.45	1.38
1	1A	2564	OMU	C3'-C4'	3.55	1.62	1.53
1	1A	2263	OMG	C2-N3	3.49	1.41	1.33
1	1A	2263	OMG	C5-C4	-3.47	1.34	1.43
32	2a	527	G7M	C2-N2	3.45	1.42	1.34
32	2a	1207	2MG	C4-N3	3.43	1.45	1.37
32	2a	516	PSU	C6-N1	3.42	1.41	1.36
1	2A	2251	OMG	C5-C4	-3.41	1.34	1.43
32	1a	516	PSU	C6-N1	3.36	1.41	1.36
32	1a	516	PSU	C2-N1	3.35	1.41	1.36
32	2a	1402	4OC	O2-C2	-3.32	1.17	1.23
32	1a	966	M2G	C4-N3	3.31	1.45	1.37
1	1A	1942	OMC	C2-N1	3.28	1.47	1.40
1	1A	2515	2MA	C2-N3	3.27	1.38	1.31
1	2A	2503	2MA	C5-C4	-3.26	1.34	1.43
1	1A	2617	PSU	C6-C5	-3.20	1.31	1.35
32	2a	966	M2G	C4-N3	3.18	1.45	1.37
1	2A	2605	PSU	C2-N1	3.15	1.41	1.36
1	1A	1933	PSU	C2-N1	3.14	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1920	OMC	O2-C2	-3.12	1.17	1.23
1	2A	1915	5MU	C2-N3	3.09	1.43	1.38
32	1a	1207	2MG	C4-N3	3.07	1.44	1.37
32	2a	527	G7M	C4-N3	3.04	1.44	1.37
1	1A	2617	PSU	C1'-C5	-3.02	1.43	1.50
1	1A	1942	OMC	O2-C2	-3.00	1.18	1.23
32	2a	966	M2G	C2-N1	2.96	1.44	1.36
32	1a	1400	5MC	C2-N1	2.95	1.46	1.40
32	1a	966	M2G	C5-C4	-2.92	1.35	1.43
32	1a	527	G7M	C4-N3	2.91	1.44	1.37
1	1A	2617	PSU	C6-N1	2.90	1.41	1.36
32	1a	1404	5MC	CM5-C5	-2.85	1.43	1.50
32	2a	1402	4OC	C2-N1	2.82	1.46	1.40
32	2a	516	PSU	O4'-C1'	-2.82	1.39	1.43
32	2a	1519	MA6	C2-N3	2.77	1.36	1.32
1	1A	1937	5MU	C2-N3	2.75	1.42	1.38
32	2a	1404	5MC	C6-C5	2.73	1.39	1.34
32	1a	1518	MA6	C5-C4	-2.67	1.33	1.40
1	2A	1920	OMC	C5-C4	2.67	1.49	1.42
1	2A	1911	PSU	C6-N1	2.66	1.40	1.36
1	1A	2515	2MA	C5-C4	-2.66	1.36	1.43
32	2a	966	M2G	C6-N1	2.65	1.41	1.37
32	2a	966	M2G	C5-C6	2.64	1.52	1.47
32	2a	966	M2G	C5-C4	-2.64	1.36	1.43
1	1A	2263	OMG	C4-N3	2.64	1.43	1.37
32	1a	966	M2G	C2-N1	2.64	1.43	1.36
32	2a	1519	MA6	C5-C4	-2.61	1.34	1.40
32	2a	527	G7M	C2-N1	2.59	1.44	1.37
1	2A	2605	PSU	C6-N1	2.58	1.40	1.36
1	2A	1911	PSU	C4-N3	2.58	1.43	1.38
32	2a	1518	MA6	C2-N3	2.56	1.36	1.32
1	1A	1964	5MC	C6-C5	2.52	1.38	1.34
1	1A	2617	PSU	O3'-C3'	-2.51	1.37	1.43
1	2A	1962	5MC	CM5-C5	-2.50	1.44	1.50
32	1a	967	5MC	C6-C5	2.48	1.38	1.34
32	2a	1207	2MG	CM2-N2	-2.44	1.41	1.45
1	1A	1961	5MU	C4-C5	-2.43	1.40	1.44
32	2a	1498	UR3	C3U-N3	-2.41	1.42	1.47
1	2A	1917	PSU	C6-N1	2.41	1.40	1.36
1	1A	1939	PSU	C6-N1	2.41	1.40	1.36
1	2A	1962	5MC	C4-N4	2.40	1.40	1.34
32	1a	967	5MC	C2-N3	2.40	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	967	5MC	C6-C5	2.39	1.38	1.34
32	1a	1519	MA6	C2-N3	2.37	1.35	1.32
1	1A	2263	OMG	C2-N2	2.35	1.39	1.34
32	2a	1498	UR3	C2-N1	2.35	1.41	1.38
32	1a	1404	5MC	C4-N4	2.34	1.40	1.34
32	1a	1402	4OC	CM4-N4	-2.33	1.41	1.45
32	1a	1207	2MG	C5-C4	-2.33	1.37	1.43
1	1A	2515	2MA	C2-N1	2.31	1.43	1.36
1	2A	1939	5MU	C5M-C5	-2.30	1.45	1.50
32	1a	1519	MA6	C5-C4	-2.29	1.34	1.40
1	1A	1984	5MC	CM5-C5	-2.27	1.45	1.50
1	2A	1915	5MU	C6-C5	2.26	1.38	1.34
32	1a	516	PSU	O4'-C1'	-2.25	1.40	1.43
1	2A	1942	5MC	C2-N3	2.25	1.40	1.36
1	1A	1942	OMC	C5-C4	2.21	1.48	1.42
1	2A	2552	OMU	O2'-C2'	2.20	1.48	1.42
1	1A	2515	2MA	C8-N7	2.20	1.38	1.35
1	2A	1962	5MC	C2-N3	2.17	1.40	1.36
1	2A	1920	OMC	C4-N3	2.17	1.39	1.34
1	1A	1961	5MU	C5M-C5	-2.16	1.45	1.50
1	1A	2515	2MA	O2'-C2'	-2.16	1.37	1.43
1	2A	2251	OMG	C4-N3	2.16	1.42	1.37
32	1a	1404	5MC	C2-N3	2.15	1.40	1.36
32	2a	1404	5MC	CM5-C5	-2.13	1.45	1.50
44	1l	92	0TD	CA-N	-2.12	1.41	1.47
1	1A	2263	OMG	C8-N7	2.10	1.38	1.35
1	2A	1962	5MC	O2-C2	-2.10	1.19	1.23
1	1A	1933	PSU	C6-N1	2.07	1.39	1.36
1	1A	2263	OMG	C2-N1	2.06	1.42	1.37
32	1a	1498	UR3	O2-C2	-2.03	1.18	1.22
1	1A	1984	5MC	C6-N1	-2.01	1.34	1.38

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1519	MA6	N1-C6-N6	-19.44	96.59	117.06
32	2a	1518	MA6	N1-C6-N6	-19.01	97.05	117.06
32	1a	1518	MA6	N1-C6-N6	-18.08	98.03	117.06
32	1a	1519	MA6	N1-C6-N6	-17.64	98.49	117.06
1	2A	2552	OMU	C5-C4-N3	7.23	125.65	114.84
44	1l	92	0TD	CSB-SB-CB	7.18	115.42	102.44
32	2a	516	PSU	C6-C5-C4	6.82	122.96	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	516	PSU	C6-C5-C4	6.74	122.91	118.20
1	1A	2564	OMU	C5-C4-N3	6.60	124.70	114.84
1	2A	2552	OMU	C4-N3-C2	-6.12	118.51	126.58
32	1a	1518	MA6	C1'-N9-C4	-6.00	116.09	126.64
1	1A	2564	OMU	O4-C4-C5	-5.79	114.98	125.16
32	2a	1518	MA6	C1'-N9-C4	-5.72	116.60	126.64
1	1A	2564	OMU	O2'-C2'-C1'	-5.55	98.25	109.08
1	1A	2515	2MA	CM2-C2-N1	5.47	128.40	116.23
1	1A	2617	PSU	C6-C5-C4	5.45	122.01	118.20
44	1l	92	0TD	CB-CA-N	-5.38	97.63	109.10
32	1a	1498	UR3	C4-N3-C2	-5.27	119.60	124.56
1	1A	1939	PSU	C6-C5-C4	5.23	121.85	118.20
32	1a	1518	MA6	N3-C2-N1	-5.19	120.57	128.68
32	2a	967	5MC	C5-C6-N1	-5.14	118.05	123.34
32	2a	1519	MA6	N3-C2-N1	-5.12	120.68	128.68
1	2A	2605	PSU	C6-C5-C4	4.98	121.68	118.20
32	2a	1519	MA6	C1'-N9-C4	-4.90	118.03	126.64
32	1a	1519	MA6	N3-C2-N1	-4.89	121.04	128.68
44	2l	92	0TD	CSB-SB-CB	4.84	111.20	102.44
1	2A	2552	OMU	O2-C2-N1	-4.84	116.36	122.79
1	2A	1917	PSU	C6-C5-C4	4.77	121.53	118.20
1	1A	1984	5MC	C5-C6-N1	-4.72	118.48	123.34
1	2A	2552	OMU	N3-C2-N1	4.64	121.06	114.89
1	1A	2564	OMU	C4-N3-C2	-4.59	120.52	126.58
32	1a	1404	5MC	C5-C6-N1	-4.37	118.84	123.34
32	2a	1498	UR3	C4-N3-C2	-4.30	120.52	124.56
32	2a	1518	MA6	N3-C2-N1	-4.23	122.07	128.68
1	1A	2515	2MA	C5-C6-N1	4.06	121.03	114.02
32	1a	1519	MA6	C1'-N9-C4	-4.06	119.51	126.64
1	1A	1984	5MC	C4-N3-C2	-4.05	115.21	120.69
1	2A	1962	5MC	C5-C6-N1	-4.05	119.17	123.34
1	1A	1961	5MU	C4-N3-C2	-4.03	122.14	127.35
32	2a	1404	5MC	C5-C6-N1	-4.00	119.22	123.34
32	2a	966	M2G	N1-C2-N2	3.99	121.44	118.04
1	2A	1962	5MC	C4-N3-C2	-3.97	115.33	120.69
32	1a	1407	5MC	C5-C4-N3	3.90	125.89	121.67
1	1A	1933	PSU	C6-C5-C4	3.84	120.88	118.20
1	1A	1984	5MC	C5-C4-N3	3.78	125.75	121.67
1	1A	2564	OMU	C6-C5-C4	-3.77	114.36	119.52
32	1a	967	5MC	C5-C4-N3	3.76	125.73	121.67
44	1l	92	0TD	OD2-CG-CB	3.76	121.27	113.15
32	2a	1407	5MC	C5-C4-N3	3.76	125.73	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1961	5MU	C5-C4-N3	3.75	118.51	115.31
32	2a	1402	4OC	C6-C5-C4	3.68	121.46	116.96
32	1a	516	PSU	C6-N1-C2	-3.66	118.94	122.68
32	1a	1404	5MC	C4-N3-C2	-3.66	115.74	120.69
1	2A	1911	PSU	C6-C5-C4	3.61	120.72	118.20
32	1a	967	5MC	C5-C6-N1	-3.58	119.65	123.34
44	2l	92	0TD	OD2-CG-CB	3.57	120.86	113.15
1	2A	2552	OMU	O4-C4-C5	-3.56	118.91	125.16
32	2a	1400	5MC	C5-C6-N1	-3.55	119.69	123.34
32	1a	1400	5MC	C5-C4-N3	3.53	125.48	121.67
32	1a	1207	2MG	C8-N7-C5	3.52	109.70	102.99
1	2A	1939	5MU	C4-N3-C2	-3.49	122.83	127.35
32	2a	967	5MC	C4-N3-C2	-3.48	115.98	120.69
1	1A	2263	OMG	C8-N7-C5	3.48	109.61	102.99
32	1a	1400	5MC	C1'-N1-C6	-3.42	115.43	121.12
32	2a	1498	UR3	O2-C2-N1	-3.41	114.73	122.72
1	1A	2515	2MA	CM2-C2-N3	-3.33	109.63	119.47
1	1A	2564	OMU	C2'-C1'-N1	-3.33	107.76	114.22
1	1A	2564	OMU	N3-C2-N1	3.31	119.28	114.89
1	1A	2564	OMU	C1'-N1-C2	3.30	123.55	117.57
32	2a	1404	5MC	C4-N3-C2	-3.29	116.24	120.69
1	2A	2251	OMG	C5-C6-N1	3.28	119.73	113.95
1	1A	1937	5MU	C4-N3-C2	-3.26	123.13	127.35
1	2A	2251	OMG	C2-N1-C6	-3.23	119.16	125.10
1	2A	1939	5MU	C6-C5-C4	3.19	120.70	118.03
44	2l	92	0TD	CB-CA-N	-3.19	102.30	109.10
1	2A	1915	5MU	C1'-N1-C2	3.18	123.32	117.57
1	2A	2251	OMG	C8-N7-C5	3.17	109.03	102.99
32	1a	966	M2G	C5-C6-N1	3.17	119.55	113.95
1	1A	2564	OMU	C3'-C2'-C1'	3.16	108.84	102.89
1	2A	1939	5MU	C5-C6-N1	-3.16	120.08	123.34
1	2A	2552	OMU	C6-C5-C4	-3.13	115.23	119.52
1	2A	1917	PSU	O2-C2-N1	-3.13	119.34	122.79
32	2a	1407	5MC	C5-C6-N1	-3.12	120.12	123.34
1	1A	1937	5MU	C6-C5-C4	3.12	120.64	118.03
1	1A	1937	5MU	C1'-N1-C2	3.12	123.22	117.57
32	1a	516	PSU	N1-C2-N3	3.12	118.66	115.13
32	2a	967	5MC	C5-C4-N3	3.11	125.03	121.67
1	1A	1939	PSU	O2-C2-N1	-3.10	119.38	122.79
1	1A	2564	OMU	O2-C2-N1	-3.09	118.68	122.79
32	2a	1400	5MC	C5-C4-N3	3.08	125.00	121.67
32	2a	1404	5MC	C5-C4-N3	3.06	124.97	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	C5-C6-N1	3.04	119.26	114.02
32	1a	966	M2G	N1-C2-N2	3.03	120.62	118.04
1	2A	1915	5MU	C6-C5-C4	3.01	120.55	118.03
32	1a	1207	2MG	C5-C6-N1	3.00	119.25	113.95
32	1a	1400	5MC	CM5-C5-C6	-2.93	118.93	122.85
1	1A	1964	5MC	C5-C6-N1	-2.91	120.35	123.34
1	2A	1942	5MC	C5-C4-N3	2.86	124.76	121.67
32	1a	1400	5MC	C5-C6-N1	-2.84	120.42	123.34
1	1A	1961	5MU	C5-C6-N1	-2.83	120.43	123.34
1	1A	1933	PSU	O2-C2-N1	-2.82	119.69	122.79
32	1a	1207	2MG	O3'-C3'-C4'	2.82	119.20	111.05
32	1a	1407	5MC	N4-C4-N3	-2.81	113.35	118.48
1	1A	2617	PSU	O4-C4-N3	-2.79	114.76	120.12
1	2A	1942	5MC	C5-C6-N1	-2.79	120.47	123.34
32	2a	967	5MC	N4-C4-N3	-2.78	113.40	118.48
32	1a	967	5MC	C4-N3-C2	-2.78	116.93	120.69
1	2A	1915	5MU	C4-N3-C2	-2.77	123.76	127.35
1	1A	1984	5MC	CM5-C5-C6	-2.76	119.16	122.85
32	2a	1407	5MC	C4-N3-C2	-2.75	116.97	120.69
1	1A	1961	5MU	C6-C5-C4	2.73	120.31	118.03
1	2A	1920	OMC	O2-C2-N3	-2.72	117.91	122.33
32	2a	1400	5MC	C4-N3-C2	-2.69	117.05	120.69
32	1a	1400	5MC	C4-N3-C2	-2.68	117.06	120.69
32	1a	1407	5MC	C4-N3-C2	-2.67	117.07	120.69
1	1A	1942	OMC	C2'-C1'-N1	-2.67	109.05	114.22
32	1a	966	M2G	C2-N1-C6	-2.66	119.29	123.71
1	1A	2564	OMU	O4'-C1'-C2'	-2.66	101.91	106.57
1	1A	2263	OMG	N2-C2-N1	2.66	122.37	116.71
32	2a	1207	2MG	C8-N7-C5	2.64	108.03	102.99
44	1l	92	0TD	OD2-CG-OD1	-2.64	118.10	124.09
1	2A	2552	OMU	O4-C4-N3	-2.63	115.44	119.31
32	1a	1407	5MC	CM5-C5-C6	-2.63	119.33	122.85
32	2a	966	M2G	C8-N7-C5	2.62	107.97	102.99
1	2A	2552	OMU	O2'-C2'-C1'	-2.61	103.99	109.08
32	2a	516	PSU	N1-C2-N3	2.60	118.07	115.13
1	1A	2263	OMG	C5-C6-N1	2.60	118.54	113.95
1	1A	1964	5MC	C4-N3-C2	-2.58	117.20	120.69
1	1A	1937	5MU	C1'-N1-C6	-2.58	116.83	121.12
1	1A	1942	OMC	O2-C2-N3	-2.58	118.14	122.33
1	2A	2605	PSU	N1-C2-N3	2.58	118.05	115.13
32	2a	1498	UR3	O2-C2-N3	2.57	124.96	121.34
32	1a	1498	UR3	C3U-N3-C2	2.53	121.75	117.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2263	OMG	O6-C6-N1	-2.53	117.67	120.65
1	1A	1937	5MU	C5M-C5-C6	-2.52	119.48	122.85
32	1a	1207	2MG	O3'-C3'-C2'	2.52	119.98	111.82
32	2a	516	PSU	C6-N1-C2	-2.51	120.11	122.68
32	1a	516	PSU	O4'-C1'-C2'	2.51	108.68	105.14
1	2A	1939	5MU	C5-C4-N3	2.50	117.45	115.31
1	1A	1984	5MC	N4-C4-N3	-2.50	113.92	118.48
32	2a	1400	5MC	CM5-C5-C6	-2.48	119.53	122.85
1	2A	2605	PSU	O4-C4-N3	-2.47	115.39	120.12
32	2a	516	PSU	O4'-C1'-C2'	2.46	108.62	105.14
32	2a	1498	UR3	C3U-N3-C4	2.46	121.41	117.89
1	2A	1962	5MC	CM5-C5-C6	-2.45	119.58	122.85
1	2A	1915	5MU	C1'-N1-C6	-2.43	117.07	121.12
1	1A	1964	5MC	C5-C4-N3	2.43	124.30	121.67
1	1A	1939	PSU	N1-C2-N3	2.43	117.88	115.13
32	1a	966	M2G	C8-N7-C5	2.42	107.60	102.99
1	1A	2617	PSU	O2'-C2'-C1'	-2.40	105.50	111.23
32	1a	527	G7M	C2-N1-C6	-2.40	120.67	125.10
1	2A	2251	OMG	O6-C6-N1	-2.40	117.82	120.65
1	2A	1911	PSU	O4-C4-N3	-2.39	115.54	120.12
1	1A	2617	PSU	C6-N1-C2	-2.38	120.25	122.68
1	1A	2617	PSU	O4-C4-C5	2.37	130.25	124.05
32	2a	1404	5MC	N4-C4-N3	-2.36	114.16	118.48
32	2a	1402	4OC	C5-C4-N3	-2.35	118.81	122.59
1	2A	1917	PSU	O4-C4-N3	-2.34	115.64	120.12
32	2a	1400	5MC	N4-C4-N3	-2.32	114.24	118.48
32	2a	1207	2MG	C5-C6-N1	2.30	118.02	113.95
32	2a	966	M2G	C5-C6-N1	2.30	118.01	113.95
44	2l	92	0TD	OD2-CG-OD1	-2.27	118.94	124.09
32	1a	1400	5MC	N4-C4-N3	-2.26	114.35	118.48
1	1A	1942	OMC	CM2-O2'-C2'	-2.26	108.61	114.52
32	1a	967	5MC	N4-C4-N3	-2.25	114.37	118.48
1	2A	1917	PSU	N1-C2-N3	2.23	117.66	115.13
32	1a	1498	UR3	C5-C6-N1	-2.21	118.10	121.81
32	2a	516	PSU	O4-C4-N3	-2.20	115.90	120.12
1	1A	1937	5MU	C5-C4-N3	2.16	117.16	115.31
32	1a	1404	5MC	C5-C4-N3	2.16	124.00	121.67
1	2A	1917	PSU	C4-N3-C2	-2.12	123.29	126.34
1	2A	2605	PSU	C4-N3-C2	-2.12	123.29	126.34
32	1a	1207	2MG	C3'-C2'-C1'	-2.09	97.83	100.98
32	2a	527	G7M	C2-N1-C6	-2.09	121.26	125.10
1	2A	1962	5MC	C5-C4-N3	2.09	123.92	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	966	M2G	O6-C6-C5	-2.07	120.33	124.37
1	1A	1933	PSU	C4-N3-C2	-2.07	123.36	126.34
1	1A	1939	PSU	C4-N3-C2	-2.07	123.36	126.34
1	2A	2605	PSU	O2-C2-N1	-2.07	120.52	122.79
1	2A	2251	OMG	CM2-O2'-C2'	-2.06	109.11	114.52
32	1a	1407	5MC	O2-C2-N3	-2.06	118.97	122.33
1	2A	1920	OMC	C2'-C1'-N1	-2.04	110.26	114.22
32	1a	966	M2G	CM2-N2-CM1	2.04	122.09	115.77
1	1A	1939	PSU	O4-C4-N3	-2.03	116.23	120.12
1	2A	1942	5MC	C4-N3-C2	-2.03	117.95	120.69
1	2A	2503	2MA	C8-N7-C5	2.02	106.84	102.99
1	1A	2263	OMG	N1-C2-N3	-2.01	119.57	123.32
32	2a	527	G7M	N1-C2-N3	-2.00	119.58	123.32
1	2A	1915	5MU	O4'-C1'-N1	2.00	112.94	108.36

There are no chirality outliers.

All (43) 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	C3'-C4'-C5'-O5'
1	1A	1937	5MU	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C9
44	1l	92	0TD	CA-CB-SB-CSB
44	1l	92	0TD	SB-CB-CG-OD2
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
32	2a	516	PSU	C2'-C1'-C5-C4
32	2a	1518	MA6	C5-C6-N6-C9
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	N1-C6-N6-C9
32	2a	1518	MA6	N1-C6-N6-C9
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	527	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
44	2l	92	0TD	CG-CB-SB-CSB
44	1l	92	0TD	SB-CB-CG-OD1
44	2l	92	0TD	CA-CB-CG-OD2
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	516	PSU	O4'-C1'-C5-C4
32	2a	516	PSU	O4'-C1'-C5-C4
1	1A	1942	OMC	O4'-C4'-C5'-O5'
1	1A	1942	OMC	C3'-C4'-C5'-O5'
32	1a	516	PSU	O4'-C1'-C5-C6
44	1l	92	0TD	CG-CB-SB-CSB
32	2a	516	PSU	O4'-C1'-C5-C6
1	1A	1942	OMC	C2'-C1'-N1-C2
1	2A	1920	OMC	C2'-C1'-N1-C2
1	1A	2515	2MA	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	1984	5MC	O4'-C1'-N1-C6
1	1A	1984	5MC	C2'-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, 2432 are monoatomic and 1 is 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
57	SF4	1d	501	36	0,12,12	-	-	-		
57	SF4	2d	501	36	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
57	SF4	1d	501	36	-	-	0/6/5/5
57	SF4	2d	501	36	-	-	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	3.56

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1A	2861/2915 (98%)	0.20	153 (5%) 26 17	18, 37, 90, 99	0
1	2A	2856/2915 (97%)	0.13	161 (5%) 24 16	33, 58, 91, 100	0
2	1B	120/120 (100%)	-0.35	0 100 100	33, 56, 67, 89	0
2	2B	120/120 (100%)	-0.34	0 100 100	63, 76, 81, 86	0
3	1D	275/275 (100%)	-0.29	0 100 100	17, 38, 53, 70	0
3	2D	275/275 (100%)	-0.25	0 100 100	32, 52, 64, 74	0
4	1E	204/204 (100%)	-0.40	0 100 100	19, 41, 61, 70	0
4	2E	204/204 (100%)	-0.23	1 (0%) 91 88	34, 57, 70, 78	0
5	1F	203/203 (100%)	-0.28	2 (0%) 82 77	17, 44, 70, 86	0
5	2F	203/203 (100%)	-0.28	0 100 100	38, 64, 78, 84	0
6	1G	181/181 (100%)	-0.42	2 (1%) 80 75	52, 68, 78, 88	0
6	2G	181/181 (100%)	0.56	15 (8%) 11 6	74, 80, 86, 91	0
7	1H	174/174 (100%)	-0.47	1 (0%) 89 86	39, 55, 66, 70	0
7	2H	173/174 (99%)	0.77	27 (15%) 2 1	65, 79, 85, 87	0
8	1I	147/147 (100%)	-0.26	0 100 100	41, 70, 78, 81	0
8	2I	146/147 (99%)	0.24	5 (3%) 45 35	53, 74, 82, 87	0
9	1N	140/140 (100%)	-0.39	0 100 100	23, 39, 62, 75	0
9	2N	140/140 (100%)	-0.26	0 100 100	48, 63, 73, 82	0
10	1O	122/122 (100%)	-0.33	0 100 100	30, 43, 59, 64	0
10	2O	122/122 (100%)	-0.36	0 100 100	44, 55, 67, 73	0
11	1P	149/149 (100%)	-0.25	0 100 100	19, 46, 65, 78	0
11	2P	149/149 (100%)	0.23	3 (2%) 65 56	42, 66, 79, 82	0
12	1Q	141/141 (100%)	-0.18	0 100 100	28, 43, 56, 69	0
12	2Q	141/141 (100%)	-0.38	2 (1%) 75 70	47, 63, 74, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	-0.16	0 100 100	26, 38, 55, 63	0
13	2R	118/118 (100%)	-0.21	0 100 100	40, 54, 64, 70	0
14	1S	110/110 (100%)	-0.36	0 100 100	44, 55, 67, 71	0
14	2S	110/110 (100%)	0.21	3 (2%) 54 44	64, 72, 78, 82	0
15	1T	131/131 (100%)	-0.34	1 (0%) 86 81	34, 47, 70, 79	0
15	2T	131/131 (100%)	-0.36	0 100 100	50, 60, 75, 83	0
16	1U	116/116 (100%)	-0.25	0 100 100	22, 32, 48, 64	0
16	2U	116/116 (100%)	-0.12	0 100 100	45, 60, 72, 81	0
17	1V	101/101 (100%)	-0.41	0 100 100	22, 41, 60, 71	0
17	2V	101/101 (100%)	-0.24	0 100 100	42, 68, 76, 83	0
18	1W	112/112 (100%)	-0.35	2 (1%) 68 61	22, 32, 54, 85	0
18	2W	112/112 (100%)	-0.30	0 100 100	39, 52, 66, 81	0
19	1X	95/95 (100%)	-0.31	0 100 100	28, 42, 64, 72	0
19	2X	95/95 (100%)	-0.06	1 (1%) 80 75	48, 62, 72, 76	0
20	1Y	107/107 (100%)	-0.35	1 (0%) 84 80	38, 51, 67, 75	0
20	2Y	107/107 (100%)	0.34	12 (11%) 5 3	53, 68, 79, 86	0
21	1Z	203/203 (100%)	-0.40	1 (0%) 91 88	45, 62, 74, 82	0
21	2Z	201/203 (99%)	0.11	3 (1%) 73 68	65, 75, 82, 87	0
22	10	77/77 (100%)	-0.28	0 100 100	29, 41, 58, 63	0
22	20	77/77 (100%)	0.16	2 (2%) 56 46	52, 63, 71, 75	0
23	11	97/97 (100%)	-0.11	1 (1%) 82 77	27, 45, 68, 77	0
23	21	97/97 (100%)	-0.14	1 (1%) 82 77	46, 59, 75, 79	0
24	12	70/70 (100%)	-0.28	0 100 100	40, 51, 63, 77	0
24	22	70/70 (100%)	-0.07	0 100 100	60, 69, 77, 79	0
25	13	59/59 (100%)	-0.32	0 100 100	28, 40, 62, 77	0
25	23	59/59 (100%)	0.32	2 (3%) 45 35	54, 63, 74, 79	0
26	14	69/69 (100%)	0.34	12 (17%) 1 1	64, 79, 87, 91	0
26	24	69/69 (100%)	1.28	21 (30%) 0 0	76, 85, 89, 94	0
27	15	59/59 (100%)	-0.30	0 100 100	18, 38, 57, 66	0
27	25	59/59 (100%)	-0.20	0 100 100	38, 55, 71, 75	0
28	16	53/53 (100%)	-0.43	0 100 100	38, 48, 60, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/53 (100%)	-0.21	0 100 100	56, 64, 71, 77	0
29	17	48/48 (100%)	-0.16	0 100 100	20, 27, 58, 68	0
29	27	48/48 (100%)	-0.10	0 100 100	34, 44, 67, 78	0
30	18	64/64 (100%)	-0.17	0 100 100	28, 35, 46, 59	0
30	28	64/64 (100%)	0.04	0 100 100	46, 58, 65, 70	0
31	19	37/37 (100%)	-0.11	0 100 100	35, 46, 63, 70	0
31	29	37/37 (100%)	0.28	1 (2%) 54 44	63, 69, 75, 75	0
32	1a	1488/1521 (97%)	0.02	59 (3%) 38 28	35, 72, 91, 100	0
32	2a	1492/1521 (98%)	0.01	58 (3%) 39 29	44, 74, 91, 97	0
33	1x	97/97 (100%)	-0.08	1 (1%) 82 77	55, 67, 76, 80	0
33	2x	96/97 (98%)	1.75	40 (41%) 0 0	70, 78, 87, 89	0
34	1b	231/231 (100%)	0.15	18 (7%) 13 7	65, 77, 84, 90	0
34	2b	231/231 (100%)	0.23	14 (6%) 21 13	66, 79, 85, 89	0
35	1c	206/206 (100%)	0.25	13 (6%) 20 12	67, 78, 84, 90	0
35	2c	206/206 (100%)	0.52	16 (7%) 13 7	72, 81, 86, 90	0
36	1d	208/208 (100%)	-0.13	2 (0%) 82 77	59, 73, 80, 87	0
36	2d	208/208 (100%)	-0.16	3 (1%) 75 70	58, 71, 80, 84	0
37	1e	148/148 (100%)	-0.24	0 100 100	45, 68, 75, 89	0
37	2e	148/148 (100%)	-0.27	0 100 100	57, 70, 77, 82	0
38	1f	100/100 (100%)	-0.44	0 100 100	54, 72, 77, 80	0
38	2f	100/100 (100%)	-0.48	0 100 100	59, 68, 78, 80	0
39	1g	155/155 (100%)	-0.03	4 (2%) 56 46	66, 74, 82, 85	0
39	2g	155/155 (100%)	0.35	14 (9%) 9 5	69, 77, 82, 87	0
40	1h	137/137 (100%)	-0.05	1 (0%) 87 84	58, 68, 74, 82	0
40	2h	137/137 (100%)	-0.19	0 100 100	62, 69, 76, 80	0
41	1i	127/127 (100%)	0.58	8 (6%) 20 12	67, 80, 86, 89	0
41	2i	126/127 (99%)	1.16	34 (26%) 0 0	72, 81, 86, 89	0
42	1j	97/97 (100%)	1.13	20 (20%) 1 0	68, 81, 87, 90	0
42	2j	96/97 (98%)	1.06	19 (19%) 1 0	73, 82, 87, 89	0
43	1k	114/114 (100%)	-0.38	0 100 100	44, 64, 75, 81	0
43	2k	114/114 (100%)	-0.29	1 (0%) 84 80	54, 69, 80, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1l	121/122 (99%)	-0.23	2 (1%) 70 63	51, 64, 72, 79	0
44	2l	121/122 (99%)	-0.17	1 (0%) 86 81	56, 66, 74, 77	0
45	1m	116/116 (100%)	0.33	8 (6%) 16 10	69, 77, 82, 83	0
45	2m	114/116 (98%)	0.48	11 (9%) 8 4	75, 81, 85, 88	0
46	1n	60/60 (100%)	0.35	4 (6%) 17 10	69, 77, 81, 83	0
46	2n	60/60 (100%)	0.83	10 (16%) 1 1	73, 81, 84, 88	0
47	1o	88/88 (100%)	-0.01	1 (1%) 80 75	52, 66, 76, 82	0
47	2o	88/88 (100%)	-0.17	1 (1%) 80 75	54, 69, 78, 81	0
48	1p	82/82 (100%)	0.15	3 (3%) 41 31	63, 74, 80, 87	0
48	2p	82/82 (100%)	0.15	2 (2%) 59 49	58, 69, 76, 84	0
49	1q	99/99 (100%)	-0.12	2 (2%) 65 56	54, 68, 77, 79	0
49	2q	99/99 (100%)	-0.26	0 100 100	57, 68, 76, 78	0
50	1r	68/68 (100%)	0.11	5 (7%) 14 8	57, 67, 75, 80	0
50	2r	68/68 (100%)	-0.07	2 (2%) 51 41	62, 69, 77, 79	0
51	1s	83/83 (100%)	0.88	16 (19%) 1 0	73, 79, 84, 85	0
51	2s	83/83 (100%)	1.73	32 (38%) 0 0	77, 83, 88, 90	0
52	1t	96/98 (97%)	0.17	3 (3%) 49 39	63, 72, 81, 83	0
52	2t	98/98 (100%)	0.10	1 (1%) 82 77	59, 69, 78, 80	0
53	1u	23/23 (100%)	1.18	5 (21%) 0 0	72, 75, 78, 81	0
53	2u	23/23 (100%)	1.71	9 (39%) 0 0	76, 79, 82, 84	0
54	1y	16/16 (100%)	0.46	2 (12%) 3 2	36, 50, 60, 61	0
54	2y	16/16 (100%)	1.09	5 (31%) 0 0	53, 59, 69, 72	0
All	All	20798/20986 (99%)	0.04	886 (4%) 35 25	17, 64, 85, 100	0

All (886) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1133	G	17.3
1	1A	1135	G	15.6
1	1A	1137	G	14.1
1	1A	1118	C	12.4
1	1A	1136	U	11.7
1	1A	1149	A	11.4
1	1A	1120	G	11.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1A	1127	U	10.5
1	1A	1132	A	10.3
1	1A	1134	A	10.1
1	1A	1123	A	10.1
1	1A	1121	C	10.0
1	1A	1139	G	9.8
1	1A	1126	C	9.7
1	1A	1109	G	9.6
1	1A	1113	A	9.5
1	1A	1125	C	9.3
1	1A	1110	C	9.1
1	1A	1122	C	9.0
1	1A	1117	G	8.7
1	1A	1138	C	8.7
1	1A	1128	U	8.6
1	1A	1112	U	8.2
32	2a	1001(A)	G	8.1
1	1A	1129	U	8.1
32	2a	1030(B)	C	8.0
1	2A	2125	G	7.9
32	1a	1036	G	7.9
1	2A	2802	G	7.9
1	1A	1124	U	7.8
1	1A	1119	A	7.7
32	1a	1030(B)	C	7.6
1	2A	2147	G	7.6
1	2A	2123	G	7.5
32	2a	1030(A)	G	7.4
33	2x	9	GLN	7.3
42	1j	10	GLY	7.3
1	1A	1148	C	7.2
32	2a	1001	A	7.2
26	14	52	THR	7.2
1	1A	1150	C	7.1
1	2A	2126	A	6.9
1	2A	2139	C	6.9
1	2A	2162	G	6.7
1	1A	1103	A	6.6
1	2A	2169	A	6.6
1	2A	2174	C	6.6
1	2A	1046	A	6.5
1	2A	1085	A	6.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	1a	1031	G	6.5
1	2A	2124	G	6.4
33	2x	64	SER	6.3
1	1A	2139	A	6.3
1	2A	2168	G	6.3
1	2A	2146	C	6.2
32	1a	1001	A	6.1
1	1A	1111	U	6.1
1	1A	2138	G	6.1
32	1a	1034	G	6.1
32	1a	1001(A)	G	6.0
45	1m	115	LYS	6.0
1	1A	2145	G	5.9
32	1a	1030(C)	G	5.9
1	2A	1064	C	5.9
1	2A	2803	C	5.9
1	2A	2118	U	5.9
1	2A	2801(A)	A	5.8
1	2A	2131	G	5.8
1	2A	2154	G	5.8
1	2A	2155	G	5.8
32	2a	80	G	5.8
1	1A	1114	G	5.7
33	2x	73	ALA	5.7
32	1a	1037	C	5.7
32	2a	1036	G	5.7
1	1A	1131	A	5.6
1	2A	1067	A	5.6
1	2A	2176	A	5.6
1	2A	2173	A	5.6
32	1a	1002	G	5.5
1	2A	2107	C	5.5
32	2a	1257	U	5.5
20	2Y	1	MET	5.5
1	2A	2179	C	5.5
32	2a	1030(C)	G	5.5
1	2A	888	C	5.5
1	2A	2145	C	5.5
1	2A	2153	G	5.4
1	2A	2133	G	5.4
1	2A	2141	G	5.4
1	1A	2166	U	5.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
41	2i	102	LEU	5.3
1	2A	2165	G	5.3
1	1A	2806	G	5.3
1	1A	2188	G	5.3
1	2A	229	A	5.2
32	1a	1035	A	5.2
1	1A	935	C	5.2
51	2s	71	LEU	5.2
26	24	49	PHE	5.2
42	2j	6	ILE	5.2
34	1b	136	VAL	5.2
41	1i	15	ALA	5.2
33	2x	42	SER	5.2
26	24	63	TYR	5.2
1	1A	1130	A	5.2
1	1A	2195	A	5.1
1	2A	2128	C	5.1
1	2A	2127	G	5.1
32	2a	1026	G	5.1
1	2A	1083	U	5.1
1	2A	2119	A	5.1
32	2a	1027	C	5.1
1	1A	2816	G	5.1
42	1j	100	THR	5.1
32	2a	1030(D)	A	5.1
32	1a	1005	A	5.0
1	2A	2106	G	5.0
39	2g	156	TRP	5.0
39	2g	154	TYR	5.0
1	1A	2161	C	5.0
1	2A	2157	G	5.0
32	1a	1032	G	5.0
1	2A	2896	C	5.0
32	1a	1003	G	4.9
35	1c	193	TYR	4.9
1	1A	2169	G	4.9
26	24	45	GLY	4.9
1	2A	1095	A	4.9
1	2A	2138	C	4.9
32	2a	1034	G	4.9
1	1A	2183	C	4.9
1	1A	2154	U	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2159	G	4.8
32	1a	1026	G	4.8
32	1a	1286	A	4.8
23	11	2	SER	4.8
1	2A	1082	U	4.8
39	2g	82	GLY	4.8
1	2A	2166	G	4.8
32	1a	1030	C	4.7
32	2a	1002	G	4.7
1	1A	2134	G	4.7
1	2A	2132	U	4.7
1	2A	2120	G	4.7
1	1A	2807	C	4.6
1	2A	2804	C	4.6
42	2j	74	ILE	4.6
1	2A	2110	G	4.6
32	2a	1035	A	4.6
1	1A	1108	G	4.6
1	1A	1141	A	4.6
39	1g	156	TRP	4.6
1	1A	2163	G	4.6
32	1a	1028	C	4.6
33	2x	41	LEU	4.5
51	1s	40	ILE	4.5
1	2A	1079	C	4.5
1	2A	2148	G	4.5
51	2s	12	ASP	4.5
1	2A	2142	C	4.5
32	1a	1024	G	4.5
32	2a	1031	G	4.5
32	1a	1004	A	4.4
1	1A	2814	C	4.4
1	2A	1076	C	4.4
1	2A	2164	C	4.4
32	2a	998	G	4.4
1	2A	1088	A	4.4
1	1A	2147	G	4.4
1	2A	2112	G	4.4
1	2A	2140	C	4.4
33	2x	10	MET	4.4
33	2x	46	GLN	4.4
41	1i	106	ALA	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2121	G	4.4
32	1a	1257	U	4.3
32	1a	1033	G	4.3
45	1m	2	ALA	4.3
1	1A	1555	C	4.3
1	1A	2151	C	4.3
1	2A	2793	G	4.3
32	2a	1040	U	4.3
14	2S	58	LEU	4.3
51	1s	56	GLN	4.3
1	1A	2148	A	4.3
26	14	54	GLY	4.3
32	1a	1030(A)	G	4.3
41	2i	72	GLY	4.3
32	1a	202	U	4.3
46	2n	13	THR	4.3
1	1A	2181	G	4.3
32	1a	1027	C	4.3
32	2a	1033	G	4.3
1	2A	2897	U	4.3
51	2s	64	GLU	4.3
34	1b	133	LYS	4.3
1	2A	2143	C	4.2
1	1A	2137	G	4.2
1	2A	2152	G	4.2
1	1A	2177	G	4.2
26	24	69	LYS	4.2
1	1A	2162	C	4.2
1	1A	2175	G	4.2
1	2A	1509	C	4.2
1	1A	2149	G	4.1
1	2A	2170	A	4.1
26	24	50	VAL	4.1
1	2A	2122	U	4.1
1	2A	2144	U	4.1
1	2A	2792	G	4.1
33	2x	63	ALA	4.1
32	1a	1030(D)	A	4.1
1	2A	2111	C	4.1
41	1i	78	LYS	4.1
1	2A	2136	C	4.1
53	1u	18	TYR	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1A	2198	A	4.1
1	1A	2160	C	4.1
1	1A	2165	C	4.1
1	2A	2134	A	4.1
42	2j	36	GLY	4.0
1	1A	2191	A	4.0
1	1A	2130	C	4.0
32	1a	1038	C	4.0
32	2a	1030	C	4.0
42	2j	85	LEU	4.0
1	2A	652(B)	A	4.0
1	2A	2137	C	4.0
1	2A	2175	C	4.0
1	2A	6	A	4.0
32	2a	1041	A	4.0
32	1a	1006	C	4.0
6	2G	62	LEU	4.0
1	1A	2194	U	4.0
1	1A	2189	U	4.0
1	2A	2158	A	3.9
1	1A	2167	C	3.9
34	1b	135	GLN	3.9
26	14	59	PHE	3.9
33	2x	65	GLY	3.9
33	2x	50	ALA	3.9
26	24	68	ARG	3.9
1	2A	1104	C	3.9
32	1a	1029	C	3.9
1	1A	2141	A	3.9
1	1A	1104	G	3.9
1	2A	2805	G	3.9
32	1a	204	U	3.9
1	2A	2105	C	3.9
33	2x	38	HIS	3.9
1	1A	2190	G	3.9
42	1j	8	LEU	3.9
51	2s	13	ASP	3.9
46	2n	12	ARG	3.9
1	1A	1221	G	3.9
1	1A	2182	G	3.9
1	1A	2178	G	3.9
32	2a	1003	G	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2151	G	3.8
26	24	64	GLY	3.8
7	2H	103	LEU	3.8
1	2A	2167	U	3.8
1	2A	2108	C	3.8
34	2b	232	PRO	3.8
42	2j	20	ALA	3.8
1	1A	2813	G	3.8
51	2s	48	THR	3.8
1	1A	2164	C	3.8
26	14	65	ASP	3.8
46	2n	38	GLY	3.8
32	2a	1286	A	3.7
32	2a	1042	G	3.7
1	1A	2815	C	3.7
32	2a	89	C	3.7
42	1j	5	ARG	3.7
33	2x	49	VAL	3.7
54	2y	16	ILE	3.7
7	2H	29	PRO	3.7
1	2A	2109	U	3.7
35	2c	158	GLY	3.7
1	2A	2178	C	3.7
1	1A	2187	G	3.7
7	2H	128	PRO	3.7
42	1j	96	ILE	3.7
1	2A	2171	A	3.7
7	2H	30	LYS	3.7
1	2A	2156	G	3.7
1	1A	2168	C	3.7
1	2A	2163	C	3.7
32	2a	1029	C	3.7
1	2A	889	C	3.6
1	2A	2116	G	3.6
52	1t	55	ILE	3.6
34	1b	130	ARG	3.6
1	2A	2177	C	3.6
20	2Y	90	LEU	3.6
1	2A	1080	C	3.6
1	2A	2794	C	3.6
35	2c	190	ARG	3.6
33	2x	75	ASN	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	2a	1037	C	3.6
34	1b	129	GLU	3.6
33	2x	68	GLU	3.6
7	2H	82	GLY	3.6
34	1b	128	GLU	3.6
33	2x	8	LYS	3.5
1	1A	2180	A	3.5
32	2a	1004	A	3.5
34	1b	131	PRO	3.5
1	1A	2186	C	3.5
11	2P	91	PHE	3.5
33	2x	11	GLU	3.5
6	2G	49	ASP	3.5
41	2i	7	THR	3.5
8	2I	74	ASN	3.5
1	2A	2172	U	3.5
51	2s	53	ASN	3.5
33	1x	95	ARG	3.5
32	2a	90	U	3.5
51	2s	16	LEU	3.5
1	1A	1099	C	3.4
35	1c	101	LEU	3.4
46	2n	25	VAL	3.4
32	1a	1039	C	3.4
1	1A	2170	G	3.4
1	1A	2129	C	3.4
6	2G	2	PRO	3.4
26	24	66	SER	3.4
34	1b	232	PRO	3.4
33	2x	45	PRO	3.4
1	2A	2160	G	3.4
34	2b	133	LYS	3.4
23	2I	2	SER	3.4
1	2A	2149	G	3.4
6	2G	48	GLU	3.4
7	2H	50	VAL	3.4
43	2k	13	GLN	3.3
39	2g	32	ARG	3.3
1	2A	2150	U	3.3
7	2H	48	GLY	3.3
42	1j	98	ILE	3.3
42	1j	85	LEU	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	2b	123	ALA	3.3
41	2i	30	GLY	3.3
32	2a	1024	G	3.3
32	1a	841	U	3.3
14	2S	20	ARG	3.3
42	1j	75	ILE	3.3
39	1g	16	LEU	3.3
32	2a	79	G	3.3
1	1A	1116	A	3.3
1	1A	1143	U	3.3
53	2u	11	GLY	3.3
1	1A	2171	G	3.3
1	2A	2894	G	3.3
32	2a	1032	G	3.3
34	2b	70	PHE	3.3
51	2s	63	THR	3.3
1	2A	2129	C	3.2
1	1A	2193	A	3.2
32	2a	848	C	3.2
51	1s	58	VAL	3.2
1	1A	2155	G	3.2
1	1A	2905	C	3.2
1	2A	11	G	3.2
7	2H	47	GLU	3.2
34	1b	123	ALA	3.2
32	2a	1006	C	3.2
42	2j	40	LEU	3.2
1	1A	2152	U	3.2
26	24	67	TYR	3.2
1	1A	2131	U	3.2
26	24	52	THR	3.2
53	1u	19	GLY	3.2
6	1G	80	PHE	3.2
46	2n	11	LYS	3.1
45	2m	82	MET	3.1
33	2x	20	VAL	3.1
49	1q	98	LEU	3.1
1	2A	1075	C	3.1
1	2A	2113	U	3.1
26	14	64	GLY	3.1
51	2s	82	GLY	3.1
7	2H	159	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
33	2x	48	PHE	3.1
1	1A	1105	G	3.1
32	2a	1021	G	3.1
1	1A	2202	U	3.1
26	24	54	GLY	3.1
1	2A	887	A	3.1
34	1b	228	GLY	3.1
1	1A	2176	G	3.1
33	2x	77	LEU	3.1
32	1a	203	U	3.1
41	1i	46	ALA	3.1
35	1c	87	LEU	3.1
54	2y	13	PRO	3.1
1	1A	2812	A	3.1
41	2i	127	LYS	3.1
53	2u	14	TRP	3.1
6	2G	19	LEU	3.0
53	2u	6	ARG	3.0
32	1a	1000	U	3.0
33	2x	88	LEU	3.0
6	2G	67	LYS	3.0
35	2c	124	ILE	3.0
42	2j	72	VAL	3.0
1	1A	2150	C	3.0
1	2A	1086	A	3.0
32	2a	202	U	3.0
39	2g	79	ARG	3.0
1	2A	1087	G	3.0
42	2j	89	ASP	3.0
51	2s	49	ILE	3.0
54	2y	15	PRO	3.0
32	2a	994	A	3.0
20	2Y	58	GLY	3.0
1	1A	2173	G	3.0
1	1A	2906	U	3.0
32	2a	841	U	3.0
46	2n	10	ALA	3.0
1	1A	2140	U	3.0
1	2A	614(A)	U	3.0
1	1A	696	C	3.0
1	1A	1144	A	3.0
46	1n	17	LYS	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	1a	1025	U	3.0
32	2a	723	U	3.0
1	2A	2161	C	3.0
32	2a	1039	C	3.0
42	2j	98	ILE	3.0
35	2c	64	VAL	3.0
42	2j	27	ALA	2.9
7	2H	95	ARG	2.9
51	1s	71	LEU	2.9
33	2x	39	ILE	2.9
51	2s	81	ARG	2.9
1	1A	1220	U	2.9
50	1r	24	ALA	2.9
1	1A	1145	G	2.9
19	2X	68	ARG	2.9
34	2b	124	SER	2.9
7	2H	102	ALA	2.9
1	1A	1147	U	2.9
1	1A	2144	U	2.9
45	1m	87	TYR	2.9
1	2A	652(T)	C	2.9
32	1a	1007	C	2.9
41	1i	47	LEU	2.9
1	1A	2179	G	2.9
32	1a	216	G	2.9
50	2r	58	LEU	2.9
32	1a	1136	U	2.9
26	14	45	GLY	2.9
26	24	56	VAL	2.9
1	1A	2196	C	2.9
1	1A	1140	U	2.9
51	1s	60	VAL	2.9
32	2a	1023	G	2.9
42	1j	7	LYS	2.8
14	2S	35	ILE	2.8
42	2j	86	MET	2.8
1	2A	890	A	2.8
1	2A	2807	G	2.8
18	1W	111	HIS	2.8
34	2b	122	PHE	2.8
41	2i	18	PHE	2.8
51	2s	20	LEU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2130	U	2.8
26	24	27	THR	2.8
36	1d	23	GLY	2.8
1	2A	614(B)	G	2.8
45	2m	87	TYR	2.8
42	1j	77	PRO	2.8
1	1A	697	C	2.8
51	2s	80	TYR	2.8
1	1A	2174	G	2.8
1	2A	1057	A	2.8
20	2Y	91	GLU	2.8
32	1a	217	C	2.8
51	1s	47	HIS	2.8
7	2H	18	GLU	2.8
45	2m	116	THR	2.8
1	2A	1043	C	2.8
51	2s	52	TYR	2.8
1	1A	2146	G	2.8
1	2A	10	G	2.8
53	1u	22	ARG	2.8
1	1A	2135	U	2.7
1	2A	2180	U	2.7
35	1c	96	GLY	2.7
45	2m	78	ILE	2.7
1	2A	1044	G	2.7
11	2P	125	VAL	2.7
41	2i	27	THR	2.7
1	2A	2135	A	2.7
7	2H	13	LYS	2.7
33	2x	58	ASN	2.7
33	2x	92	GLY	2.7
6	2G	82	LEU	2.7
1	1A	2153	G	2.7
45	2m	92	HIS	2.7
1	1A	218	A	2.7
50	1r	29	PHE	2.7
1	1A	2805	G	2.7
21	2Z	143	GLY	2.7
1	2A	645	C	2.7
26	24	59	PHE	2.7
51	2s	15	LEU	2.7
35	1c	2	GLY	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	1081	U	2.7
45	2m	84	ILE	2.7
6	2G	75	LYS	2.7
21	2Z	199	LYS	2.7
33	2x	80	LYS	2.7
7	2H	113	VAL	2.7
46	2n	8	GLU	2.7
35	2c	159	GLY	2.7
1	2A	1066	U	2.7
41	2i	83	ARG	2.7
7	2H	43	VAL	2.7
20	2Y	55	TYR	2.7
20	2Y	89	PHE	2.7
39	1g	154	TYR	2.7
1	1A	1151	U	2.7
32	2a	84	U	2.7
39	2g	6	ARG	2.7
6	1G	49	ASP	2.7
1	2A	2181	G	2.7
34	1b	125	PRO	2.7
34	2b	227	GLY	2.7
32	2a	1005	A	2.7
45	1m	116	THR	2.7
1	2A	1068	G	2.7
42	2j	29	ARG	2.7
53	1u	6	ARG	2.7
32	1a	1020	U	2.6
32	2a	1136	U	2.6
40	1h	58	TYR	2.6
26	14	50	VAL	2.6
32	2a	91	C	2.6
39	2g	155	ARG	2.6
53	2u	10	ARG	2.6
1	1A	2203	G	2.6
32	2a	1020	U	2.6
11	2P	122	PRO	2.6
32	1a	1137	C	2.6
20	1Y	1	MET	2.6
51	2s	40	ILE	2.6
1	2A	1059	G	2.6
32	1a	1023	G	2.6
41	2i	8	GLY	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	2b	33	TYR	2.6
42	1j	30	SER	2.6
44	1l	64	TYR	2.6
46	2n	35	ARG	2.6
51	2s	30	LEU	2.6
18	1W	112	GLY	2.6
42	1j	72	VAL	2.6
1	2A	652(C)	G	2.6
1	2A	1042	G	2.6
1	2A	1103	A	2.6
32	1a	344	A	2.6
32	1a	201	C	2.6
51	2s	11	VAL	2.6
6	2G	79	ASN	2.6
1	1A	2136	A	2.6
39	2g	81	GLY	2.6
41	2i	54	ASP	2.6
46	1n	25	VAL	2.6
20	2Y	56	PRO	2.6
44	2l	28	LYS	2.6
39	2g	86	GLN	2.6
42	2j	87	THR	2.6
1	1A	2192	A	2.6
1	2A	2602	A	2.6
7	2H	41	MET	2.6
7	2H	105	LEU	2.6
32	2a	1000	U	2.6
8	2I	3	VAL	2.6
39	2g	33	ASP	2.6
45	2m	80	ARG	2.6
33	2x	15	ALA	2.6
33	2x	70	MET	2.5
51	1s	66	MET	2.5
1	1A	2185	C	2.5
26	24	57	GLU	2.5
33	2x	76	GLU	2.5
35	2c	89	GLU	2.5
53	2u	8	THR	2.5
33	2x	95	ARG	2.5
41	2i	59	PHE	2.5
46	2n	2	ALA	2.5
1	2A	2114	A	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
42	2j	84	GLN	2.5
1	2A	2187	G	2.5
46	1n	55	GLY	2.5
46	1n	11	LYS	2.5
42	1j	90	LEU	2.5
50	1r	78	LEU	2.5
32	1a	77	G	2.5
1	1A	2199	C	2.5
1	1A	2803	A	2.5
32	1a	161	A	2.5
51	2s	66	MET	2.5
1	1A	2126	G	2.5
39	2g	8	GLU	2.5
42	1j	40	LEU	2.5
53	2u	13	ILE	2.5
42	2j	34	VAL	2.5
33	2x	67	HIS	2.5
42	2j	68	HIS	2.5
41	2i	5	TYR	2.5
34	2b	130	ARG	2.5
51	2s	45	VAL	2.5
1	2A	2117	A	2.5
1	1A	1101	G	2.5
35	2c	8	ILE	2.5
41	2i	79	LEU	2.5
1	1A	2200	C	2.4
32	2a	1043	C	2.4
33	2x	7	SER	2.4
1	1A	934	A	2.4
35	1c	206	GLU	2.4
42	1j	70	ARG	2.4
45	2m	94	ARG	2.4
45	2m	102	ARG	2.4
1	2A	2104	G	2.4
32	1a	78	G	2.4
1	1A	34	C	2.4
4	2E	1	MET	2.4
20	2Y	60	PHE	2.4
32	2a	1018	C	2.4
32	2a	1028	C	2.4
1	1A	2156	A	2.4
34	2b	201	ILE	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
35	1c	124	ILE	2.4
39	1g	42	ILE	2.4
1	2A	652(V)	C	2.4
1	2A	2895	U	2.4
26	24	46	GLN	2.4
21	2Z	201	LYS	2.4
33	2x	12	ILE	2.4
45	2m	41	PRO	2.4
54	1y	10	PRO	2.4
1	1A	2172	U	2.4
32	2a	1019	C	2.4
1	1A	2206	G	2.4
26	24	44	THR	2.4
33	2x	71	TYR	2.4
8	2I	142	VAL	2.4
41	2i	90	PRO	2.4
41	2i	92	TYR	2.4
41	2i	103	THR	2.4
42	2j	21	GLN	2.4
1	2A	1106	G	2.4
1	2A	2100	G	2.4
7	2H	115	VAL	2.4
26	14	56	VAL	2.4
26	24	7	PRO	2.4
51	2s	84	GLY	2.4
20	2Y	65	ALA	2.4
41	2i	45	ALA	2.4
1	1A	2210	C	2.4
48	2p	19	ILE	2.4
50	1r	31	LEU	2.4
1	1A	2184	G	2.4
41	2i	42	ARG	2.4
34	1b	227	GLY	2.4
35	2c	206	GLU	2.4
36	2d	180	GLY	2.4
1	1A	2157	A	2.4
1	2A	34	C	2.4
51	1s	30	LEU	2.4
20	2Y	57	GLN	2.4
41	2i	36	TYR	2.4
1	2A	1084	A	2.4
48	1p	50	LYS	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	1a	218	C	2.4
20	2Y	45	VAL	2.3
26	24	19	GLY	2.3
35	2c	71	ALA	2.3
45	2m	93	ARG	2.3
35	1c	39	ILE	2.3
7	2H	34	GLU	2.3
1	1A	2197	C	2.3
32	1a	91	C	2.3
51	2s	68	GLY	2.3
53	1u	9	ARG	2.3
1	1A	2128	G	2.3
52	1t	9	ASN	2.3
33	2x	47	GLY	2.3
35	1c	194	GLY	2.3
39	2g	141	VAL	2.3
22	20	74	ARG	2.3
51	1s	59	PRO	2.3
41	2i	88	TYR	2.3
51	1s	61	TYR	2.3
44	1l	61	THR	2.3
51	2s	28	LYS	2.3
1	2A	1056	G	2.3
35	1c	180	ALA	2.3
35	2c	189	ALA	2.3
1	2A	652(U)	G	2.3
32	1a	999	C	2.3
35	2c	193	TYR	2.3
51	2s	24	ALA	2.3
45	1m	114	ARG	2.3
5	1F	15	SER	2.3
21	1Z	192	ALA	2.3
51	1s	74	PHE	2.3
41	2i	87	GLN	2.3
41	2i	105	ASP	2.3
41	2i	94	ALA	2.3
33	2x	87	LYS	2.3
33	2x	91	LYS	2.3
1	1A	2204	G	2.3
8	2I	81	VAL	2.2
33	2x	79	ASN	2.2
50	1r	25	THR	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
53	2u	15	ARG	2.2
31	29	37	GLY	2.2
41	1i	81	ILE	2.2
51	2s	32	LYS	2.2
1	1A	1146	C	2.2
42	1j	47	PHE	2.2
26	14	55	ARG	2.2
1	1A	2142	G	2.2
32	1a	1040	U	2.2
32	2a	204	U	2.2
6	2G	152	LEU	2.2
22	20	76	GLY	2.2
41	2i	19	LEU	2.2
32	2a	1038	C	2.2
6	2G	136	ARG	2.2
25	23	59	VAL	2.2
35	1c	64	VAL	2.2
41	2i	86	VAL	2.2
1	1A	6	A	2.2
32	2a	1531	A	2.2
6	2G	3	LEU	2.2
51	2s	8	GLY	2.2
1	1A	2201	C	2.2
1	2A	2892	A	2.2
32	1a	162	A	2.2
34	2b	43	ASP	2.2
41	1i	30	GLY	2.2
51	1s	57	HIS	2.2
1	1A	2132	G	2.2
1	2A	2184	G	2.2
46	2n	24	CYS	2.2
1	2A	1041	C	2.2
32	1a	840	C	2.2
25	23	26	LEU	2.2
34	1b	134	GLU	2.2
51	2s	17	GLU	2.2
12	2Q	5	ARG	2.2
42	1j	27	ALA	2.2
42	2j	35	SER	2.2
36	2d	158	ILE	2.2
51	1s	50	ALA	2.2
1	1A	694	G	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1A	698	G	2.2
1	2A	2893	G	2.2
26	24	43	TYR	2.2
32	2a	1017	G	2.2
26	14	57	GLU	2.2
32	1a	163	C	2.2
32	2a	1007	C	2.2
32	2a	1045	C	2.2
41	2i	110	GLU	2.2
41	2i	75	ASP	2.2
1	1A	2143	G	2.2
1	2A	1062	G	2.2
1	2A	1089	G	2.2
32	2a	1022	G	2.2
47	2o	6	GLU	2.2
34	2b	228	GLY	2.2
1	1A	936	C	2.2
26	14	68	ARG	2.2
41	2i	66	ARG	2.2
48	2p	48	TRP	2.2
26	14	18	CYS	2.2
50	2r	24	ALA	2.2
33	2x	72	THR	2.2
49	1q	99	SER	2.2
51	1s	69	HIS	2.2
12	2Q	59	ARG	2.2
41	1i	80	GLY	2.2
42	1j	9	ARG	2.2
41	2i	52	ALA	2.2
42	2j	47	PHE	2.2
26	24	29	PRO	2.2
39	2g	153	HIS	2.2
34	1b	126	GLU	2.2
36	1d	135	LEU	2.1
1	2A	1058	G	2.1
1	2A	2115	G	2.1
35	1c	89	GLU	2.1
7	2H	106	THR	2.1
6	2G	25	TYR	2.1
41	2i	62	TYR	2.1
34	1b	132	LYS	2.1
35	2c	65	ALA	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
52	1t	100	ILE	2.1
52	2t	55	ILE	2.1
34	2b	131	PRO	2.1
1	1A	1102	G	2.1
51	2s	69	HIS	2.1
7	2H	114	VAL	2.1
39	2g	80	VAL	2.1
1	2A	653	A	2.1
34	1b	122	PHE	2.1
1	2A	1065	U	2.1
6	2G	39	ILE	2.1
7	2H	97	ARG	2.1
54	2y	12	PRO	2.1
7	1H	2	SER	2.1
1	2A	1533	G	2.1
32	1a	156	G	2.1
6	2G	146	TYR	2.1
48	1p	39	TYR	2.1
20	2Y	50	ARG	2.1
42	1j	33	GLN	2.1
51	2s	36	ARG	2.1
15	1T	38	ASN	2.1
32	2a	999	C	2.1
34	1b	121	LEU	2.1
1	2A	1099	G	2.1
32	1a	1212	U	2.1
33	2x	40	ILE	2.1
33	2x	74	ILE	2.1
35	2c	157	ILE	2.1
7	2H	25	LYS	2.1
47	1o	89	GLY	2.1
1	1A	2158	C	2.1
35	2c	154	SER	2.1
51	2s	35	SER	2.1
51	2s	47	HIS	2.1
5	1F	16	GLY	2.1
1	2A	1045	A	2.1
7	2H	6	ARG	2.1
7	2H	101	ARG	2.1
1	2A	652(D)	C	2.1
1	2A	886	C	2.1
1	2A	2103	C	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	1b	231	GLU	2.1
41	2i	4	TYR	2.1
51	1s	12	ASP	2.1
34	2b	137	ARG	2.1
45	1m	93	ARG	2.1
1	2A	2629	A	2.1
35	2c	87	LEU	2.1
45	1m	90	LEU	2.1
51	2s	56	GLN	2.1
8	2I	144	VAL	2.1
45	1m	117	VAL	2.1
51	1s	38	SER	2.0
41	2i	82	ALA	2.0
53	2u	9	ARG	2.0
54	2y	14	ARG	2.0
7	2H	44	VAL	2.0
1	2A	2182	G	2.0
32	1a	79	G	2.0
1	1A	1115	A	2.0
1	2A	1054	A	2.0
32	1a	723	U	2.0
35	2c	160	ALA	2.0
36	2d	149	ALA	2.0
42	1j	36	GLY	2.0
7	2H	45	VAL	2.0
35	1c	63	ASN	2.0
1	1A	2207	C	2.0
1	2A	1170	G	2.0
32	1a	1021	G	2.0
32	1a	1493	A	2.0
54	1y	11	THR	2.0
41	2i	6	GLY	2.0
1	1A	1072	U	2.0
1	2A	1060	U	2.0
1	2A	883	G	2.0
1	2A	2186	G	2.0
48	1p	57	ARG	2.0
53	2u	17	THR	2.0
41	2i	21	PRO	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	PSU	1A	1939	20/21	0.91	0.22	60,73,87,88	0
1	5MU	1A	1937	21/22	0.92	0.23	73,79,94,111	0
32	2MG	2a	1207	24/25	0.92	0.21	76,85,87,93	0
32	5MC	2a	967	21/22	0.93	0.15	67,70,79,85	0
32	M2G	2a	966	25/26	0.93	0.14	64,71,79,91	0
32	PSU	2a	516	20/21	0.94	0.16	70,80,85,85	0
32	PSU	1a	516	20/21	0.94	0.15	62,72,77,77	0
1	PSU	2A	1911	20/21	0.94	0.11	68,72,78,81	0
1	PSU	2A	1917	20/21	0.94	0.14	67,76,84,95	0
32	2MG	1a	1207	24/25	0.95	0.12	71,78,82,84	0
32	G7M	2a	527	24/25	0.95	0.17	64,71,75,80	0
32	M2G	1a	966	25/26	0.95	0.14	58,63,73,75	0
1	5MU	2A	1915	21/22	0.95	0.18	76,82,87,102	0
32	5MC	1a	967	21/22	0.95	0.14	62,67,74,77	0
32	5MC	2a	1404	21/22	0.95	0.16	51,55,61,66	0
32	5MC	1a	1407	21/22	0.96	0.17	42,55,59,61	0
32	5MC	2a	1400	21/22	0.96	0.18	61,70,74,75	0
32	4OC	2a	1402	22/23	0.96	0.16	54,61,66,70	0
1	OMC	2A	1920	21/22	0.96	0.15	59,65,69,74	0
44	0TD	2l	92	10/11	0.96	0.12	68,70,74,84	0
1	5MC	2A	1962	21/22	0.97	0.14	38,46,53,61	0
1	2MA	2A	2503	23/24	0.97	0.23	33,38,41,42	0
1	PSU	2A	2605	20/21	0.97	0.18	34,38,44,44	0
32	UR3	1a	1498	21/22	0.97	0.18	48,53,58,64	0
32	MA6	1a	1518	24/25	0.97	0.20	42,51,58,62	0
32	MA6	1a	1519	24/25	0.97	0.18	46,53,58,61	0
44	0TD	1l	92	10/11	0.97	0.13	64,65,70,78	0
1	PSU	1A	1933	20/21	0.97	0.14	62,68,71,72	0
32	G7M	1a	527	24/25	0.97	0.16	50,60,66,69	0
32	4OC	1a	1402	22/23	0.97	0.17	50,53,57,60	0
1	OMC	1A	1942	21/22	0.97	0.14	51,61,63,67	0
32	5MC	2a	1407	21/22	0.97	0.14	51,59,66,69	0
32	UR3	2a	1498	21/22	0.97	0.15	50,60,64,67	0
32	MA6	2a	1518	24/25	0.97	0.17	54,63,68,69	0
32	MA6	2a	1519	24/25	0.97	0.19	51,61,65,68	0
1	5MC	2A	1942	21/22	0.97	0.16	47,52,55,56	0
1	5MU	1A	1961	21/22	0.98	0.17	24,28,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MU	2A	1939	21/22	0.98	0.16	36,39,45,46	0
1	5MC	1A	1964	21/22	0.98	0.13	29,37,42,45	0
1	5MC	1A	1984	21/22	0.98	0.14	31,37,39,44	0
1	OMG	2A	2251	24/25	0.98	0.16	37,44,46,51	0
1	OMG	1A	2263	24/25	0.98	0.18	19,25,27,30	0
1	OMU	1A	2564	21/22	0.98	0.18	23,29,31,33	0
32	5MC	1a	1400	21/22	0.98	0.14	57,61,66,67	0
1	PSU	1A	2617	20/21	0.98	0.21	23,27,33,34	0
32	5MC	1a	1404	21/22	0.98	0.15	45,50,54,55	0
1	2MA	1A	2515	23/24	0.99	0.21	16,20,24,24	0
1	OMU	2A	2552	21/22	0.99	0.16	32,43,45,45	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3411	1/1	0.20	0.94	88,88,88,88	0
55	MG	2A	3090	1/1	0.34	0.34	78,78,78,78	0
55	MG	2a	1791	1/1	0.34	0.31	102,102,102,102	0
55	MG	2A	3532	1/1	0.38	0.28	87,87,87,87	0
55	MG	1A	3898	1/1	0.44	0.53	53,53,53,53	0
55	MG	2A	3549	1/1	0.46	0.47	72,72,72,72	0
55	MG	2A	3554	1/1	0.48	0.75	62,62,62,62	0
55	MG	2A	3506	1/1	0.48	0.52	72,72,72,72	0
55	MG	2N	201	1/1	0.49	0.43	90,90,90,90	0
55	MG	2A	3717	1/1	0.50	0.15	89,89,89,89	0
55	MG	1B	206	1/1	0.52	0.17	66,66,66,66	0
55	MG	2A	3454	1/1	0.52	1.21	67,67,67,67	0
55	MG	1A	3758	1/1	0.52	0.60	60,60,60,60	0
55	MG	1A	3496	1/1	0.53	0.08	73,73,73,73	0
55	MG	1A	3185	1/1	0.53	0.18	74,74,74,74	0
55	MG	1A	3359	1/1	0.54	0.12	80,80,80,80	0
55	MG	1a	3078	1/1	0.54	0.71	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1722	1/1	0.54	0.12	77,77,77,77	0
55	MG	2a	1750	1/1	0.54	0.20	103,103,103,103	0
55	MG	1A	3254	1/1	0.54	0.52	59,59,59,59	0
55	MG	2a	1741	1/1	0.55	0.46	91,91,91,91	0
55	MG	2A	3475	1/1	0.55	0.53	66,66,66,66	0
55	MG	1a	3151	1/1	0.55	0.14	81,81,81,81	0
55	MG	2A	3562	1/1	0.56	0.46	81,81,81,81	0
55	MG	1A	3712	1/1	0.56	0.23	96,96,96,96	0
55	MG	2A	3791	1/1	0.56	0.76	73,73,73,73	0
55	MG	2A	3555	1/1	0.56	0.68	70,70,70,70	0
55	MG	1a	3077	1/1	0.57	0.76	68,68,68,68	0
55	MG	1A	3854	1/1	0.57	0.14	74,74,74,74	0
55	MG	2A	3810	1/1	0.58	0.15	68,68,68,68	0
55	MG	1a	3058	1/1	0.58	0.58	81,81,81,81	0
55	MG	1a	3168	1/1	0.58	0.07	75,75,75,75	0
55	MG	2d	504	1/1	0.58	0.25	93,93,93,93	0
55	MG	1A	3213	1/1	0.59	0.52	56,56,56,56	0
55	MG	1A	3886	1/1	0.59	0.22	39,39,39,39	0
55	MG	2A	3113	1/1	0.59	0.23	66,66,66,66	0
55	MG	2B	3013	1/1	0.60	0.06	77,77,77,77	0
55	MG	2a	1719	1/1	0.61	0.23	75,75,75,75	0
55	MG	2A	3103	1/1	0.61	0.25	64,64,64,64	0
55	MG	2A	3773	1/1	0.61	0.10	81,81,81,81	0
55	MG	1A	3609	1/1	0.62	0.40	63,63,63,63	0
55	MG	1D	313	1/1	0.62	0.25	54,54,54,54	0
55	MG	2A	3133	1/1	0.62	0.48	64,64,64,64	0
55	MG	2A	3610	1/1	0.62	0.10	82,82,82,82	0
55	MG	2n	502	1/1	0.62	0.48	77,77,77,77	0
55	MG	2A	3178	1/1	0.63	0.23	73,73,73,73	0
55	MG	1B	220	1/1	0.63	0.22	57,57,57,57	0
55	MG	1A	3721	1/1	0.63	0.24	71,71,71,71	0
55	MG	2A	3635	1/1	0.63	0.23	97,97,97,97	0
55	MG	2A	3695	1/1	0.63	0.10	82,82,82,82	0
55	MG	1H	8001	1/1	0.63	0.23	91,91,91,91	0
55	MG	1A	3608	1/1	0.64	0.18	76,76,76,76	0
55	MG	1A	3839	1/1	0.64	0.18	68,68,68,68	0
55	MG	2A	3574	1/1	0.65	0.31	99,99,99,99	0
55	MG	2A	3727	1/1	0.65	0.61	64,64,64,64	0
55	MG	2A	3128	1/1	0.65	0.59	83,83,83,83	0
55	MG	2a	1731	1/1	0.65	0.13	88,88,88,88	0
55	MG	2A	3627	1/1	0.65	0.19	67,67,67,67	0
55	MG	2A	3049	1/1	0.65	1.70	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3813	1/1	0.65	0.49	59,59,59,59	0
55	MG	1A	3095	1/1	0.65	0.41	58,58,58,58	0
55	MG	2D	302	1/1	0.65	0.35	67,67,67,67	0
55	MG	1B	222	1/1	0.66	0.10	78,78,78,78	0
55	MG	2a	1753	1/1	0.66	0.22	84,84,84,84	0
55	MG	2A	3752	1/1	0.66	0.41	77,77,77,77	0
55	MG	2d	503	1/1	0.66	0.24	72,72,72,72	0
55	MG	2A	3136	1/1	0.66	0.47	59,59,59,59	0
55	MG	2l	201	1/1	0.66	0.80	106,106,106,106	0
55	MG	2P	202	1/1	0.66	0.31	74,74,74,74	0
55	MG	2A	3473	1/1	0.67	0.13	71,71,71,71	0
55	MG	2A	3675	1/1	0.67	0.16	75,75,75,75	0
55	MG	2A	3474	1/1	0.67	0.10	78,78,78,78	0
55	MG	1A	3201	1/1	0.67	0.30	61,61,61,61	0
55	MG	1a	3210	1/1	0.67	0.15	76,76,76,76	0
55	MG	1A	3112	1/1	0.68	0.38	50,50,50,50	0
55	MG	1B	207	1/1	0.68	0.24	60,60,60,60	0
55	MG	2B	3012	1/1	0.68	0.07	80,80,80,80	0
55	MG	1A	3135	1/1	0.69	0.17	71,71,71,71	0
55	MG	2A	3501	1/1	0.69	0.21	57,57,57,57	0
55	MG	1E	303	1/1	0.69	0.29	64,64,64,64	0
55	MG	2A	3376	1/1	0.69	0.15	89,89,89,89	0
55	MG	2A	3672	1/1	0.69	0.32	67,67,67,67	0
55	MG	1F	309	1/1	0.69	0.25	59,59,59,59	0
55	MG	1A	3912	1/1	0.69	0.26	52,52,52,52	0
55	MG	2B	3017	1/1	0.69	0.21	91,91,91,91	0
55	MG	1A	3701	1/1	0.69	0.35	44,44,44,44	0
55	MG	2A	3042	1/1	0.69	0.63	59,59,59,59	0
55	MG	2A	3748	1/1	0.69	0.11	66,66,66,66	0
55	MG	1A	3130	1/1	0.70	0.24	65,65,65,65	0
55	MG	1A	3855	1/1	0.70	0.23	51,51,51,51	0
55	MG	2A	3678	1/1	0.70	0.09	91,91,91,91	0
55	MG	2A	3131	1/1	0.70	0.51	71,71,71,71	0
55	MG	1A	3861	1/1	0.70	0.08	75,75,75,75	0
55	MG	2B	3015	1/1	0.70	0.12	79,79,79,79	0
55	MG	1A	3530	1/1	0.70	0.17	63,63,63,63	0
55	MG	1A	3832	1/1	0.70	0.08	72,72,72,72	0
55	MG	2A	3258	1/1	0.70	0.21	84,84,84,84	0
55	MG	1A	3243	1/1	0.70	0.26	62,62,62,62	0
55	MG	2a	1654	1/1	0.70	0.69	79,79,79,79	0
58	A	2A	3816	1/23	0.70	1.02	85,85,85,85	0
55	MG	1a	3140	1/1	0.71	0.20	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3484	1/1	0.71	0.32	62,62,62,62	0
55	MG	1a	3149	1/1	0.71	0.24	97,97,97,97	0
55	MG	1A	3072	1/1	0.71	0.38	42,42,42,42	0
55	MG	2a	1604	1/1	0.71	0.17	61,61,61,61	0
55	MG	2A	3602	1/1	0.71	0.14	73,73,73,73	0
55	MG	2A	3606	1/1	0.71	0.15	69,69,69,69	0
55	MG	1A	3514	1/1	0.71	0.43	38,38,38,38	0
55	MG	2A	3340	1/1	0.71	0.18	72,72,72,72	0
55	MG	2a	1643	1/1	0.72	0.16	78,78,78,78	0
55	MG	2A	3255	1/1	0.72	0.40	67,67,67,67	0
55	MG	1A	3531	1/1	0.72	0.20	68,68,68,68	0
55	MG	2A	3834	1/1	0.72	0.27	68,68,68,68	0
55	MG	2B	3011	1/1	0.72	0.15	88,88,88,88	0
55	MG	1a	3063	1/1	0.72	0.89	65,65,65,65	0
55	MG	1a	3176	1/1	0.72	0.17	91,91,91,91	0
55	MG	1a	3049	1/1	0.72	0.67	78,78,78,78	0
55	MG	2A	3509	1/1	0.72	0.16	99,99,99,99	0
55	MG	2A	3444	1/1	0.72	0.29	57,57,57,57	0
55	MG	2A	3170	1/1	0.72	0.21	71,71,71,71	0
55	MG	2A	3028	1/1	0.72	0.40	61,61,61,61	0
55	MG	2A	3801	1/1	0.72	0.31	86,86,86,86	0
55	MG	2a	1624	1/1	0.72	0.14	78,78,78,78	0
55	MG	2A	3138	1/1	0.73	0.42	53,53,53,53	0
55	MG	1A	3030	1/1	0.73	0.20	39,39,39,39	0
55	MG	1A	3642	1/1	0.73	0.34	28,28,28,28	0
55	MG	2A	3814	1/1	0.73	0.20	76,76,76,76	0
55	MG	1A	3661	1/1	0.73	0.11	55,55,55,55	0
55	MG	2A	3057	1/1	0.73	0.38	48,48,48,48	0
55	MG	2A	3276	1/1	0.73	0.10	61,61,61,61	0
55	MG	1A	3700	1/1	0.73	0.42	47,47,47,47	0
55	MG	1A	3062	1/1	0.73	0.63	49,49,49,49	0
55	MG	1A	3433	1/1	0.73	0.07	81,81,81,81	0
55	MG	1A	3195	1/1	0.73	0.28	46,46,46,46	0
55	MG	2D	304	1/1	0.73	0.87	58,58,58,58	0
55	MG	1A	3887	1/1	0.73	0.19	58,58,58,58	0
55	MG	1A	3757	1/1	0.73	0.40	59,59,59,59	0
55	MG	1A	3904	1/1	0.73	0.58	53,53,53,53	0
55	MG	1A	3805	1/1	0.74	0.14	72,72,72,72	0
55	MG	2A	3519	1/1	0.74	0.17	68,68,68,68	0
55	MG	1a	3038	1/1	0.74	0.77	78,78,78,78	0
55	MG	2a	1603	1/1	0.74	0.74	65,65,65,65	0
55	MG	2A	3075	1/1	0.74	0.30	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1620	1/1	0.74	0.45	76,76,76,76	0
55	MG	1A	3226	1/1	0.74	0.29	31,31,31,31	0
55	MG	1A	3728	1/1	0.74	0.17	53,53,53,53	0
55	MG	2A	3104	1/1	0.74	0.34	57,57,57,57	0
55	MG	1A	3311	1/1	0.74	0.29	52,52,52,52	0
55	MG	2A	3589	1/1	0.74	0.28	80,80,80,80	0
55	MG	2a	1727	1/1	0.74	0.24	92,92,92,92	0
55	MG	1a	3069	1/1	0.74	0.29	65,65,65,65	0
55	MG	1a	3217	1/1	0.74	0.17	81,81,81,81	0
55	MG	2A	3815	1/1	0.74	0.43	79,79,79,79	0
55	MG	1a	3218	1/1	0.74	0.24	82,82,82,82	0
55	MG	2A	3013	1/1	0.74	0.23	65,65,65,65	0
55	MG	2A	3631	1/1	0.74	0.44	80,80,80,80	0
55	MG	1A	3035	1/1	0.74	0.21	42,42,42,42	0
55	MG	2A	3150	1/1	0.74	0.26	50,50,50,50	0
55	MG	2A	3160	1/1	0.74	0.39	52,52,52,52	0
55	MG	1A	3760	1/1	0.74	0.12	60,60,60,60	0
55	MG	1A	3150	1/1	0.75	0.23	62,62,62,62	0
55	MG	2A	3804	1/1	0.75	0.10	75,75,75,75	0
55	MG	2A	3101	1/1	0.75	0.27	66,66,66,66	0
55	MG	1A	3219	1/1	0.75	0.87	76,76,76,76	0
55	MG	1a	3066	1/1	0.75	0.11	75,75,75,75	0
55	MG	1A	3454	1/1	0.75	0.39	61,61,61,61	0
55	MG	2a	1655	1/1	0.75	0.37	70,70,70,70	0
55	MG	2a	1718	1/1	0.75	0.17	88,88,88,88	0
55	MG	2A	3829	1/1	0.75	0.39	60,60,60,60	0
55	MG	1A	3665	1/1	0.75	0.22	49,49,49,49	0
55	MG	1a	3005	1/1	0.75	0.17	67,67,67,67	0
55	MG	1a	3013	1/1	0.75	0.10	79,79,79,79	0
55	MG	2A	3412	1/1	0.75	0.17	72,72,72,72	0
55	MG	2a	1746	1/1	0.75	0.12	89,89,89,89	0
55	MG	1A	3093	1/1	0.75	0.24	41,41,41,41	0
55	MG	1a	3039	1/1	0.75	0.43	68,68,68,68	0
55	MG	2a	1773	1/1	0.75	0.10	91,91,91,91	0
55	MG	2B	3018	1/1	0.75	0.19	74,74,74,74	0
55	MG	2A	3464	1/1	0.75	0.15	83,83,83,83	0
55	MG	2A	3582	1/1	0.75	0.28	67,67,67,67	0
55	MG	2A	3058	1/1	0.75	0.20	60,60,60,60	0
55	MG	1A	3845	1/1	0.75	0.18	47,47,47,47	0
55	MG	2Q	204	1/1	0.75	0.51	69,69,69,69	0
55	MG	2A	3299	1/1	0.76	0.15	46,46,46,46	0
55	MG	2a	1633	1/1	0.76	0.36	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3302	1/1	0.76	0.14	47,47,47,47	0
55	MG	1a	3150	1/1	0.76	0.23	94,94,94,94	0
55	MG	2A	3141	1/1	0.76	0.48	51,51,51,51	0
55	MG	2A	3533	1/1	0.76	1.28	79,79,79,79	0
55	MG	2A	3694	1/1	0.76	0.10	61,61,61,61	0
55	MG	2A	3148	1/1	0.76	0.27	72,72,72,72	0
55	MG	1A	3171	1/1	0.76	0.29	48,48,48,48	0
55	MG	2A	3151	1/1	0.76	0.92	50,50,50,50	0
55	MG	2a	1732	1/1	0.76	0.13	83,83,83,83	0
55	MG	1A	3319	1/1	0.76	0.21	64,64,64,64	0
55	MG	2A	3457	1/1	0.76	0.16	77,77,77,77	0
55	MG	1A	3877	1/1	0.76	0.14	69,69,69,69	0
55	MG	1a	3136	1/1	0.76	0.57	82,82,82,82	0
55	MG	1A	3880	1/1	0.76	0.09	73,73,73,73	0
55	MG	1A	3724	1/1	0.76	0.41	40,40,40,40	0
55	MG	2X	102	1/1	0.76	0.44	82,82,82,82	0
55	MG	28	101	1/1	0.76	0.60	67,67,67,67	0
55	MG	2A	3808	1/1	0.76	0.31	73,73,73,73	0
55	MG	2A	3260	1/1	0.76	0.31	74,74,74,74	0
55	MG	1d	505	1/1	0.76	0.10	76,76,76,76	0
55	MG	2A	3594	1/1	0.77	0.12	55,55,55,55	0
55	MG	1A	3766	1/1	0.77	0.08	58,58,58,58	0
55	MG	2A	3337	1/1	0.77	0.04	74,74,74,74	0
55	MG	1a	3175	1/1	0.77	0.17	87,87,87,87	0
55	MG	10	101	1/1	0.77	0.38	51,51,51,51	0
55	MG	2a	1729	1/1	0.77	0.19	68,68,68,68	0
55	MG	1a	3074	1/1	0.77	0.48	70,70,70,70	0
55	MG	1A	3139	1/1	0.77	0.30	38,38,38,38	0
55	MG	2a	1733	1/1	0.77	0.53	66,66,66,66	0
55	MG	2A	3424	1/1	0.77	0.21	76,76,76,76	0
55	MG	1B	216	1/1	0.77	0.17	74,74,74,74	0
55	MG	2a	1601	1/1	0.77	0.31	59,59,59,59	0
55	MG	1a	3117	1/1	0.77	0.32	71,71,71,71	0
55	MG	2a	1771	1/1	0.77	0.37	83,83,83,83	0
55	MG	1A	3890	1/1	0.77	0.20	45,45,45,45	0
55	MG	1A	3396	1/1	0.77	0.32	40,40,40,40	0
55	MG	2A	3706	1/1	0.77	0.07	93,93,93,93	0
55	MG	1A	3899	1/1	0.77	0.10	52,52,52,52	0
55	MG	2a	1641	1/1	0.77	0.96	65,65,65,65	0
55	MG	1A	3685	1/1	0.77	0.13	31,31,31,31	0
55	MG	1A	3567	1/1	0.77	0.18	51,51,51,51	0
55	MG	2A	3183	1/1	0.78	0.58	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3188	1/1	0.78	0.43	57,57,57,57	0
55	MG	1a	3114	1/1	0.78	0.10	79,79,79,79	0
55	MG	1a	3048	1/1	0.78	0.13	75,75,75,75	0
55	MG	1a	3129	1/1	0.78	0.11	83,83,83,83	0
55	MG	2a	1659	1/1	0.78	0.13	76,76,76,76	0
55	MG	2A	3008	1/1	0.78	0.37	68,68,68,68	0
55	MG	2A	3292	1/1	0.78	0.08	55,55,55,55	0
55	MG	1F	301	1/1	0.78	0.20	51,51,51,51	0
55	MG	1A	3131	1/1	0.78	0.21	44,44,44,44	0
55	MG	1A	3816	1/1	0.78	0.27	72,72,72,72	0
55	MG	1A	3179	1/1	0.78	0.35	44,44,44,44	0
55	MG	2A	3538	1/1	0.78	0.07	73,73,73,73	0
55	MG	1A	3725	1/1	0.78	0.25	33,33,33,33	0
55	MG	2G	3003	1/1	0.78	0.10	83,83,83,83	0
55	MG	1a	3152	1/1	0.78	0.14	90,90,90,90	0
55	MG	1a	3073	1/1	0.78	0.17	75,75,75,75	0
55	MG	2A	3754	1/1	0.78	0.18	85,85,85,85	0
55	MG	2A	3416	1/1	0.78	0.53	50,50,50,50	0
55	MG	27	102	1/1	0.78	0.17	72,72,72,72	0
55	MG	2A	3787	1/1	0.78	0.18	84,84,84,84	0
55	MG	2A	3422	1/1	0.78	0.12	71,71,71,71	0
55	MG	1A	3123	1/1	0.78	0.18	61,61,61,61	0
55	MG	2A	3161	1/1	0.78	0.28	83,83,83,83	0
55	MG	1A	3848	1/1	0.78	0.27	60,60,60,60	0
55	MG	1A	3920	1/1	0.78	0.40	45,45,45,45	0
55	MG	2A	3132	1/1	0.79	0.72	68,68,68,68	0
55	MG	2A	3263	1/1	0.79	0.17	65,65,65,65	0
55	MG	2A	3811	1/1	0.79	0.48	57,57,57,57	0
55	MG	1A	3647	1/1	0.79	0.05	85,85,85,85	0
55	MG	2a	1636	1/1	0.79	0.30	67,67,67,67	0
55	MG	1A	3655	1/1	0.79	0.18	72,72,72,72	0
55	MG	1B	224	1/1	0.79	0.18	55,55,55,55	0
55	MG	1A	3169	1/1	0.79	0.36	37,37,37,37	0
55	MG	2A	3303	1/1	0.79	0.09	73,73,73,73	0
55	MG	1A	3174	1/1	0.79	0.71	60,60,60,60	0
55	MG	2a	1714	1/1	0.79	0.36	73,73,73,73	0
55	MG	2A	3682	1/1	0.79	0.21	68,68,68,68	0
55	MG	1A	3501	1/1	0.79	0.19	58,58,58,58	0
55	MG	1a	3194	1/1	0.79	0.11	80,80,80,80	0
55	MG	2a	1725	1/1	0.79	0.12	89,89,89,89	0
55	MG	1A	3729	1/1	0.79	0.17	68,68,68,68	0
55	MG	1A	3622	1/1	0.79	0.27	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3561	1/1	0.79	0.17	55,55,55,55	0
55	MG	1a	3144	1/1	0.79	0.39	74,74,74,74	0
55	MG	2F	305	1/1	0.79	0.19	51,51,51,51	0
55	MG	2A	3105	1/1	0.79	0.14	83,83,83,83	0
55	MG	2A	3439	1/1	0.79	0.15	73,73,73,73	0
55	MG	2A	3765	1/1	0.79	0.42	60,60,60,60	0
55	MG	2A	3766	1/1	0.79	0.13	78,78,78,78	0
55	MG	2R	8001	1/1	0.79	0.35	77,77,77,77	0
55	MG	2V	202	1/1	0.79	0.17	70,70,70,70	0
55	MG	2A	3002	1/1	0.79	0.23	68,68,68,68	0
55	MG	20	103	1/1	0.79	0.20	77,77,77,77	0
55	MG	2A	3228	1/1	0.79	0.33	84,84,84,84	0
55	MG	10	103	1/1	0.79	0.11	51,51,51,51	0
55	MG	2A	3011	1/1	0.79	0.41	57,57,57,57	0
55	MG	2A	3605	1/1	0.79	0.38	68,68,68,68	0
55	MG	1A	3723	1/1	0.80	0.10	77,77,77,77	0
55	MG	1A	3482	1/1	0.80	0.27	64,64,64,64	0
55	MG	2A	3795	1/1	0.80	0.59	61,61,61,61	0
55	MG	2A	3798	1/1	0.80	0.14	81,81,81,81	0
55	MG	1a	3022	1/1	0.80	0.68	66,66,66,66	0
55	MG	2A	3250	1/1	0.80	0.15	68,68,68,68	0
55	MG	2A	3109	1/1	0.80	0.50	63,63,63,63	0
55	MG	2A	3461	1/1	0.80	0.25	72,72,72,72	0
55	MG	1A	3806	1/1	0.80	0.18	59,59,59,59	0
55	MG	1A	3143	1/1	0.80	0.48	69,69,69,69	0
55	MG	2a	1644	1/1	0.80	0.29	71,71,71,71	0
55	MG	1A	3824	1/1	0.80	0.15	57,57,57,57	0
55	MG	1D	303	1/1	0.80	0.62	48,48,48,48	0
55	MG	2A	3819	1/1	0.80	0.86	51,51,51,51	0
55	MG	2A	3671	1/1	0.80	0.14	76,76,76,76	0
55	MG	1a	3057	1/1	0.80	0.48	89,89,89,89	0
55	MG	2B	3005	1/1	0.80	0.14	71,71,71,71	0
55	MG	1A	3536	1/1	0.80	0.17	56,56,56,56	0
55	MG	2A	3041	1/1	0.80	0.83	62,62,62,62	0
55	MG	2A	3681	1/1	0.80	0.06	65,65,65,65	0
55	MG	1A	3628	1/1	0.80	0.20	66,66,66,66	0
55	MG	2A	3513	1/1	0.80	0.85	62,62,62,62	0
55	MG	2A	3327	1/1	0.80	0.20	88,88,88,88	0
55	MG	1A	3752	1/1	0.80	0.14	65,65,65,65	0
55	MG	1a	3157	1/1	0.80	0.11	75,75,75,75	0
55	MG	2F	303	1/1	0.80	0.31	57,57,57,57	0
55	MG	2a	1747	1/1	0.80	0.15	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3725	1/1	0.80	0.09	58,58,58,58	0
55	MG	2A	3343	1/1	0.80	0.29	79,79,79,79	0
55	MG	1A	3547	1/1	0.80	0.23	29,29,29,29	0
55	MG	1A	3021	1/1	0.80	0.12	50,50,50,50	0
55	MG	2A	3076	1/1	0.80	0.34	50,50,50,50	0
55	MG	2A	3558	1/1	0.80	0.19	67,67,67,67	0
55	MG	1A	3258	1/1	0.80	0.14	53,53,53,53	0
55	MG	1A	3856	1/1	0.80	0.26	53,53,53,53	0
55	MG	2A	3777	1/1	0.80	0.21	83,83,83,83	0
55	MG	2A	3785	1/1	0.80	0.08	53,53,53,53	0
55	MG	2A	3803	1/1	0.81	0.20	47,47,47,47	0
55	MG	1A	3528	1/1	0.81	0.20	61,61,61,61	0
55	MG	2A	3129	1/1	0.81	0.17	64,64,64,64	0
55	MG	2A	3130	1/1	0.81	0.41	66,66,66,66	0
55	MG	2A	3668	1/1	0.81	0.14	72,72,72,72	0
55	MG	2A	3481	1/1	0.81	0.56	57,57,57,57	0
55	MG	1A	3849	1/1	0.81	0.23	86,86,86,86	0
55	MG	1A	3026	1/1	0.81	0.21	59,59,59,59	0
55	MG	1a	3146	1/1	0.81	0.12	71,71,71,71	0
55	MG	2a	1645	1/1	0.81	0.21	64,64,64,64	0
55	MG	2A	3035	1/1	0.81	0.16	53,53,53,53	0
55	MG	2A	3305	1/1	0.81	0.09	52,52,52,52	0
55	MG	2A	3686	1/1	0.81	0.10	93,93,93,93	0
55	MG	2a	1682	1/1	0.81	0.16	78,78,78,78	0
55	MG	2a	1708	1/1	0.81	0.10	89,89,89,89	0
55	MG	1A	3170	1/1	0.81	0.31	40,40,40,40	0
55	MG	1A	3374	1/1	0.81	0.08	74,74,74,74	0
55	MG	1A	3240	1/1	0.81	0.31	42,42,42,42	0
55	MG	2A	3712	1/1	0.81	0.14	69,69,69,69	0
55	MG	2A	3050	1/1	0.81	0.20	63,63,63,63	0
55	MG	1A	3862	1/1	0.81	0.36	55,55,55,55	0
55	MG	1A	3550	1/1	0.81	0.37	47,47,47,47	0
55	MG	1A	3878	1/1	0.81	0.13	36,36,36,36	0
55	MG	1A	3697	1/1	0.81	0.31	64,64,64,64	0
55	MG	1A	3147	1/1	0.81	0.21	62,62,62,62	0
55	MG	2G	3002	1/1	0.81	0.18	79,79,79,79	0
55	MG	2A	3564	1/1	0.81	0.13	58,58,58,58	0
55	MG	1A	3246	1/1	0.81	0.12	87,87,87,87	0
55	MG	2P	201	1/1	0.81	0.33	67,67,67,67	0
55	MG	2A	3771	1/1	0.81	0.15	65,65,65,65	0
55	MG	2A	3427	1/1	0.81	0.43	81,81,81,81	0
55	MG	1A	3252	1/1	0.81	0.80	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3200	1/1	0.81	0.53	65,65,65,65	0
55	MG	1A	3101	1/1	0.81	0.52	55,55,55,55	0
55	MG	1A	3209	1/1	0.81	0.43	49,49,49,49	0
55	MG	1A	3623	1/1	0.81	0.34	43,43,43,43	0
55	MG	1A	3177	1/1	0.81	0.54	54,54,54,54	0
56	ZN	14	501	1/1	0.81	0.05	149,149,149,149	0
55	MG	2A	3621	1/1	0.81	0.73	64,64,64,64	0
55	MG	1a	3197	1/1	0.82	0.12	78,78,78,78	0
55	MG	2A	3380	1/1	0.82	0.10	83,83,83,83	0
55	MG	2A	3690	1/1	0.82	0.22	82,82,82,82	0
55	MG	2A	3821	1/1	0.82	0.30	54,54,54,54	0
55	MG	2A	3545	1/1	0.82	0.07	84,84,84,84	0
55	MG	2A	3173	1/1	0.82	0.97	72,72,72,72	0
55	MG	2B	3002	1/1	0.82	0.12	67,67,67,67	0
55	MG	2a	1652	1/1	0.82	0.11	65,65,65,65	0
55	MG	1A	3267	1/1	0.82	0.12	77,77,77,77	0
55	MG	1A	3166	1/1	0.82	0.18	54,54,54,54	0
55	MG	2a	1657	1/1	0.82	0.34	64,64,64,64	0
55	MG	1A	3167	1/1	0.82	0.11	54,54,54,54	0
55	MG	2A	3194	1/1	0.82	0.08	83,83,83,83	0
55	MG	2a	1696	1/1	0.82	0.07	78,78,78,78	0
55	MG	2a	1697	1/1	0.82	0.07	79,79,79,79	0
55	MG	1A	3207	1/1	0.82	0.29	35,35,35,35	0
55	MG	2a	1710	1/1	0.82	0.16	84,84,84,84	0
55	MG	1A	3236	1/1	0.82	0.27	53,53,53,53	0
55	MG	1A	3382	1/1	0.82	0.54	58,58,58,58	0
55	MG	2A	3009	1/1	0.82	0.69	64,64,64,64	0
55	MG	1A	3632	1/1	0.82	0.29	53,53,53,53	0
55	MG	2F	301	1/1	0.82	0.30	52,52,52,52	0
55	MG	1A	3257	1/1	0.82	0.54	44,44,44,44	0
55	MG	2A	3019	1/1	0.82	0.20	43,43,43,43	0
55	MG	1A	3118	1/1	0.82	0.31	39,39,39,39	0
55	MG	2A	3774	1/1	0.82	0.22	81,81,81,81	0
55	MG	1A	3444	1/1	0.82	0.22	57,57,57,57	0
55	MG	1A	3260	1/1	0.82	0.18	75,75,75,75	0
55	MG	2A	3479	1/1	0.82	0.11	73,73,73,73	0
55	MG	1A	3907	1/1	0.82	0.44	58,58,58,58	0
55	MG	1A	3477	1/1	0.82	0.17	40,40,40,40	0
55	MG	2A	3647	1/1	0.82	0.19	77,77,77,77	0
55	MG	2a	1755	1/1	0.82	0.13	66,66,66,66	0
55	MG	2A	3650	1/1	0.82	0.35	57,57,57,57	0
55	MG	2A	3802	1/1	0.82	0.68	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2I	102	1/1	0.82	0.19	66,66,66,66	0
55	MG	1A	3670	1/1	0.82	0.27	51,51,51,51	0
55	MG	1a	3184	1/1	0.82	0.15	82,82,82,82	0
55	MG	2A	3329	1/1	0.82	0.44	72,72,72,72	0
55	MG	1a	3186	1/1	0.82	0.08	69,69,69,69	0
55	MG	1A	3683	1/1	0.82	0.16	50,50,50,50	0
55	MG	1a	3196	1/1	0.82	0.13	82,82,82,82	0
55	MG	20	102	1/1	0.83	0.31	63,63,63,63	0
55	MG	1g	3001	1/1	0.83	0.25	79,79,79,79	0
55	MG	1h	3001	1/1	0.83	0.56	52,52,52,52	0
55	MG	2A	3768	1/1	0.83	0.44	94,94,94,94	0
55	MG	2A	3326	1/1	0.83	0.13	69,69,69,69	0
55	MG	1A	3039	1/1	0.83	0.34	55,55,55,55	0
55	MG	1a	3131	1/1	0.83	0.17	70,70,70,70	0
55	MG	2A	3336	1/1	0.83	0.80	76,76,76,76	0
55	MG	1A	3558	1/1	0.83	0.19	72,72,72,72	0
55	MG	2A	3010	1/1	0.83	0.20	62,62,62,62	0
55	MG	1A	3431	1/1	0.83	0.58	53,53,53,53	0
55	MG	2A	3585	1/1	0.83	0.19	75,75,75,75	0
55	MG	2a	1638	1/1	0.83	0.86	70,70,70,70	0
55	MG	1A	3142	1/1	0.83	0.47	43,43,43,43	0
55	MG	1a	3019	1/1	0.83	0.15	67,67,67,67	0
55	MG	2A	3385	1/1	0.83	0.23	86,86,86,86	0
55	MG	2A	3027	1/1	0.83	0.35	66,66,66,66	0
55	MG	2a	1646	1/1	0.83	0.41	62,62,62,62	0
55	MG	1A	3919	1/1	0.83	0.45	33,33,33,33	0
55	MG	1A	3786	1/1	0.83	0.30	58,58,58,58	0
55	MG	2A	3162	1/1	0.83	0.76	79,79,79,79	0
55	MG	1A	3803	1/1	0.83	0.10	78,78,78,78	0
55	MG	2A	3172	1/1	0.83	0.39	64,64,64,64	0
55	MG	2A	3431	1/1	0.83	0.15	74,74,74,74	0
55	MG	2A	3638	1/1	0.83	0.19	85,85,85,85	0
55	MG	2A	3641	1/1	0.83	0.16	72,72,72,72	0
55	MG	2A	3643	1/1	0.83	0.51	56,56,56,56	0
55	MG	1A	3857	1/1	0.83	0.16	67,67,67,67	0
55	MG	1A	3804	1/1	0.83	0.10	71,71,71,71	0
55	MG	2A	3655	1/1	0.83	0.24	60,60,60,60	0
55	MG	2A	3179	1/1	0.83	0.72	63,63,63,63	0
55	MG	2B	3007	1/1	0.83	0.14	79,79,79,79	0
55	MG	1B	217	1/1	0.83	0.08	57,57,57,57	0
55	MG	1A	3603	1/1	0.83	0.48	46,46,46,46	0
55	MG	2A	3674	1/1	0.83	0.12	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2B	3014	1/1	0.83	0.09	73,73,73,73	0
55	MG	1A	3188	1/1	0.83	0.35	44,44,44,44	0
55	MG	1A	3034	1/1	0.83	0.19	60,60,60,60	0
55	MG	2a	1737	1/1	0.83	0.84	87,87,87,87	0
55	MG	2A	3203	1/1	0.83	1.25	58,58,58,58	0
55	MG	2A	3209	1/1	0.83	0.07	89,89,89,89	0
55	MG	1A	3468	1/1	0.83	0.17	30,30,30,30	0
55	MG	2A	3243	1/1	0.83	0.46	55,55,55,55	0
55	MG	2a	1752	1/1	0.83	0.49	69,69,69,69	0
55	MG	1A	3882	1/1	0.83	0.19	67,67,67,67	0
55	MG	2A	3486	1/1	0.83	0.15	57,57,57,57	0
55	MG	1A	3215	1/1	0.83	0.21	51,51,51,51	0
55	MG	2A	3707	1/1	0.83	0.15	73,73,73,73	0
55	MG	1A	3245	1/1	0.83	0.10	74,74,74,74	0
55	MG	1A	3840	1/1	0.83	0.26	64,64,64,64	0
55	MG	1a	3216	1/1	0.83	0.11	96,96,96,96	0
55	MG	1a	3079	1/1	0.83	0.14	54,54,54,54	0
55	MG	1A	3843	1/1	0.83	0.22	47,47,47,47	0
55	MG	1a	3226	1/1	0.83	0.41	74,74,74,74	0
55	MG	1P	202	1/1	0.83	0.19	85,85,85,85	0
55	MG	1A	3903	1/1	0.84	0.10	34,34,34,34	0
55	MG	2A	3612	1/1	0.84	0.18	41,41,41,41	0
55	MG	2a	1607	1/1	0.84	0.88	73,73,73,73	0
55	MG	2A	3229	1/1	0.84	0.46	64,64,64,64	0
55	MG	1A	3552	1/1	0.84	0.20	64,64,64,64	0
55	MG	2A	3030	1/1	0.84	0.25	66,66,66,66	0
55	MG	1a	3208	1/1	0.84	0.29	70,70,70,70	0
55	MG	2A	3462	1/1	0.84	0.19	62,62,62,62	0
55	MG	1A	3164	1/1	0.84	0.29	78,78,78,78	0
55	MG	1A	3182	1/1	0.84	0.41	38,38,38,38	0
55	MG	1A	3259	1/1	0.84	0.24	36,36,36,36	0
55	MG	2A	3147	1/1	0.84	0.17	81,81,81,81	0
55	MG	2A	3277	1/1	0.84	0.17	54,54,54,54	0
55	MG	1F	302	1/1	0.84	0.43	37,37,37,37	0
55	MG	2A	3297	1/1	0.84	0.13	68,68,68,68	0
55	MG	2A	3053	1/1	0.84	0.96	60,60,60,60	0
55	MG	2A	3835	1/1	0.84	1.05	65,65,65,65	0
55	MG	2A	3838	1/1	0.84	0.38	54,54,54,54	0
55	MG	1a	3222	1/1	0.84	0.35	72,72,72,72	0
55	MG	2A	3154	1/1	0.84	0.73	53,53,53,53	0
55	MG	1A	3572	1/1	0.84	0.23	67,67,67,67	0
55	MG	1A	3932	1/1	0.84	0.33	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1B	204	1/1	0.84	0.27	72,72,72,72	0
55	MG	2A	3169	1/1	0.84	0.29	73,73,73,73	0
55	MG	2A	3085	1/1	0.84	0.17	67,67,67,67	0
55	MG	2A	3534	1/1	0.84	0.16	82,82,82,82	0
55	MG	1a	3071	1/1	0.84	0.28	56,56,56,56	0
55	MG	2A	3542	1/1	0.84	0.23	75,75,75,75	0
55	MG	1y	101	1/1	0.84	0.35	50,50,50,50	0
55	MG	2A	3177	1/1	0.84	0.98	50,50,50,50	0
55	MG	2a	1730	1/1	0.84	0.13	84,84,84,84	0
55	MG	2A	3716	1/1	0.84	0.10	85,85,85,85	0
55	MG	2A	3553	1/1	0.84	0.13	66,66,66,66	0
55	MG	2A	3347	1/1	0.84	0.05	72,72,72,72	0
55	MG	2F	309	1/1	0.84	0.14	72,72,72,72	0
55	MG	2A	3374	1/1	0.84	0.59	60,60,60,60	0
55	MG	1A	3218	1/1	0.84	0.22	53,53,53,53	0
55	MG	2A	3378	1/1	0.84	0.07	58,58,58,58	0
55	MG	1A	3253	1/1	0.84	0.42	63,63,63,63	0
55	MG	1A	3541	1/1	0.84	0.30	55,55,55,55	0
55	MG	1A	3671	1/1	0.84	0.17	46,46,46,46	0
55	MG	2A	3192	1/1	0.84	0.66	64,64,64,64	0
55	MG	2a	1769	1/1	0.84	0.23	83,83,83,83	0
55	MG	1A	3211	1/1	0.84	0.40	41,41,41,41	0
55	MG	2A	3197	1/1	0.84	0.28	53,53,53,53	0
55	MG	2a	1785	1/1	0.84	0.17	83,83,83,83	0
55	MG	2A	3115	1/1	0.84	0.29	65,65,65,65	0
55	MG	2A	3603	1/1	0.84	0.12	70,70,70,70	0
55	MG	2A	3604	1/1	0.84	0.30	77,77,77,77	0
55	MG	2g	3001	1/1	0.84	0.18	75,75,75,75	0
55	MG	27	101	1/1	0.84	0.33	57,57,57,57	0
55	MG	1A	3315	1/1	0.84	0.07	74,74,74,74	0
55	MG	1a	3036	1/1	0.84	0.20	50,50,50,50	0
55	MG	2A	3608	1/1	0.84	0.15	63,63,63,63	0
55	MG	1A	3566	1/1	0.85	0.18	70,70,70,70	0
55	MG	2A	3644	1/1	0.85	0.44	66,66,66,66	0
55	MG	2A	3499	1/1	0.85	0.38	51,51,51,51	0
55	MG	2A	3159	1/1	0.85	0.43	53,53,53,53	0
55	MG	1A	3876	1/1	0.85	0.07	61,61,61,61	0
55	MG	2A	3658	1/1	0.85	0.26	76,76,76,76	0
55	MG	2A	3054	1/1	0.85	0.34	54,54,54,54	0
55	MG	18	3302	1/1	0.85	0.60	43,43,43,43	0
55	MG	2A	3166	1/1	0.85	0.28	54,54,54,54	0
55	MG	1A	3287	1/1	0.85	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3162	1/1	0.85	0.24	62,62,62,62	0
55	MG	2A	3338	1/1	0.85	0.22	55,55,55,55	0
55	MG	1a	3018	1/1	0.85	0.11	66,66,66,66	0
55	MG	2A	3077	1/1	0.85	0.34	58,58,58,58	0
55	MG	1A	3472	1/1	0.85	0.15	64,64,64,64	0
55	MG	1d	502	1/1	0.85	0.28	71,71,71,71	0
55	MG	1d	504	1/1	0.85	0.21	77,77,77,77	0
55	MG	1A	3837	1/1	0.85	0.13	78,78,78,78	0
55	MG	2A	3184	1/1	0.85	0.64	57,57,57,57	0
55	MG	1a	3033	1/1	0.85	0.12	56,56,56,56	0
55	MG	1A	3392	1/1	0.85	0.37	57,57,57,57	0
55	MG	1A	3148	1/1	0.85	0.47	48,48,48,48	0
55	MG	2a	1721	1/1	0.85	0.14	86,86,86,86	0
55	MG	2A	3110	1/1	0.85	0.61	58,58,58,58	0
55	MG	2A	3579	1/1	0.85	0.17	61,61,61,61	0
55	MG	2a	1726	1/1	0.85	0.15	73,73,73,73	0
55	MG	2A	3581	1/1	0.85	0.09	73,73,73,73	0
55	MG	2A	3737	1/1	0.85	0.12	79,79,79,79	0
55	MG	1A	3104	1/1	0.85	0.21	42,42,42,42	0
55	MG	2A	3749	1/1	0.85	0.06	81,81,81,81	0
55	MG	1a	3041	1/1	0.85	0.11	76,76,76,76	0
55	MG	2A	3587	1/1	0.85	0.06	63,63,63,63	0
55	MG	1D	301	1/1	0.85	0.45	54,54,54,54	0
55	MG	1A	3499	1/1	0.85	0.13	62,62,62,62	0
55	MG	1D	312	1/1	0.85	0.26	65,65,65,65	0
55	MG	2A	3240	1/1	0.85	0.15	50,50,50,50	0
55	MG	1A	3551	1/1	0.85	0.27	36,36,36,36	0
55	MG	1A	3357	1/1	0.85	0.06	75,75,75,75	0
55	MG	20	101	1/1	0.85	0.27	84,84,84,84	0
55	MG	2A	3458	1/1	0.85	0.12	74,74,74,74	0
55	MG	2a	1759	1/1	0.85	0.04	86,86,86,86	0
55	MG	1A	3706	1/1	0.85	0.40	70,70,70,70	0
55	MG	1a	3180	1/1	0.85	0.20	97,97,97,97	0
55	MG	1A	3793	1/1	0.85	0.33	60,60,60,60	0
55	MG	2a	1780	1/1	0.85	0.27	73,73,73,73	0
55	MG	1a	3070	1/1	0.85	0.35	60,60,60,60	0
55	MG	1A	3505	1/1	0.85	0.38	50,50,50,50	0
55	MG	1A	3720	1/1	0.85	0.36	64,64,64,64	0
55	MG	2A	3634	1/1	0.85	0.20	81,81,81,81	0
55	MG	2e	202	1/1	0.85	0.31	73,73,73,73	0
55	MG	2A	3045	1/1	0.85	0.11	75,75,75,75	0
55	MG	2h	3002	1/1	0.85	0.24	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3280	1/1	0.85	0.16	33,33,33,33	0
55	MG	2a	1608	1/1	0.85	0.30	57,57,57,57	0
55	MG	2a	1610	1/1	0.85	0.96	70,70,70,70	0
55	MG	2A	3152	1/1	0.85	0.24	66,66,66,66	0
55	MG	25	104	1/1	0.86	0.16	83,83,83,83	0
55	MG	1A	3002	1/1	0.86	0.23	55,55,55,55	0
55	MG	2A	3731	1/1	0.86	0.07	65,65,65,65	0
55	MG	1A	3834	1/1	0.86	0.17	73,73,73,73	0
55	MG	2A	3266	1/1	0.86	0.20	66,66,66,66	0
55	MG	1a	3020	1/1	0.86	0.34	71,71,71,71	0
55	MG	1A	3036	1/1	0.86	0.25	40,40,40,40	0
55	MG	1A	3152	1/1	0.86	0.17	46,46,46,46	0
55	MG	1A	3518	1/1	0.86	0.21	71,71,71,71	0
55	MG	1A	3073	1/1	0.86	0.19	44,44,44,44	0
55	MG	2a	1612	1/1	0.86	0.19	54,54,54,54	0
55	MG	2a	1615	1/1	0.86	1.49	78,78,78,78	0
55	MG	1a	3201	1/1	0.86	0.10	80,80,80,80	0
55	MG	1A	3180	1/1	0.86	0.15	64,64,64,64	0
55	MG	1A	3629	1/1	0.86	0.16	63,63,63,63	0
55	MG	1a	3046	1/1	0.86	0.30	50,50,50,50	0
55	MG	1A	3138	1/1	0.86	0.29	57,57,57,57	0
55	MG	1A	3636	1/1	0.86	0.41	27,27,27,27	0
55	MG	1a	3050	1/1	0.86	0.25	54,54,54,54	0
55	MG	1a	3223	1/1	0.86	0.22	65,65,65,65	0
55	MG	1a	3056	1/1	0.86	0.09	74,74,74,74	0
55	MG	1A	3733	1/1	0.86	0.26	42,42,42,42	0
55	MG	2a	1648	1/1	0.86	0.08	82,82,82,82	0
55	MG	2A	3142	1/1	0.86	0.77	57,57,57,57	0
55	MG	2A	3599	1/1	0.86	0.10	78,78,78,78	0
55	MG	1A	3734	1/1	0.86	0.25	29,29,29,29	0
55	MG	1A	3113	1/1	0.86	0.25	26,26,26,26	0
55	MG	1A	3013	1/1	0.86	0.16	62,62,62,62	0
55	MG	2a	1667	1/1	0.86	0.25	75,75,75,75	0
55	MG	1a	3068	1/1	0.86	0.23	71,71,71,71	0
55	MG	1B	225	1/1	0.86	0.34	68,68,68,68	0
55	MG	1A	3436	1/1	0.86	0.16	58,58,58,58	0
55	MG	1A	3869	1/1	0.86	0.19	40,40,40,40	0
55	MG	1A	3270	1/1	0.86	0.33	60,60,60,60	0
55	MG	1A	3190	1/1	0.86	0.17	72,72,72,72	0
55	MG	1A	3669	1/1	0.86	0.30	62,62,62,62	0
55	MG	2A	3825	1/1	0.86	1.51	60,60,60,60	0
55	MG	2A	3165	1/1	0.86	0.35	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3191	1/1	0.86	0.28	39,39,39,39	0
55	MG	1A	3881	1/1	0.86	0.20	51,51,51,51	0
55	MG	1F	308	1/1	0.86	0.56	62,62,62,62	0
55	MG	1A	3058	1/1	0.86	0.08	50,50,50,50	0
55	MG	2B	3003	1/1	0.86	0.16	71,71,71,71	0
55	MG	1A	3199	1/1	0.86	0.63	41,41,41,41	0
55	MG	2A	3032	1/1	0.86	0.35	63,63,63,63	0
55	MG	1A	3316	1/1	0.86	0.40	69,69,69,69	0
55	MG	1A	3127	1/1	0.86	0.14	36,36,36,36	0
55	MG	1A	3895	1/1	0.86	0.37	45,45,45,45	0
55	MG	2A	3463	1/1	0.86	0.18	77,77,77,77	0
55	MG	2A	3664	1/1	0.86	0.13	81,81,81,81	0
55	MG	1a	3143	1/1	0.86	0.10	82,82,82,82	0
55	MG	11	102	1/1	0.86	0.22	56,56,56,56	0
55	MG	11	103	1/1	0.86	0.20	50,50,50,50	0
55	MG	17	101	1/1	0.86	0.28	64,64,64,64	0
55	MG	1A	3809	1/1	0.86	0.14	35,35,35,35	0
55	MG	18	3303	1/1	0.86	0.04	63,63,63,63	0
55	MG	1a	3004	1/1	0.86	0.19	67,67,67,67	0
55	MG	2A	3065	1/1	0.86	0.08	70,70,70,70	0
55	MG	2A	3488	1/1	0.86	0.17	75,75,75,75	0
55	MG	2a	1775	1/1	0.86	0.10	74,74,74,74	0
55	MG	2A	3223	1/1	0.86	0.16	68,68,68,68	0
55	MG	2A	3691	1/1	0.86	0.08	75,75,75,75	0
55	MG	2a	1786	1/1	0.86	0.12	72,72,72,72	0
55	MG	2A	3693	1/1	0.86	0.06	78,78,78,78	0
55	MG	1a	3153	1/1	0.86	0.12	66,66,66,66	0
55	MG	1A	3322	1/1	0.86	0.17	49,49,49,49	0
55	MG	1a	3164	1/1	0.86	0.20	68,68,68,68	0
55	MG	2A	3512	1/1	0.86	0.59	59,59,59,59	0
55	MG	2A	3078	1/1	0.86	0.23	50,50,50,50	0
55	MG	1a	3007	1/1	0.86	0.28	71,71,71,71	0
55	MG	1A	3602	1/1	0.86	0.18	56,56,56,56	0
55	MG	2A	3721	1/1	0.86	0.23	50,50,50,50	0
55	MG	2A	3098	1/1	0.86	0.23	60,60,60,60	0
55	MG	1A	3217	1/1	0.87	0.45	35,35,35,35	0
55	MG	28	102	1/1	0.87	0.07	73,73,73,73	0
55	MG	2A	3139	1/1	0.87	0.20	51,51,51,51	0
55	MG	2A	3140	1/1	0.87	0.34	56,56,56,56	0
55	MG	1A	3859	1/1	0.87	0.19	81,81,81,81	0
55	MG	2A	3756	1/1	0.87	0.64	86,86,86,86	0
55	MG	2A	3563	1/1	0.87	0.28	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3139	1/1	0.87	0.28	67,67,67,67	0
55	MG	1A	3607	1/1	0.87	0.19	67,67,67,67	0
55	MG	1A	3049	1/1	0.87	0.57	36,36,36,36	0
55	MG	2a	1618	1/1	0.87	0.59	66,66,66,66	0
55	MG	1A	3866	1/1	0.87	0.25	62,62,62,62	0
55	MG	1A	3532	1/1	0.87	0.13	56,56,56,56	0
55	MG	2A	3583	1/1	0.87	0.11	72,72,72,72	0
55	MG	2A	3782	1/1	0.87	0.19	79,79,79,79	0
55	MG	2A	3783	1/1	0.87	0.31	93,93,93,93	0
55	MG	1a	3028	1/1	0.87	0.30	63,63,63,63	0
55	MG	2a	1642	1/1	0.87	0.16	82,82,82,82	0
55	MG	1A	3870	1/1	0.87	0.36	54,54,54,54	0
55	MG	1A	3063	1/1	0.87	0.52	45,45,45,45	0
55	MG	2A	3033	1/1	0.87	0.62	66,66,66,66	0
55	MG	1A	3255	1/1	0.87	0.23	41,41,41,41	0
55	MG	2A	3037	1/1	0.87	0.43	48,48,48,48	0
55	MG	1A	3546	1/1	0.87	0.24	40,40,40,40	0
55	MG	1a	3040	1/1	0.87	0.25	73,73,73,73	0
55	MG	2A	3043	1/1	0.87	0.18	68,68,68,68	0
55	MG	1a	3163	1/1	0.87	0.16	79,79,79,79	0
55	MG	1A	3052	1/1	0.87	0.54	24,24,24,24	0
55	MG	1D	306	1/1	0.87	0.22	45,45,45,45	0
55	MG	2a	1676	1/1	0.87	0.14	65,65,65,65	0
55	MG	1D	310	1/1	0.87	0.13	68,68,68,68	0
55	MG	1A	3235	1/1	0.87	0.42	72,72,72,72	0
55	MG	1A	3054	1/1	0.87	0.22	41,41,41,41	0
55	MG	2a	1707	1/1	0.87	0.10	82,82,82,82	0
55	MG	2A	3445	1/1	0.87	0.41	61,61,61,61	0
55	MG	2A	3448	1/1	0.87	0.15	80,80,80,80	0
55	MG	1a	3054	1/1	0.87	0.19	79,79,79,79	0
55	MG	2a	1717	1/1	0.87	0.06	71,71,71,71	0
55	MG	2A	3063	1/1	0.87	0.22	65,65,65,65	0
55	MG	1A	3638	1/1	0.87	0.25	35,35,35,35	0
55	MG	1A	3836	1/1	0.87	0.14	54,54,54,54	0
55	MG	1A	3889	1/1	0.87	0.09	55,55,55,55	0
55	MG	1A	3239	1/1	0.87	0.45	50,50,50,50	0
55	MG	1a	3199	1/1	0.87	0.14	71,71,71,71	0
55	MG	1A	3089	1/1	0.87	0.19	48,48,48,48	0
55	MG	1A	3090	1/1	0.87	0.22	41,41,41,41	0
55	MG	2A	3661	1/1	0.87	0.11	88,88,88,88	0
55	MG	2A	3094	1/1	0.87	1.35	58,58,58,58	0
55	MG	1A	3044	1/1	0.87	0.23	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1R	203	1/1	0.87	0.26	48,48,48,48	0
55	MG	2a	1734	1/1	0.87	0.06	73,73,73,73	0
55	MG	1A	3406	1/1	0.87	0.21	37,37,37,37	0
55	MG	2A	3673	1/1	0.87	0.22	70,70,70,70	0
55	MG	1A	3568	1/1	0.87	0.29	53,53,53,53	0
55	MG	2A	3244	1/1	0.87	0.06	87,87,87,87	0
55	MG	1A	3193	1/1	0.87	0.36	29,29,29,29	0
55	MG	2A	3254	1/1	0.87	0.12	87,87,87,87	0
55	MG	1A	3853	1/1	0.87	0.09	22,22,22,22	0
55	MG	2A	3256	1/1	0.87	0.14	61,61,61,61	0
55	MG	1a	3225	1/1	0.87	0.10	74,74,74,74	0
55	MG	2G	3001	1/1	0.87	0.19	82,82,82,82	0
55	MG	1A	3579	1/1	0.87	0.52	41,41,41,41	0
55	MG	2A	3114	1/1	0.87	0.40	62,62,62,62	0
55	MG	2A	3528	1/1	0.87	0.09	67,67,67,67	0
55	MG	1A	3764	1/1	0.87	0.09	41,41,41,41	0
55	MG	2A	3705	1/1	0.87	0.21	65,65,65,65	0
55	MG	1a	3096	1/1	0.87	0.17	81,81,81,81	0
55	MG	1a	3097	1/1	0.87	0.10	58,58,58,58	0
55	MG	2a	1792	1/1	0.87	0.20	74,74,74,74	0
55	MG	2A	3536	1/1	0.87	0.15	62,62,62,62	0
55	MG	2A	3537	1/1	0.87	0.73	65,65,65,65	0
55	MG	1A	3929	1/1	0.87	0.64	40,40,40,40	0
55	MG	2A	3540	1/1	0.87	0.07	70,70,70,70	0
55	MG	1A	3299	1/1	0.87	0.21	37,37,37,37	0
55	MG	1a	3124	1/1	0.87	0.30	88,88,88,88	0
55	MG	1B	203	1/1	0.87	0.25	66,66,66,66	0
55	MG	2q	201	1/1	0.87	0.39	63,63,63,63	0
55	MG	2A	3736	1/1	0.87	0.14	88,88,88,88	0
55	MG	2A	3004	1/1	0.87	0.23	52,52,52,52	0
55	MG	2A	3134	1/1	0.88	0.89	70,70,70,70	0
55	MG	1a	3133	1/1	0.88	0.42	77,77,77,77	0
55	MG	1A	3594	1/1	0.88	0.18	59,59,59,59	0
55	MG	1A	3922	1/1	0.88	0.21	39,39,39,39	0
55	MG	1A	3159	1/1	0.88	0.87	40,40,40,40	0
55	MG	2A	3732	1/1	0.88	0.56	60,60,60,60	0
55	MG	2A	3544	1/1	0.88	0.14	89,89,89,89	0
55	MG	1A	3176	1/1	0.88	0.29	45,45,45,45	0
55	MG	2A	3547	1/1	0.88	0.06	67,67,67,67	0
55	MG	2A	3318	1/1	0.88	0.06	77,77,77,77	0
55	MG	1A	3940	1/1	0.88	0.23	40,40,40,40	0
55	MG	2A	3753	1/1	0.88	0.09	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1616	1/1	0.88	0.12	55,55,55,55	0
55	MG	2A	3144	1/1	0.88	0.15	78,78,78,78	0
55	MG	1A	3606	1/1	0.88	0.23	62,62,62,62	0
55	MG	2a	1621	1/1	0.88	0.11	80,80,80,80	0
55	MG	2A	3757	1/1	0.88	0.25	64,64,64,64	0
55	MG	2A	3762	1/1	0.88	0.63	57,57,57,57	0
55	MG	1A	3220	1/1	0.88	0.22	61,61,61,61	0
55	MG	2a	1637	1/1	0.88	0.48	87,87,87,87	0
55	MG	1A	3515	1/1	0.88	0.28	63,63,63,63	0
55	MG	1A	3517	1/1	0.88	0.20	51,51,51,51	0
55	MG	1a	3035	1/1	0.88	1.05	69,69,69,69	0
55	MG	2A	3568	1/1	0.88	0.31	46,46,46,46	0
55	MG	1A	3198	1/1	0.88	0.26	30,30,30,30	0
55	MG	2A	3576	1/1	0.88	0.52	57,57,57,57	0
55	MG	2A	3157	1/1	0.88	0.26	63,63,63,63	0
55	MG	2a	1647	1/1	0.88	0.23	60,60,60,60	0
55	MG	1a	3154	1/1	0.88	0.12	90,90,90,90	0
55	MG	2a	1649	1/1	0.88	0.11	71,71,71,71	0
55	MG	1A	3521	1/1	0.88	0.30	66,66,66,66	0
55	MG	1A	3384	1/1	0.88	0.11	70,70,70,70	0
55	MG	1A	3234	1/1	0.88	0.26	43,43,43,43	0
55	MG	2A	3794	1/1	0.88	0.10	70,70,70,70	0
55	MG	1A	3737	1/1	0.88	0.39	38,38,38,38	0
55	MG	2A	3400	1/1	0.88	0.28	77,77,77,77	0
55	MG	1A	3749	1/1	0.88	0.10	50,50,50,50	0
55	MG	2A	3596	1/1	0.88	0.16	63,63,63,63	0
55	MG	1A	3160	1/1	0.88	0.26	52,52,52,52	0
55	MG	1a	3179	1/1	0.88	0.04	73,73,73,73	0
55	MG	2A	3420	1/1	0.88	0.15	58,58,58,58	0
55	MG	1A	3032	1/1	0.88	0.39	53,53,53,53	0
55	MG	1A	3203	1/1	0.88	0.36	38,38,38,38	0
55	MG	2A	3174	1/1	0.88	0.39	47,47,47,47	0
55	MG	1D	308	1/1	0.88	0.13	46,46,46,46	0
55	MG	2A	3437	1/1	0.88	0.06	75,75,75,75	0
55	MG	1A	3285	1/1	0.88	0.22	49,49,49,49	0
55	MG	1A	3644	1/1	0.88	0.43	51,51,51,51	0
55	MG	1A	3206	1/1	0.88	0.28	42,42,42,42	0
55	MG	2A	3446	1/1	0.88	0.13	78,78,78,78	0
55	MG	1A	3774	1/1	0.88	0.22	79,79,79,79	0
55	MG	2A	3185	1/1	0.88	0.44	65,65,65,65	0
55	MG	2A	3637	1/1	0.88	0.05	63,63,63,63	0
55	MG	2A	3455	1/1	0.88	0.25	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3200	1/1	0.88	0.08	87,87,87,87	0
55	MG	2A	3642	1/1	0.88	0.07	80,80,80,80	0
55	MG	2A	3080	1/1	0.88	0.26	66,66,66,66	0
55	MG	1A	3442	1/1	0.88	0.13	80,80,80,80	0
55	MG	1A	3792	1/1	0.88	0.08	63,63,63,63	0
55	MG	1A	3443	1/1	0.88	0.27	59,59,59,59	0
55	MG	2A	3653	1/1	0.88	0.23	70,70,70,70	0
55	MG	1A	3078	1/1	0.88	0.29	50,50,50,50	0
55	MG	2B	3016	1/1	0.88	0.29	81,81,81,81	0
55	MG	2a	1751	1/1	0.88	0.12	77,77,77,77	0
55	MG	1A	3667	1/1	0.88	0.09	74,74,74,74	0
55	MG	2A	3102	1/1	0.88	0.39	55,55,55,55	0
55	MG	1a	3072	1/1	0.88	0.09	59,59,59,59	0
55	MG	2a	1756	1/1	0.88	0.17	76,76,76,76	0
55	MG	1A	3079	1/1	0.88	0.78	45,45,45,45	0
55	MG	2A	3234	1/1	0.88	0.10	71,71,71,71	0
55	MG	1R	201	1/1	0.88	0.22	59,59,59,59	0
55	MG	1A	3312	1/1	0.88	0.17	61,61,61,61	0
55	MG	1W	3001	1/1	0.88	0.31	44,44,44,44	0
55	MG	2A	3498	1/1	0.88	0.11	68,68,68,68	0
55	MG	1A	3080	1/1	0.88	0.32	45,45,45,45	0
55	MG	1A	3682	1/1	0.88	0.44	61,61,61,61	0
55	MG	2a	1788	1/1	0.88	0.10	83,83,83,83	0
55	MG	1A	3823	1/1	0.88	0.16	32,32,32,32	0
55	MG	2A	3127	1/1	0.88	0.18	76,76,76,76	0
55	MG	1a	3106	1/1	0.88	0.06	56,56,56,56	0
55	MG	1A	3476	1/1	0.88	0.10	33,33,33,33	0
55	MG	1A	3011	1/1	0.88	0.49	48,48,48,48	0
55	MG	2A	3520	1/1	0.88	0.15	70,70,70,70	0
55	MG	2A	3523	1/1	0.88	0.07	65,65,65,65	0
55	MG	2A	3524	1/1	0.88	0.10	47,47,47,47	0
55	MG	1A	3038	1/1	0.88	0.23	50,50,50,50	0
55	MG	1A	3116	1/1	0.88	0.14	49,49,49,49	0
55	MG	1A	3348	1/1	0.88	0.09	42,42,42,42	0
55	MG	2A	3291	1/1	0.88	0.17	40,40,40,40	0
55	MG	2A	3005	1/1	0.89	0.20	47,47,47,47	0
55	MG	1A	3328	1/1	0.89	0.10	40,40,40,40	0
55	MG	1a	3084	1/1	0.89	0.30	58,58,58,58	0
55	MG	2A	3646	1/1	0.89	0.36	57,57,57,57	0
55	MG	1A	3790	1/1	0.89	0.07	38,38,38,38	0
55	MG	1A	3333	1/1	0.89	0.19	29,29,29,29	0
55	MG	2U	201	1/1	0.89	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3225	1/1	0.89	0.20	32,32,32,32	0
55	MG	1A	3074	1/1	0.89	0.68	39,39,39,39	0
55	MG	2A	3026	1/1	0.89	0.14	37,37,37,37	0
55	MG	1A	3204	1/1	0.89	0.30	43,43,43,43	0
55	MG	1a	3120	1/1	0.89	0.08	65,65,65,65	0
55	MG	20	105	1/1	0.89	0.21	80,80,80,80	0
55	MG	1A	3571	1/1	0.89	0.45	33,33,33,33	0
55	MG	25	101	1/1	0.89	0.31	58,58,58,58	0
55	MG	2A	3456	1/1	0.89	0.25	91,91,91,91	0
55	MG	1A	3263	1/1	0.89	0.15	48,48,48,48	0
55	MG	15	202	1/1	0.89	0.25	39,39,39,39	0
55	MG	1a	3132	1/1	0.89	0.11	71,71,71,71	0
55	MG	1A	3902	1/1	0.89	0.32	25,25,25,25	0
55	MG	1A	3576	1/1	0.89	0.16	77,77,77,77	0
55	MG	2a	1602	1/1	0.89	0.40	76,76,76,76	0
55	MG	1A	3577	1/1	0.89	0.18	68,68,68,68	0
55	MG	2A	3469	1/1	0.89	0.09	62,62,62,62	0
55	MG	1a	3001	1/1	0.89	0.07	73,73,73,73	0
55	MG	2A	3689	1/1	0.89	0.18	66,66,66,66	0
55	MG	1A	3906	1/1	0.89	0.36	40,40,40,40	0
55	MG	2A	3046	1/1	0.89	0.10	72,72,72,72	0
55	MG	1A	3504	1/1	0.89	0.12	66,66,66,66	0
55	MG	2A	3480	1/1	0.89	0.16	65,65,65,65	0
55	MG	1A	3586	1/1	0.89	0.19	60,60,60,60	0
55	MG	2A	3189	1/1	0.89	0.33	53,53,53,53	0
55	MG	2A	3051	1/1	0.89	0.42	53,53,53,53	0
55	MG	1A	3830	1/1	0.89	0.07	51,51,51,51	0
55	MG	2a	1630	1/1	0.89	0.16	83,83,83,83	0
55	MG	2A	3195	1/1	0.89	0.18	60,60,60,60	0
55	MG	1A	3588	1/1	0.89	0.06	41,41,41,41	0
55	MG	2A	3055	1/1	0.89	0.30	56,56,56,56	0
55	MG	2A	3502	1/1	0.89	0.52	69,69,69,69	0
55	MG	2A	3505	1/1	0.89	0.25	44,44,44,44	0
55	MG	2A	3201	1/1	0.89	0.27	50,50,50,50	0
55	MG	1A	3704	1/1	0.89	0.34	57,57,57,57	0
55	MG	2A	3207	1/1	0.89	0.15	65,65,65,65	0
55	MG	1A	3205	1/1	0.89	0.19	34,34,34,34	0
55	MG	1A	3598	1/1	0.89	0.13	76,76,76,76	0
55	MG	2A	3740	1/1	0.89	0.26	78,78,78,78	0
55	MG	2A	3742	1/1	0.89	0.59	61,61,61,61	0
55	MG	1A	3838	1/1	0.89	0.22	46,46,46,46	0
55	MG	2a	1651	1/1	0.89	0.77	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3521	1/1	0.89	0.13	74,74,74,74	0
55	MG	2A	3522	1/1	0.89	0.15	67,67,67,67	0
55	MG	2A	3066	1/1	0.89	0.29	64,64,64,64	0
55	MG	1a	3029	1/1	0.89	0.14	55,55,55,55	0
55	MG	2A	3525	1/1	0.89	0.18	77,77,77,77	0
55	MG	2A	3236	1/1	0.89	0.09	65,65,65,65	0
55	MG	1a	3030	1/1	0.89	1.08	75,75,75,75	0
55	MG	2A	3242	1/1	0.89	0.07	75,75,75,75	0
55	MG	1a	3032	1/1	0.89	0.16	39,39,39,39	0
55	MG	1a	3166	1/1	0.89	0.13	70,70,70,70	0
55	MG	1A	3944	1/1	0.89	0.77	47,47,47,47	0
55	MG	2A	3083	1/1	0.89	0.29	60,60,60,60	0
55	MG	1a	3170	1/1	0.89	0.22	80,80,80,80	0
55	MG	1a	3173	1/1	0.89	0.23	68,68,68,68	0
55	MG	2A	3091	1/1	0.89	0.23	52,52,52,52	0
55	MG	1A	3717	1/1	0.89	0.16	69,69,69,69	0
55	MG	2A	3095	1/1	0.89	0.23	58,58,58,58	0
55	MG	1A	3719	1/1	0.89	0.10	70,70,70,70	0
55	MG	2A	3552	1/1	0.89	0.55	57,57,57,57	0
55	MG	2A	3271	1/1	0.89	0.10	58,58,58,58	0
55	MG	1A	3507	1/1	0.89	0.32	32,32,32,32	0
55	MG	1A	3055	1/1	0.89	0.21	48,48,48,48	0
55	MG	1B	213	1/1	0.89	0.09	54,54,54,54	0
55	MG	1A	3273	1/1	0.89	0.11	35,35,35,35	0
55	MG	1A	3004	1/1	0.89	0.16	50,50,50,50	0
55	MG	2A	3107	1/1	0.89	0.12	58,58,58,58	0
55	MG	2A	3567	1/1	0.89	0.22	72,72,72,72	0
55	MG	1A	3404	1/1	0.89	0.15	62,62,62,62	0
55	MG	2a	1735	1/1	0.89	0.17	74,74,74,74	0
55	MG	2A	3569	1/1	0.89	0.17	56,56,56,56	0
55	MG	1A	3050	1/1	0.89	0.25	37,37,37,37	0
55	MG	2A	3112	1/1	0.89	1.04	68,68,68,68	0
55	MG	2A	3315	1/1	0.89	0.12	68,68,68,68	0
55	MG	1A	3084	1/1	0.89	0.56	43,43,43,43	0
55	MG	2A	3322	1/1	0.89	0.21	69,69,69,69	0
55	MG	1a	3052	1/1	0.89	0.30	59,59,59,59	0
55	MG	1A	3732	1/1	0.89	0.70	34,34,34,34	0
55	MG	1a	3055	1/1	0.89	0.32	44,44,44,44	0
55	MG	2A	3588	1/1	0.89	0.17	66,66,66,66	0
55	MG	2A	3332	1/1	0.89	0.18	63,63,63,63	0
55	MG	2A	3593	1/1	0.89	0.23	72,72,72,72	0
55	MG	1A	3172	1/1	0.89	0.53	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3308	1/1	0.89	0.31	38,38,38,38	0
55	MG	1A	3441	1/1	0.89	0.17	21,21,21,21	0
55	MG	2a	1776	1/1	0.89	0.09	74,74,74,74	0
55	MG	1A	3214	1/1	0.89	0.23	33,33,33,33	0
55	MG	1a	3064	1/1	0.89	0.34	82,82,82,82	0
55	MG	1a	3065	1/1	0.89	0.53	67,67,67,67	0
55	MG	2A	3359	1/1	0.89	0.08	64,64,64,64	0
55	MG	1A	3865	1/1	0.89	0.11	82,82,82,82	0
55	MG	1A	3173	1/1	0.89	0.22	45,45,45,45	0
55	MG	1A	3051	1/1	0.89	0.17	35,35,35,35	0
55	MG	1A	3031	1/1	0.89	0.21	27,27,27,27	0
55	MG	1E	304	1/1	0.89	0.25	35,35,35,35	0
55	MG	2A	3393	1/1	0.89	0.14	67,67,67,67	0
55	MG	1A	3465	1/1	0.89	0.18	28,28,28,28	0
55	MG	1A	3163	1/1	0.89	0.27	69,69,69,69	0
55	MG	1o	3001	1/1	0.89	0.46	62,62,62,62	0
55	MG	1A	3029	1/1	0.89	0.17	39,39,39,39	0
55	MG	1A	3773	1/1	0.89	0.15	53,53,53,53	0
55	MG	1A	3659	1/1	0.89	0.33	61,61,61,61	0
55	MG	1A	3457	1/1	0.90	0.48	70,70,70,70	0
55	MG	2A	3320	1/1	0.90	0.17	71,71,71,71	0
55	MG	1A	3244	1/1	0.90	0.28	49,49,49,49	0
55	MG	2A	3021	1/1	0.90	0.27	50,50,50,50	0
55	MG	2A	3719	1/1	0.90	0.07	67,67,67,67	0
55	MG	1A	3937	1/1	0.90	1.57	52,52,52,52	0
55	MG	1A	3161	1/1	0.90	0.66	38,38,38,38	0
55	MG	1A	3584	1/1	0.90	0.08	48,48,48,48	0
55	MG	2A	3729	1/1	0.90	0.42	72,72,72,72	0
55	MG	1A	3755	1/1	0.90	0.18	44,44,44,44	0
55	MG	1a	3148	1/1	0.90	0.23	88,88,88,88	0
55	MG	1A	3756	1/1	0.90	0.16	38,38,38,38	0
55	MG	2a	1614	1/1	0.90	0.42	61,61,61,61	0
55	MG	1A	3402	1/1	0.90	0.07	62,62,62,62	0
55	MG	1a	3031	1/1	0.90	0.12	71,71,71,71	0
55	MG	2A	3550	1/1	0.90	0.11	75,75,75,75	0
55	MG	2a	1619	1/1	0.90	0.57	76,76,76,76	0
55	MG	2A	3744	1/1	0.90	0.26	72,72,72,72	0
55	MG	2A	3344	1/1	0.90	0.12	78,78,78,78	0
55	MG	1A	3474	1/1	0.90	0.20	50,50,50,50	0
55	MG	1A	3759	1/1	0.90	0.19	61,61,61,61	0
55	MG	1A	3077	1/1	0.90	0.29	48,48,48,48	0
55	MG	2a	1634	1/1	0.90	0.34	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1635	1/1	0.90	0.60	81,81,81,81	0
55	MG	2A	3556	1/1	0.90	0.15	63,63,63,63	0
55	MG	1A	3674	1/1	0.90	0.39	51,51,51,51	0
55	MG	1a	3161	1/1	0.90	0.60	67,67,67,67	0
55	MG	1A	3067	1/1	0.90	0.74	47,47,47,47	0
55	MG	1A	3600	1/1	0.90	0.46	81,81,81,81	0
55	MG	1A	3534	1/1	0.90	0.09	40,40,40,40	0
55	MG	2A	3395	1/1	0.90	0.12	76,76,76,76	0
55	MG	2A	3398	1/1	0.90	0.10	45,45,45,45	0
55	MG	1A	3782	1/1	0.90	0.14	59,59,59,59	0
55	MG	2A	3403	1/1	0.90	0.05	67,67,67,67	0
55	MG	2A	3404	1/1	0.90	0.11	47,47,47,47	0
55	MG	1B	226	1/1	0.90	0.11	72,72,72,72	0
55	MG	2a	1650	1/1	0.90	0.08	84,84,84,84	0
55	MG	1A	3689	1/1	0.90	0.16	62,62,62,62	0
55	MG	1a	3174	1/1	0.90	0.11	70,70,70,70	0
55	MG	2A	3417	1/1	0.90	0.12	52,52,52,52	0
55	MG	1A	3874	1/1	0.90	0.17	67,67,67,67	0
55	MG	2A	3059	1/1	0.90	1.20	55,55,55,55	0
55	MG	2A	3180	1/1	0.90	0.43	72,72,72,72	0
55	MG	2A	3590	1/1	0.90	0.38	63,63,63,63	0
55	MG	2a	1671	1/1	0.90	0.16	80,80,80,80	0
55	MG	1A	3478	1/1	0.90	0.12	33,33,33,33	0
55	MG	1A	3791	1/1	0.90	0.16	58,58,58,58	0
55	MG	2a	1686	1/1	0.90	0.20	61,61,61,61	0
55	MG	1A	3409	1/1	0.90	0.17	48,48,48,48	0
55	MG	2A	3072	1/1	0.90	0.64	64,64,64,64	0
55	MG	2A	3074	1/1	0.90	0.39	51,51,51,51	0
55	MG	1a	3183	1/1	0.90	0.15	82,82,82,82	0
55	MG	2a	1709	1/1	0.90	0.16	87,87,87,87	0
55	MG	1A	3493	1/1	0.90	0.14	46,46,46,46	0
55	MG	2a	1712	1/1	0.90	0.40	68,68,68,68	0
55	MG	1A	3237	1/1	0.90	0.28	42,42,42,42	0
55	MG	2A	3452	1/1	0.90	0.11	63,63,63,63	0
55	MG	1A	3498	1/1	0.90	0.41	67,67,67,67	0
55	MG	1A	3621	1/1	0.90	0.14	58,58,58,58	0
55	MG	2A	3611	1/1	0.90	0.30	79,79,79,79	0
55	MG	2A	3822	1/1	0.90	0.78	65,65,65,65	0
55	MG	2a	1723	1/1	0.90	0.21	98,98,98,98	0
55	MG	1A	3087	1/1	0.90	0.46	34,34,34,34	0
55	MG	1A	3888	1/1	0.90	0.28	54,54,54,54	0
55	MG	2A	3832	1/1	0.90	0.90	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3500	1/1	0.90	0.14	67,67,67,67	0
55	MG	1A	3553	1/1	0.90	0.06	47,47,47,47	0
55	MG	2A	3211	1/1	0.90	0.15	64,64,64,64	0
55	MG	1F	311	1/1	0.90	0.22	67,67,67,67	0
55	MG	1A	3369	1/1	0.90	0.16	70,70,70,70	0
55	MG	2A	3097	1/1	0.90	0.23	39,39,39,39	0
55	MG	2A	3470	1/1	0.90	0.17	75,75,75,75	0
55	MG	1a	3213	1/1	0.90	0.16	67,67,67,67	0
55	MG	2a	1740	1/1	0.90	0.06	73,73,73,73	0
55	MG	1A	3722	1/1	0.90	0.08	50,50,50,50	0
55	MG	1A	3371	1/1	0.90	0.12	62,62,62,62	0
55	MG	1A	3900	1/1	0.90	0.45	57,57,57,57	0
55	MG	1U	203	1/1	0.90	0.19	51,51,51,51	0
55	MG	2A	3649	1/1	0.90	0.38	52,52,52,52	0
55	MG	1A	3831	1/1	0.90	0.20	43,43,43,43	0
55	MG	1A	3098	1/1	0.90	0.21	37,37,37,37	0
55	MG	1A	3833	1/1	0.90	0.13	70,70,70,70	0
55	MG	10	107	1/1	0.90	0.43	46,46,46,46	0
55	MG	1A	3276	1/1	0.90	0.23	35,35,35,35	0
55	MG	2a	1765	1/1	0.90	0.07	88,88,88,88	0
55	MG	2a	1767	1/1	0.90	0.09	74,74,74,74	0
55	MG	1A	3508	1/1	0.90	0.12	72,72,72,72	0
55	MG	2A	3666	1/1	0.90	0.07	63,63,63,63	0
55	MG	2A	3500	1/1	0.90	0.11	78,78,78,78	0
55	MG	1A	3909	1/1	0.90	0.28	38,38,38,38	0
55	MG	1A	3383	1/1	0.90	0.14	53,53,53,53	0
55	MG	2a	1777	1/1	0.90	0.05	85,85,85,85	0
55	MG	2A	3118	1/1	0.90	0.39	54,54,54,54	0
55	MG	2A	3267	1/1	0.90	0.13	50,50,50,50	0
55	MG	2A	3508	1/1	0.90	0.97	52,52,52,52	0
55	MG	1l	201	1/1	0.90	0.14	71,71,71,71	0
55	MG	2a	1789	1/1	0.90	0.53	82,82,82,82	0
55	MG	2A	3511	1/1	0.90	0.17	54,54,54,54	0
55	MG	18	3301	1/1	0.90	0.62	64,64,64,64	0
55	MG	1A	3914	1/1	0.90	0.33	68,68,68,68	0
55	MG	2A	3001	1/1	0.90	0.18	50,50,50,50	0
55	MG	1A	3730	1/1	0.90	0.10	75,75,75,75	0
55	MG	1A	3061	1/1	0.90	0.14	36,36,36,36	0
55	MG	2h	3001	1/1	0.90	0.56	64,64,64,64	0
55	MG	1A	3921	1/1	0.90	0.44	40,40,40,40	0
55	MG	1a	3130	1/1	0.90	0.34	75,75,75,75	0
55	MG	2l	202	1/1	0.90	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3575	1/1	0.90	0.56	45,45,45,45	0
55	MG	2A	3700	1/1	0.90	0.15	79,79,79,79	0
55	MG	1A	3926	1/1	0.90	0.64	44,44,44,44	0
55	MG	1a	3009	1/1	0.90	0.89	62,62,62,62	0
55	MG	1A	3549	1/1	0.91	0.24	52,52,52,52	0
55	MG	1A	3489	1/1	0.91	0.19	46,46,46,46	0
55	MG	2A	3146	1/1	0.91	0.66	57,57,57,57	0
55	MG	1A	3913	1/1	0.91	0.42	64,64,64,64	0
55	MG	2A	3720	1/1	0.91	0.36	58,58,58,58	0
55	MG	2A	3541	1/1	0.91	0.14	85,85,85,85	0
55	MG	1A	3146	1/1	0.91	0.19	39,39,39,39	0
55	MG	2a	1609	1/1	0.91	0.20	46,46,46,46	0
55	MG	1A	3047	1/1	0.91	0.37	45,45,45,45	0
55	MG	1a	3135	1/1	0.91	0.26	77,77,77,77	0
55	MG	1A	3064	1/1	0.91	0.39	59,59,59,59	0
55	MG	1A	3426	1/1	0.91	0.12	72,72,72,72	0
55	MG	1A	3183	1/1	0.91	0.21	44,44,44,44	0
55	MG	2A	3358	1/1	0.91	0.15	59,59,59,59	0
55	MG	2A	3158	1/1	0.91	0.74	56,56,56,56	0
55	MG	1A	3924	1/1	0.91	0.93	43,43,43,43	0
55	MG	2A	3743	1/1	0.91	0.22	48,48,48,48	0
55	MG	1A	3565	1/1	0.91	0.17	26,26,26,26	0
55	MG	2A	3747	1/1	0.91	0.09	78,78,78,78	0
55	MG	1A	3168	1/1	0.91	0.27	56,56,56,56	0
55	MG	1A	3931	1/1	0.91	0.32	35,35,35,35	0
55	MG	2A	3559	1/1	0.91	0.10	51,51,51,51	0
55	MG	1a	3017	1/1	0.91	0.40	75,75,75,75	0
55	MG	1A	3132	1/1	0.91	0.60	34,34,34,34	0
55	MG	2A	3167	1/1	0.91	0.60	56,56,56,56	0
55	MG	1A	3934	1/1	0.91	0.30	30,30,30,30	0
55	MG	1A	3744	1/1	0.91	0.05	55,55,55,55	0
55	MG	1A	3747	1/1	0.91	0.14	66,66,66,66	0
55	MG	2A	3572	1/1	0.91	0.16	51,51,51,51	0
55	MG	1a	3026	1/1	0.91	0.30	64,64,64,64	0
55	MG	2A	3769	1/1	0.91	0.13	66,66,66,66	0
55	MG	2A	3405	1/1	0.91	0.23	60,60,60,60	0
55	MG	1A	3657	1/1	0.91	0.32	45,45,45,45	0
55	MG	1A	3151	1/1	0.91	0.27	48,48,48,48	0
55	MG	1A	3133	1/1	0.91	0.13	62,62,62,62	0
55	MG	1A	3275	1/1	0.91	0.20	38,38,38,38	0
55	MG	1a	3165	1/1	0.91	0.78	74,74,74,74	0
55	MG	2a	1653	1/1	0.91	0.44	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3115	1/1	0.91	0.14	69,69,69,69	0
55	MG	2A	3062	1/1	0.91	0.29	56,56,56,56	0
55	MG	1A	3668	1/1	0.91	0.55	63,63,63,63	0
55	MG	1A	3453	1/1	0.91	0.08	51,51,51,51	0
55	MG	2a	1661	1/1	0.91	0.17	74,74,74,74	0
55	MG	1A	3277	1/1	0.91	0.20	56,56,56,56	0
55	MG	1A	3863	1/1	0.91	0.28	68,68,68,68	0
55	MG	2A	3799	1/1	0.91	0.25	97,97,97,97	0
55	MG	2A	3440	1/1	0.91	0.11	78,78,78,78	0
55	MG	2a	1683	1/1	0.91	0.21	79,79,79,79	0
55	MG	2A	3193	1/1	0.91	0.09	80,80,80,80	0
55	MG	2A	3073	1/1	0.91	0.35	52,52,52,52	0
55	MG	1A	3455	1/1	0.91	0.15	21,21,21,21	0
55	MG	1A	3216	1/1	0.91	0.46	50,50,50,50	0
55	MG	1A	3526	1/1	0.91	0.08	52,52,52,52	0
55	MG	1A	3527	1/1	0.91	0.22	56,56,56,56	0
55	MG	2A	3812	1/1	0.91	0.53	68,68,68,68	0
55	MG	2A	3202	1/1	0.91	0.25	59,59,59,59	0
55	MG	1A	3593	1/1	0.91	0.05	63,63,63,63	0
55	MG	1A	3372	1/1	0.91	0.11	68,68,68,68	0
55	MG	1A	3789	1/1	0.91	0.12	89,89,89,89	0
55	MG	2A	3615	1/1	0.91	0.23	59,59,59,59	0
55	MG	1a	3188	1/1	0.91	0.24	65,65,65,65	0
55	MG	2A	3824	1/1	0.91	0.38	55,55,55,55	0
55	MG	2A	3624	1/1	0.91	0.34	55,55,55,55	0
55	MG	2A	3221	1/1	0.91	0.49	68,68,68,68	0
55	MG	2A	3831	1/1	0.91	1.10	52,52,52,52	0
55	MG	1D	307	1/1	0.91	0.38	22,22,22,22	0
55	MG	1a	3053	1/1	0.91	0.23	76,76,76,76	0
55	MG	1A	3529	1/1	0.91	0.07	45,45,45,45	0
55	MG	2A	3636	1/1	0.91	0.06	67,67,67,67	0
55	MG	1A	3281	1/1	0.91	0.14	31,31,31,31	0
55	MG	2A	3472	1/1	0.91	0.11	55,55,55,55	0
55	MG	1A	3014	1/1	0.91	0.40	41,41,41,41	0
55	MG	1A	3068	1/1	0.91	0.51	41,41,41,41	0
55	MG	1A	3883	1/1	0.91	0.06	58,58,58,58	0
55	MG	1A	3885	1/1	0.91	0.21	33,33,33,33	0
55	MG	1A	3802	1/1	0.91	0.09	41,41,41,41	0
55	MG	1A	3705	1/1	0.91	0.12	53,53,53,53	0
55	MG	2A	3648	1/1	0.91	0.08	39,39,39,39	0
55	MG	1A	3289	1/1	0.91	0.19	33,33,33,33	0
55	MG	1A	3711	1/1	0.91	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3651	1/1	0.91	0.23	56,56,56,56	0
55	MG	2A	3487	1/1	0.91	0.23	75,75,75,75	0
55	MG	1F	310	1/1	0.91	0.40	43,43,43,43	0
55	MG	2D	310	1/1	0.91	0.27	61,61,61,61	0
55	MG	2E	301	1/1	0.91	0.15	47,47,47,47	0
55	MG	2a	1764	1/1	0.91	0.50	70,70,70,70	0
55	MG	1A	3110	1/1	0.91	0.29	41,41,41,41	0
55	MG	2A	3660	1/1	0.91	0.15	80,80,80,80	0
55	MG	1A	3893	1/1	0.91	0.23	66,66,66,66	0
55	MG	1A	3111	1/1	0.91	0.22	55,55,55,55	0
55	MG	1A	3812	1/1	0.91	0.09	32,32,32,32	0
55	MG	1A	3718	1/1	0.91	0.11	46,46,46,46	0
55	MG	2A	3268	1/1	0.91	0.18	54,54,54,54	0
55	MG	2H	201	1/1	0.91	0.72	95,95,95,95	0
55	MG	2a	1779	1/1	0.91	0.20	85,85,85,85	0
55	MG	1U	202	1/1	0.91	0.32	34,34,34,34	0
55	MG	2A	3124	1/1	0.91	0.95	53,53,53,53	0
55	MG	1A	3545	1/1	0.91	0.21	30,30,30,30	0
55	MG	2A	3288	1/1	0.91	0.32	67,67,67,67	0
55	MG	1A	3615	1/1	0.91	0.04	50,50,50,50	0
55	MG	2a	1790	1/1	0.91	0.23	72,72,72,72	0
55	MG	1W	3002	1/1	0.91	0.27	51,51,51,51	0
55	MG	2A	3296	1/1	0.91	0.16	60,60,60,60	0
55	MG	2b	3001	1/1	0.91	0.18	79,79,79,79	0
55	MG	1a	3092	1/1	0.91	0.09	86,86,86,86	0
55	MG	2X	103	1/1	0.91	0.13	58,58,58,58	0
55	MG	1A	3825	1/1	0.91	0.08	67,67,67,67	0
55	MG	10	102	1/1	0.91	0.26	69,69,69,69	0
55	MG	1A	3826	1/1	0.91	0.07	65,65,65,65	0
55	MG	1a	3113	1/1	0.91	0.26	65,65,65,65	0
55	MG	10	105	1/1	0.91	0.14	63,63,63,63	0
55	MG	2A	3526	1/1	0.91	0.19	64,64,64,64	0
55	MG	10	106	1/1	0.91	0.06	73,73,73,73	0
55	MG	1A	3178	1/1	0.91	0.53	37,37,37,37	0
55	MG	1A	3488	1/1	0.91	0.22	64,64,64,64	0
56	ZN	24	501	1/1	0.91	0.14	132,132,132,132	0
55	MG	1a	3127	1/1	0.91	0.16	52,52,52,52	0
55	MG	2W	3001	1/1	0.92	0.25	57,57,57,57	0
55	MG	2A	3485	1/1	0.92	0.81	57,57,57,57	0
55	MG	1A	3037	1/1	0.92	0.11	51,51,51,51	0
55	MG	2A	3092	1/1	0.92	0.52	49,49,49,49	0
55	MG	1a	3185	1/1	0.92	0.21	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3493	1/1	0.92	0.09	75,75,75,75	0
55	MG	1A	3688	1/1	0.92	0.17	76,76,76,76	0
55	MG	1a	3051	1/1	0.92	0.39	59,59,59,59	0
55	MG	1A	3192	1/1	0.92	0.32	51,51,51,51	0
55	MG	1A	3690	1/1	0.92	0.14	21,21,21,21	0
55	MG	1A	3692	1/1	0.92	0.09	40,40,40,40	0
55	MG	1A	3800	1/1	0.92	0.06	65,65,65,65	0
55	MG	1A	3695	1/1	0.92	0.09	33,33,33,33	0
55	MG	1F	305	1/1	0.92	0.11	35,35,35,35	0
55	MG	1A	3241	1/1	0.92	0.28	32,32,32,32	0
55	MG	1a	3060	1/1	0.92	0.41	74,74,74,74	0
55	MG	1A	3596	1/1	0.92	0.17	83,83,83,83	0
55	MG	2A	3702	1/1	0.92	0.17	38,38,38,38	0
55	MG	1a	3215	1/1	0.92	0.23	74,74,74,74	0
55	MG	1A	3048	1/1	0.92	0.16	29,29,29,29	0
55	MG	1A	3894	1/1	0.92	0.04	87,87,87,87	0
55	MG	1A	3467	1/1	0.92	0.23	59,59,59,59	0
55	MG	1a	3067	1/1	0.92	0.06	66,66,66,66	0
55	MG	2A	3119	1/1	0.92	0.22	47,47,47,47	0
55	MG	1H	8002	1/1	0.92	0.19	58,58,58,58	0
55	MG	1N	8001	1/1	0.92	0.26	49,49,49,49	0
55	MG	1A	3144	1/1	0.92	0.26	33,33,33,33	0
55	MG	2A	3724	1/1	0.92	0.14	46,46,46,46	0
55	MG	1A	3145	1/1	0.92	0.15	60,60,60,60	0
55	MG	2A	3529	1/1	0.92	0.37	48,48,48,48	0
55	MG	1d	503	1/1	0.92	0.27	72,72,72,72	0
55	MG	1R	202	1/1	0.92	0.32	51,51,51,51	0
55	MG	2a	1631	1/1	0.92	0.42	52,52,52,52	0
55	MG	2A	3316	1/1	0.92	0.27	69,69,69,69	0
55	MG	1A	3814	1/1	0.92	0.25	46,46,46,46	0
55	MG	1A	3041	1/1	0.92	0.25	63,63,63,63	0
55	MG	1a	3076	1/1	0.92	0.20	69,69,69,69	0
55	MG	2A	3539	1/1	0.92	0.13	64,64,64,64	0
55	MG	1A	3820	1/1	0.92	0.24	45,45,45,45	0
55	MG	1A	3250	1/1	0.92	0.42	43,43,43,43	0
55	MG	1A	3714	1/1	0.92	0.04	80,80,80,80	0
55	MG	1A	3537	1/1	0.92	0.25	63,63,63,63	0
55	MG	1a	3087	1/1	0.92	0.11	63,63,63,63	0
55	MG	1A	3388	1/1	0.92	0.17	26,26,26,26	0
55	MG	2A	3548	1/1	0.92	0.05	72,72,72,72	0
55	MG	1A	3105	1/1	0.92	0.29	35,35,35,35	0
55	MG	1A	3480	1/1	0.92	0.28	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3342	1/1	0.92	0.19	49,49,49,49	0
55	MG	1a	3101	1/1	0.92	0.13	46,46,46,46	0
55	MG	2A	3764	1/1	0.92	0.13	80,80,80,80	0
55	MG	1A	3394	1/1	0.92	0.66	75,75,75,75	0
55	MG	2A	3149	1/1	0.92	0.23	58,58,58,58	0
55	MG	2A	3348	1/1	0.92	0.16	59,59,59,59	0
55	MG	2A	3355	1/1	0.92	0.14	58,58,58,58	0
55	MG	1A	3548	1/1	0.92	0.19	47,47,47,47	0
55	MG	2A	3772	1/1	0.92	0.10	68,68,68,68	0
55	MG	1A	3307	1/1	0.92	0.19	37,37,37,37	0
55	MG	2a	1662	1/1	0.92	0.30	61,61,61,61	0
55	MG	2A	3360	1/1	0.92	0.20	58,58,58,58	0
55	MG	2A	3015	1/1	0.92	0.36	46,46,46,46	0
55	MG	1A	3399	1/1	0.92	0.05	65,65,65,65	0
55	MG	2A	3155	1/1	0.92	0.64	42,42,42,42	0
55	MG	1A	3022	1/1	0.92	0.24	28,28,28,28	0
55	MG	2A	3786	1/1	0.92	0.14	66,66,66,66	0
55	MG	2a	1694	1/1	0.92	0.26	77,77,77,77	0
55	MG	2A	3025	1/1	0.92	0.23	53,53,53,53	0
55	MG	15	203	1/1	0.92	0.32	45,45,45,45	0
55	MG	2a	1699	1/1	0.92	0.14	67,67,67,67	0
55	MG	1A	3633	1/1	0.92	0.22	48,48,48,48	0
55	MG	2A	3396	1/1	0.92	0.04	64,64,64,64	0
55	MG	2A	3397	1/1	0.92	0.16	83,83,83,83	0
55	MG	1A	3221	1/1	0.92	0.60	32,32,32,32	0
55	MG	2A	3029	1/1	0.92	0.53	72,72,72,72	0
55	MG	2A	3584	1/1	0.92	0.18	65,65,65,65	0
55	MG	1A	3928	1/1	0.92	0.22	32,32,32,32	0
55	MG	1A	3405	1/1	0.92	0.08	59,59,59,59	0
55	MG	2A	3805	1/1	0.92	0.22	68,68,68,68	0
55	MG	19	103	1/1	0.92	0.21	63,63,63,63	0
55	MG	2A	3809	1/1	0.92	0.28	45,45,45,45	0
55	MG	2A	3034	1/1	0.92	0.17	58,58,58,58	0
55	MG	2a	1724	1/1	0.92	0.23	92,92,92,92	0
55	MG	1A	3639	1/1	0.92	0.28	30,30,30,30	0
55	MG	2A	3415	1/1	0.92	0.19	69,69,69,69	0
55	MG	1A	3554	1/1	0.92	0.18	15,15,15,15	0
55	MG	1A	3119	1/1	0.92	0.39	35,35,35,35	0
55	MG	2A	3419	1/1	0.92	0.18	58,58,58,58	0
55	MG	2A	3818	1/1	0.92	0.49	69,69,69,69	0
55	MG	1A	3136	1/1	0.92	0.62	42,42,42,42	0
55	MG	1A	3938	1/1	0.92	0.24	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3741	1/1	0.92	0.41	56,56,56,56	0
55	MG	2A	3823	1/1	0.92	0.79	53,53,53,53	0
55	MG	2A	3425	1/1	0.92	0.27	67,67,67,67	0
55	MG	1A	3942	1/1	0.92	0.32	32,32,32,32	0
55	MG	2A	3827	1/1	0.92	0.67	58,58,58,58	0
55	MG	2a	1744	1/1	0.92	0.36	69,69,69,69	0
55	MG	1A	3648	1/1	0.92	0.19	33,33,33,33	0
55	MG	2A	3830	1/1	0.92	0.70	65,65,65,65	0
55	MG	2a	1748	1/1	0.92	0.10	85,85,85,85	0
55	MG	2A	3432	1/1	0.92	0.15	58,58,58,58	0
55	MG	2A	3434	1/1	0.92	0.14	78,78,78,78	0
55	MG	2A	3181	1/1	0.92	0.58	67,67,67,67	0
55	MG	1A	3945	1/1	0.92	0.22	56,56,56,56	0
55	MG	2A	3616	1/1	0.92	0.06	57,57,57,57	0
55	MG	1A	3425	1/1	0.92	0.10	46,46,46,46	0
55	MG	2A	3441	1/1	0.92	0.29	88,88,88,88	0
55	MG	2A	3626	1/1	0.92	0.21	68,68,68,68	0
55	MG	1A	3228	1/1	0.92	0.20	76,76,76,76	0
55	MG	1a	3024	1/1	0.92	0.31	61,61,61,61	0
55	MG	2A	3632	1/1	0.92	0.37	94,94,94,94	0
55	MG	1A	3232	1/1	0.92	0.34	68,68,68,68	0
55	MG	2a	1772	1/1	0.92	0.10	81,81,81,81	0
55	MG	1a	3027	1/1	0.92	0.89	75,75,75,75	0
55	MG	2a	1774	1/1	0.92	0.07	65,65,65,65	0
55	MG	1A	3120	1/1	0.92	0.24	54,54,54,54	0
55	MG	1A	3860	1/1	0.92	0.22	56,56,56,56	0
55	MG	2A	3060	1/1	0.92	0.35	48,48,48,48	0
55	MG	2A	3640	1/1	0.92	0.17	76,76,76,76	0
55	MG	2A	3196	1/1	0.92	0.12	75,75,75,75	0
55	MG	2D	303	1/1	0.92	0.26	54,54,54,54	0
55	MG	1A	3186	1/1	0.92	0.10	58,58,58,58	0
55	MG	1A	3156	1/1	0.92	0.10	53,53,53,53	0
55	MG	1A	3344	1/1	0.92	0.20	54,54,54,54	0
55	MG	1A	3057	1/1	0.92	0.18	26,26,26,26	0
55	MG	1A	3353	1/1	0.92	0.25	62,62,62,62	0
55	MG	1A	3519	1/1	0.92	0.23	52,52,52,52	0
55	MG	2F	307	1/1	0.92	0.83	58,58,58,58	0
55	MG	1a	3169	1/1	0.92	0.25	90,90,90,90	0
55	MG	1A	3583	1/1	0.92	0.09	59,59,59,59	0
55	MG	1A	3772	1/1	0.92	0.11	48,48,48,48	0
55	MG	1A	3678	1/1	0.92	0.23	40,40,40,40	0
55	MG	1A	3679	1/1	0.92	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3043	1/1	0.92	0.61	66,66,66,66	0
55	MG	2A	3476	1/1	0.92	0.17	67,67,67,67	0
55	MG	2A	3231	1/1	0.92	0.17	74,74,74,74	0
55	MG	1a	3044	1/1	0.92	0.17	62,62,62,62	0
55	MG	2A	3665	1/1	0.92	0.09	54,54,54,54	0
55	MG	1A	3238	1/1	0.92	0.15	37,37,37,37	0
55	MG	2U	202	1/1	0.92	0.54	60,60,60,60	0
55	MG	1A	3522	1/1	0.92	0.30	57,57,57,57	0
55	MG	2Q	202	1/1	0.93	0.13	65,65,65,65	0
55	MG	2A	3662	1/1	0.93	0.07	65,65,65,65	0
55	MG	1A	3395	1/1	0.93	0.05	68,68,68,68	0
55	MG	2A	3086	1/1	0.93	0.42	60,60,60,60	0
55	MG	2A	3483	1/1	0.93	0.26	44,44,44,44	0
55	MG	2A	3253	1/1	0.93	0.09	66,66,66,66	0
55	MG	2A	3089	1/1	0.93	0.15	58,58,58,58	0
55	MG	1F	307	1/1	0.93	0.69	34,34,34,34	0
55	MG	1A	3817	1/1	0.93	0.08	21,21,21,21	0
55	MG	1A	3247	1/1	0.93	0.26	47,47,47,47	0
55	MG	2A	3489	1/1	0.93	0.26	38,38,38,38	0
55	MG	2A	3492	1/1	0.93	0.28	46,46,46,46	0
55	MG	2A	3680	1/1	0.93	0.12	63,63,63,63	0
55	MG	1a	3189	1/1	0.93	0.17	81,81,81,81	0
55	MG	1a	3193	1/1	0.93	0.41	75,75,75,75	0
55	MG	25	102	1/1	0.93	0.31	63,63,63,63	0
55	MG	2A	3684	1/1	0.93	0.13	61,61,61,61	0
55	MG	1A	3821	1/1	0.93	0.13	64,64,64,64	0
55	MG	1A	3470	1/1	0.93	0.26	52,52,52,52	0
55	MG	1A	3006	1/1	0.93	0.20	26,26,26,26	0
55	MG	1A	3329	1/1	0.93	0.11	30,30,30,30	0
55	MG	1A	3523	1/1	0.93	0.40	70,70,70,70	0
55	MG	1A	3905	1/1	0.93	0.09	58,58,58,58	0
55	MG	2A	3278	1/1	0.93	0.13	53,53,53,53	0
55	MG	1a	3205	1/1	0.93	0.06	78,78,78,78	0
55	MG	2A	3701	1/1	0.93	0.09	59,59,59,59	0
55	MG	2A	3510	1/1	0.93	0.12	82,82,82,82	0
55	MG	1Q	203	1/1	0.93	0.19	49,49,49,49	0
55	MG	1Q	204	1/1	0.93	0.16	51,51,51,51	0
55	MG	2A	3293	1/1	0.93	0.30	72,72,72,72	0
55	MG	2a	1613	1/1	0.93	0.09	50,50,50,50	0
55	MG	2A	3514	1/1	0.93	0.30	50,50,50,50	0
55	MG	2A	3518	1/1	0.93	0.20	60,60,60,60	0
55	MG	2A	3295	1/1	0.93	0.10	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3649	1/1	0.93	0.39	52,52,52,52	0
55	MG	1A	3650	1/1	0.93	0.24	45,45,45,45	0
55	MG	1A	3652	1/1	0.93	0.08	67,67,67,67	0
55	MG	2A	3723	1/1	0.93	0.07	70,70,70,70	0
55	MG	1U	201	1/1	0.93	0.30	56,56,56,56	0
55	MG	1A	3100	1/1	0.93	0.33	31,31,31,31	0
55	MG	1a	3219	1/1	0.93	0.22	68,68,68,68	0
55	MG	1A	3017	1/1	0.93	0.25	31,31,31,31	0
55	MG	1A	3042	1/1	0.93	0.23	32,32,32,32	0
55	MG	1a	3224	1/1	0.93	0.25	60,60,60,60	0
55	MG	1A	3479	1/1	0.93	0.11	31,31,31,31	0
55	MG	1Y	502	1/1	0.93	0.07	68,68,68,68	0
55	MG	1A	3735	1/1	0.93	0.29	79,79,79,79	0
55	MG	2A	3535	1/1	0.93	0.08	67,67,67,67	0
55	MG	1A	3088	1/1	0.93	0.50	34,34,34,34	0
55	MG	1A	3355	1/1	0.93	0.17	22,22,22,22	0
55	MG	2A	3746	1/1	0.93	0.07	73,73,73,73	0
55	MG	1A	3483	1/1	0.93	0.32	56,56,56,56	0
55	MG	2A	3334	1/1	0.93	0.25	71,71,71,71	0
55	MG	1d	506	1/1	0.93	0.16	86,86,86,86	0
55	MG	2A	3750	1/1	0.93	0.14	60,60,60,60	0
55	MG	2A	3751	1/1	0.93	0.20	67,67,67,67	0
55	MG	1a	3081	1/1	0.93	0.23	76,76,76,76	0
55	MG	1A	3590	1/1	0.93	0.31	77,77,77,77	0
55	MG	1A	3485	1/1	0.93	0.30	56,56,56,56	0
55	MG	2A	3341	1/1	0.93	0.04	75,75,75,75	0
55	MG	1A	3750	1/1	0.93	0.21	55,55,55,55	0
55	MG	2A	3759	1/1	0.93	0.10	84,84,84,84	0
55	MG	1t	3001	1/1	0.93	0.21	64,64,64,64	0
55	MG	1A	3019	1/1	0.93	0.45	43,43,43,43	0
55	MG	2a	1660	1/1	0.93	0.15	74,74,74,74	0
55	MG	1A	3673	1/1	0.93	0.14	29,29,29,29	0
55	MG	1A	3595	1/1	0.93	0.43	35,35,35,35	0
55	MG	2a	1665	1/1	0.93	0.35	65,65,65,65	0
55	MG	2A	3354	1/1	0.93	0.19	41,41,41,41	0
55	MG	1a	3102	1/1	0.93	0.09	48,48,48,48	0
55	MG	2a	1675	1/1	0.93	0.22	83,83,83,83	0
55	MG	1A	3676	1/1	0.93	0.15	57,57,57,57	0
55	MG	2a	1677	1/1	0.93	0.16	61,61,61,61	0
55	MG	2a	1678	1/1	0.93	0.18	75,75,75,75	0
55	MG	2a	1681	1/1	0.93	0.10	53,53,53,53	0
55	MG	1a	3107	1/1	0.93	0.22	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3677	1/1	0.93	0.24	38,38,38,38	0
55	MG	2a	1685	1/1	0.93	0.09	77,77,77,77	0
55	MG	1A	3430	1/1	0.93	0.11	54,54,54,54	0
55	MG	2a	1688	1/1	0.93	0.09	58,58,58,58	0
55	MG	2a	1690	1/1	0.93	0.22	83,83,83,83	0
55	MG	2a	1691	1/1	0.93	0.18	64,64,64,64	0
55	MG	1A	3941	1/1	0.93	0.20	54,54,54,54	0
55	MG	2A	3780	1/1	0.93	0.08	54,54,54,54	0
55	MG	1A	3540	1/1	0.93	0.08	80,80,80,80	0
55	MG	1A	3490	1/1	0.93	0.21	50,50,50,50	0
55	MG	2a	1706	1/1	0.93	0.24	90,90,90,90	0
55	MG	2A	3017	1/1	0.93	0.37	65,65,65,65	0
55	MG	1a	3003	1/1	0.93	0.21	81,81,81,81	0
55	MG	1A	3543	1/1	0.93	0.30	39,39,39,39	0
55	MG	2A	3789	1/1	0.93	0.05	68,68,68,68	0
55	MG	2A	3024	1/1	0.93	0.76	60,60,60,60	0
55	MG	2A	3573	1/1	0.93	0.06	73,73,73,73	0
55	MG	1A	3770	1/1	0.93	0.05	64,64,64,64	0
55	MG	2A	3797	1/1	0.93	0.33	88,88,88,88	0
55	MG	1a	3006	1/1	0.93	0.16	72,72,72,72	0
55	MG	2A	3577	1/1	0.93	0.10	51,51,51,51	0
55	MG	1A	3864	1/1	0.93	0.05	53,53,53,53	0
55	MG	2A	3402	1/1	0.93	0.10	80,80,80,80	0
55	MG	1A	3358	1/1	0.93	0.13	24,24,24,24	0
55	MG	1a	3134	1/1	0.93	0.18	73,73,73,73	0
55	MG	1a	3010	1/1	0.93	0.25	60,60,60,60	0
55	MG	2A	3407	1/1	0.93	0.21	70,70,70,70	0
55	MG	2a	1728	1/1	0.93	0.18	81,81,81,81	0
55	MG	2A	3586	1/1	0.93	0.14	89,89,89,89	0
55	MG	2A	3409	1/1	0.93	0.10	88,88,88,88	0
55	MG	1A	3292	1/1	0.93	0.07	34,34,34,34	0
55	MG	1B	210	1/1	0.93	0.21	60,60,60,60	0
55	MG	1B	211	1/1	0.93	0.06	59,59,59,59	0
55	MG	1A	3297	1/1	0.93	0.25	26,26,26,26	0
55	MG	1A	3124	1/1	0.93	0.18	35,35,35,35	0
55	MG	2A	3040	1/1	0.93	0.18	53,53,53,53	0
55	MG	1a	3145	1/1	0.93	0.16	79,79,79,79	0
55	MG	2A	3601	1/1	0.93	0.13	59,59,59,59	0
55	MG	1a	3021	1/1	0.93	0.31	68,68,68,68	0
55	MG	1A	3053	1/1	0.93	0.38	32,32,32,32	0
55	MG	1B	219	1/1	0.93	0.13	47,47,47,47	0
55	MG	1A	3875	1/1	0.93	0.40	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1749	1/1	0.93	0.04	72,72,72,72	0
55	MG	2A	3428	1/1	0.93	0.09	68,68,68,68	0
55	MG	2A	3048	1/1	0.93	0.14	46,46,46,46	0
55	MG	1A	3012	1/1	0.93	0.18	30,30,30,30	0
55	MG	1A	3617	1/1	0.93	0.42	47,47,47,47	0
55	MG	1A	3698	1/1	0.93	0.12	48,48,48,48	0
55	MG	1A	3310	1/1	0.93	0.15	64,64,64,64	0
55	MG	1A	3010	1/1	0.93	0.49	46,46,46,46	0
55	MG	2a	1760	1/1	0.93	0.23	71,71,71,71	0
55	MG	2a	1762	1/1	0.93	0.12	60,60,60,60	0
55	MG	2A	3837	1/1	0.93	0.77	53,53,53,53	0
55	MG	1D	302	1/1	0.93	0.33	44,44,44,44	0
55	MG	2A	3623	1/1	0.93	0.20	71,71,71,71	0
55	MG	2A	3056	1/1	0.93	0.22	47,47,47,47	0
55	MG	1a	3162	1/1	0.93	0.05	72,72,72,72	0
55	MG	1A	3222	1/1	0.93	0.12	46,46,46,46	0
55	MG	2B	3008	1/1	0.93	0.12	84,84,84,84	0
55	MG	2A	3447	1/1	0.93	0.39	47,47,47,47	0
55	MG	1a	3034	1/1	0.93	0.32	74,74,74,74	0
55	MG	1D	304	1/1	0.93	0.07	56,56,56,56	0
55	MG	2A	3061	1/1	0.93	0.87	71,71,71,71	0
55	MG	1A	3624	1/1	0.93	0.14	53,53,53,53	0
55	MG	1A	3884	1/1	0.93	0.12	22,22,22,22	0
55	MG	1A	3208	1/1	0.93	0.12	70,70,70,70	0
55	MG	2A	3214	1/1	0.93	0.16	76,76,76,76	0
55	MG	2A	3460	1/1	0.93	0.17	44,44,44,44	0
55	MG	1A	3707	1/1	0.93	0.18	55,55,55,55	0
55	MG	1a	3172	1/1	0.93	0.18	75,75,75,75	0
55	MG	2D	306	1/1	0.93	1.21	64,64,64,64	0
55	MG	2A	3225	1/1	0.93	0.11	52,52,52,52	0
55	MG	1A	3512	1/1	0.93	0.16	37,37,37,37	0
55	MG	2A	3468	1/1	0.93	0.15	64,64,64,64	0
55	MG	2F	302	1/1	0.93	0.26	58,58,58,58	0
55	MG	1A	3560	1/1	0.93	0.25	24,24,24,24	0
55	MG	1A	3114	1/1	0.93	0.08	59,59,59,59	0
55	MG	2A	3471	1/1	0.93	0.10	72,72,72,72	0
55	MG	2A	3233	1/1	0.93	0.19	48,48,48,48	0
55	MG	2A	3652	1/1	0.93	0.33	58,58,58,58	0
55	MG	1A	3634	1/1	0.93	0.13	44,44,44,44	0
55	MG	1A	3892	1/1	0.93	0.16	59,59,59,59	0
55	MG	2A	3657	1/1	0.93	0.09	55,55,55,55	0
55	MG	1A	3227	1/1	0.93	0.34	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3182	1/1	0.93	0.65	76,76,76,76	0
55	MG	1F	304	1/1	0.93	0.67	41,41,41,41	0
55	MG	1A	3492	1/1	0.94	0.23	68,68,68,68	0
55	MG	2A	3018	1/1	0.94	0.80	48,48,48,48	0
55	MG	2A	3421	1/1	0.94	0.13	52,52,52,52	0
55	MG	1a	3109	1/1	0.94	0.30	60,60,60,60	0
55	MG	1A	3400	1/1	0.94	0.18	44,44,44,44	0
55	MG	1A	3401	1/1	0.94	0.12	43,43,43,43	0
55	MG	2A	3426	1/1	0.94	0.12	62,62,62,62	0
55	MG	2A	3175	1/1	0.94	0.26	50,50,50,50	0
55	MG	1a	3115	1/1	0.94	0.58	71,71,71,71	0
55	MG	2A	3430	1/1	0.94	0.30	54,54,54,54	0
55	MG	1a	3116	1/1	0.94	0.55	80,80,80,80	0
55	MG	2Q	201	1/1	0.94	0.05	77,77,77,77	0
55	MG	1A	3570	1/1	0.94	0.27	46,46,46,46	0
55	MG	2Q	203	1/1	0.94	0.34	55,55,55,55	0
55	MG	1a	3119	1/1	0.94	0.14	78,78,78,78	0
55	MG	2A	3436	1/1	0.94	0.12	82,82,82,82	0
55	MG	2S	201	1/1	0.94	0.52	70,70,70,70	0
55	MG	1A	3497	1/1	0.94	0.21	70,70,70,70	0
55	MG	1A	3256	1/1	0.94	0.35	47,47,47,47	0
55	MG	1A	3056	1/1	0.94	0.23	47,47,47,47	0
55	MG	1A	3794	1/1	0.94	0.26	46,46,46,46	0
55	MG	2A	3443	1/1	0.94	0.17	33,33,33,33	0
55	MG	2A	3186	1/1	0.94	0.40	72,72,72,72	0
55	MG	2A	3187	1/1	0.94	0.17	41,41,41,41	0
55	MG	1A	3033	1/1	0.94	0.42	52,52,52,52	0
55	MG	1A	3233	1/1	0.94	0.23	49,49,49,49	0
55	MG	2A	3191	1/1	0.94	0.20	64,64,64,64	0
55	MG	1A	3578	1/1	0.94	0.21	68,68,68,68	0
55	MG	2A	3453	1/1	0.94	0.12	74,74,74,74	0
55	MG	1A	3503	1/1	0.94	0.20	42,42,42,42	0
55	MG	1A	3580	1/1	0.94	0.24	70,70,70,70	0
55	MG	1A	3915	1/1	0.94	0.27	64,64,64,64	0
55	MG	1A	3408	1/1	0.94	0.21	43,43,43,43	0
55	MG	1A	3140	1/1	0.94	0.36	38,38,38,38	0
55	MG	2A	3198	1/1	0.94	0.23	19,19,19,19	0
55	MG	2A	3199	1/1	0.94	0.61	54,54,54,54	0
55	MG	1A	3506	1/1	0.94	0.18	51,51,51,51	0
55	MG	1a	3141	1/1	0.94	0.12	78,78,78,78	0
55	MG	1a	3002	1/1	0.94	0.21	44,44,44,44	0
55	MG	2A	3466	1/1	0.94	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3587	1/1	0.94	0.12	35,35,35,35	0
55	MG	1A	3420	1/1	0.94	0.17	37,37,37,37	0
55	MG	2A	3683	1/1	0.94	0.08	68,68,68,68	0
55	MG	2A	3052	1/1	0.94	0.23	59,59,59,59	0
55	MG	1A	3693	1/1	0.94	0.09	38,38,38,38	0
55	MG	2A	3687	1/1	0.94	0.18	46,46,46,46	0
55	MG	2A	3213	1/1	0.94	0.13	36,36,36,36	0
55	MG	1A	3262	1/1	0.94	0.15	41,41,41,41	0
55	MG	2a	1617	1/1	0.94	0.21	67,67,67,67	0
55	MG	2A	3219	1/1	0.94	0.14	64,64,64,64	0
55	MG	1A	3592	1/1	0.94	0.17	27,27,27,27	0
55	MG	1A	3930	1/1	0.94	0.22	25,25,25,25	0
55	MG	2A	3478	1/1	0.94	0.23	55,55,55,55	0
55	MG	2a	1622	1/1	0.94	0.39	61,61,61,61	0
55	MG	1A	3081	1/1	0.94	0.37	41,41,41,41	0
55	MG	2a	1626	1/1	0.94	0.51	68,68,68,68	0
55	MG	2a	1629	1/1	0.94	0.21	61,61,61,61	0
55	MG	2A	3227	1/1	0.94	0.28	50,50,50,50	0
55	MG	1a	3012	1/1	0.94	0.22	28,28,28,28	0
55	MG	2A	3704	1/1	0.94	0.08	57,57,57,57	0
55	MG	1A	3264	1/1	0.94	0.16	73,73,73,73	0
55	MG	1a	3014	1/1	0.94	0.17	67,67,67,67	0
55	MG	2A	3232	1/1	0.94	0.07	70,70,70,70	0
55	MG	2A	3709	1/1	0.94	0.12	49,49,49,49	0
55	MG	1a	3155	1/1	0.94	0.05	76,76,76,76	0
55	MG	1a	3016	1/1	0.94	0.24	77,77,77,77	0
55	MG	1a	3158	1/1	0.94	0.08	78,78,78,78	0
55	MG	2A	3239	1/1	0.94	0.18	38,38,38,38	0
55	MG	1a	3159	1/1	0.94	0.13	79,79,79,79	0
55	MG	1A	3265	1/1	0.94	0.17	81,81,81,81	0
55	MG	2A	3722	1/1	0.94	0.07	69,69,69,69	0
55	MG	2A	3496	1/1	0.94	0.16	85,85,85,85	0
55	MG	2A	3070	1/1	0.94	0.58	52,52,52,52	0
55	MG	1A	3516	1/1	0.94	0.15	77,77,77,77	0
55	MG	2A	3249	1/1	0.94	0.07	68,68,68,68	0
55	MG	1A	3341	1/1	0.94	0.15	31,31,31,31	0
55	MG	2A	3252	1/1	0.94	0.34	54,54,54,54	0
55	MG	1A	3599	1/1	0.94	0.54	46,46,46,46	0
55	MG	2A	3734	1/1	0.94	0.04	67,67,67,67	0
55	MG	2A	3735	1/1	0.94	0.16	55,55,55,55	0
55	MG	1A	3103	1/1	0.94	0.52	41,41,41,41	0
55	MG	1A	3709	1/1	0.94	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3345	1/1	0.94	0.14	24,24,24,24	0
55	MG	2A	3257	1/1	0.94	0.22	49,49,49,49	0
55	MG	1A	3835	1/1	0.94	0.07	51,51,51,51	0
55	MG	2a	1663	1/1	0.94	0.20	64,64,64,64	0
55	MG	1A	3347	1/1	0.94	0.23	28,28,28,28	0
55	MG	2a	1666	1/1	0.94	0.08	74,74,74,74	0
55	MG	1A	3605	1/1	0.94	0.05	63,63,63,63	0
55	MG	2a	1668	1/1	0.94	0.13	63,63,63,63	0
55	MG	1A	3122	1/1	0.94	0.58	27,27,27,27	0
55	MG	2a	1672	1/1	0.94	0.04	75,75,75,75	0
55	MG	1A	3351	1/1	0.94	0.08	66,66,66,66	0
55	MG	2A	3088	1/1	0.94	0.08	73,73,73,73	0
55	MG	1A	3524	1/1	0.94	0.17	55,55,55,55	0
55	MG	1A	3841	1/1	0.94	0.08	68,68,68,68	0
55	MG	2a	1679	1/1	0.94	0.43	64,64,64,64	0
55	MG	1A	3842	1/1	0.94	0.03	68,68,68,68	0
55	MG	1A	3450	1/1	0.94	0.31	71,71,71,71	0
55	MG	2A	3279	1/1	0.94	0.08	58,58,58,58	0
55	MG	2A	3755	1/1	0.94	0.20	63,63,63,63	0
55	MG	2A	3281	1/1	0.94	0.17	39,39,39,39	0
55	MG	2A	3283	1/1	0.94	0.15	47,47,47,47	0
55	MG	1a	3181	1/1	0.94	0.11	76,76,76,76	0
55	MG	1A	3612	1/1	0.94	0.12	77,77,77,77	0
55	MG	2A	3763	1/1	0.94	0.17	41,41,41,41	0
55	MG	2a	1695	1/1	0.94	0.31	65,65,65,65	0
55	MG	2A	3531	1/1	0.94	0.09	78,78,78,78	0
55	MG	1A	3847	1/1	0.94	0.14	61,61,61,61	0
55	MG	1A	3071	1/1	0.94	0.21	32,32,32,32	0
55	MG	2A	3099	1/1	0.94	0.23	52,52,52,52	0
55	MG	1A	3045	1/1	0.94	0.22	37,37,37,37	0
55	MG	1A	3851	1/1	0.94	0.08	29,29,29,29	0
55	MG	1A	3109	1/1	0.94	0.25	41,41,41,41	0
55	MG	1a	3042	1/1	0.94	0.20	63,63,63,63	0
55	MG	2a	1711	1/1	0.94	1.00	82,82,82,82	0
55	MG	1A	3128	1/1	0.94	0.17	33,33,33,33	0
55	MG	2a	1713	1/1	0.94	0.06	68,68,68,68	0
55	MG	1A	3726	1/1	0.94	0.28	39,39,39,39	0
55	MG	1A	3460	1/1	0.94	0.07	47,47,47,47	0
55	MG	1a	3047	1/1	0.94	0.15	64,64,64,64	0
55	MG	2A	3111	1/1	0.94	0.58	57,57,57,57	0
55	MG	2a	1720	1/1	0.94	0.18	66,66,66,66	0
55	MG	1A	3278	1/1	0.94	0.10	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3546	1/1	0.94	0.15	43,43,43,43	0
55	MG	1A	3046	1/1	0.94	0.24	13,13,13,13	0
55	MG	2A	3325	1/1	0.94	0.58	68,68,68,68	0
55	MG	1A	3194	1/1	0.94	0.16	54,54,54,54	0
55	MG	2A	3792	1/1	0.94	0.16	77,77,77,77	0
55	MG	1a	3204	1/1	0.94	0.05	70,70,70,70	0
55	MG	2A	3117	1/1	0.94	0.22	56,56,56,56	0
55	MG	1A	3469	1/1	0.94	0.16	62,62,62,62	0
55	MG	2A	3333	1/1	0.94	0.08	69,69,69,69	0
55	MG	1A	3016	1/1	0.94	0.26	18,18,18,18	0
55	MG	2A	3335	1/1	0.94	0.11	70,70,70,70	0
55	MG	2A	3557	1/1	0.94	0.07	55,55,55,55	0
55	MG	1D	309	1/1	0.94	0.23	31,31,31,31	0
55	MG	2A	3125	1/1	0.94	0.18	66,66,66,66	0
55	MG	2a	1736	1/1	0.94	0.34	74,74,74,74	0
55	MG	1A	3471	1/1	0.94	0.08	67,67,67,67	0
55	MG	2a	1738	1/1	0.94	0.05	77,77,77,77	0
55	MG	1A	3196	1/1	0.94	0.11	32,32,32,32	0
55	MG	1A	3740	1/1	0.94	0.09	63,63,63,63	0
55	MG	1E	301	1/1	0.94	0.36	40,40,40,40	0
55	MG	1A	3375	1/1	0.94	0.11	69,69,69,69	0
55	MG	1A	3742	1/1	0.94	0.12	55,55,55,55	0
55	MG	1a	3220	1/1	0.94	0.10	60,60,60,60	0
55	MG	1A	3076	1/1	0.94	0.48	43,43,43,43	0
55	MG	2A	3350	1/1	0.94	0.22	54,54,54,54	0
55	MG	1A	3872	1/1	0.94	0.12	32,32,32,32	0
55	MG	1F	303	1/1	0.94	0.28	44,44,44,44	0
55	MG	2A	3356	1/1	0.94	0.21	51,51,51,51	0
55	MG	1A	3873	1/1	0.94	0.11	59,59,59,59	0
55	MG	1A	3745	1/1	0.94	0.16	30,30,30,30	0
55	MG	1A	3746	1/1	0.94	0.05	52,52,52,52	0
55	MG	2A	3363	1/1	0.94	0.24	43,43,43,43	0
55	MG	2A	3364	1/1	0.94	0.07	34,34,34,34	0
55	MG	2a	1763	1/1	0.94	0.10	55,55,55,55	0
55	MG	2A	3373	1/1	0.94	0.15	76,76,76,76	0
55	MG	1A	3290	1/1	0.94	0.17	52,52,52,52	0
55	MG	1A	3018	1/1	0.94	0.19	30,30,30,30	0
55	MG	1A	3645	1/1	0.94	0.24	35,35,35,35	0
55	MG	2A	3833	1/1	0.94	0.19	57,57,57,57	0
55	MG	2A	3379	1/1	0.94	0.07	76,76,76,76	0
55	MG	1A	3294	1/1	0.94	0.13	25,25,25,25	0
55	MG	1A	3390	1/1	0.94	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3390	1/1	0.94	0.10	48,48,48,48	0
55	MG	2A	3598	1/1	0.94	0.15	70,70,70,70	0
55	MG	1A	3481	1/1	0.94	0.14	35,35,35,35	0
55	MG	1A	3251	1/1	0.94	0.30	34,34,34,34	0
55	MG	1P	201	1/1	0.94	0.23	30,30,30,30	0
55	MG	2a	1782	1/1	0.94	0.16	75,75,75,75	0
55	MG	1A	3393	1/1	0.94	0.17	48,48,48,48	0
55	MG	2B	3009	1/1	0.94	0.12	79,79,79,79	0
55	MG	1A	3653	1/1	0.94	0.15	42,42,42,42	0
55	MG	1A	3200	1/1	0.94	0.31	37,37,37,37	0
55	MG	1a	3082	1/1	0.94	0.24	58,58,58,58	0
55	MG	1A	3761	1/1	0.94	0.61	43,43,43,43	0
55	MG	1A	3486	1/1	0.94	0.30	43,43,43,43	0
55	MG	1A	3094	1/1	0.94	0.48	34,34,34,34	0
55	MG	1A	3202	1/1	0.94	0.43	49,49,49,49	0
55	MG	2A	3408	1/1	0.94	0.15	48,48,48,48	0
55	MG	2D	301	1/1	0.94	0.58	49,49,49,49	0
55	MG	2f	8001	1/1	0.94	0.16	56,56,56,56	0
55	MG	1A	3663	1/1	0.94	0.22	68,68,68,68	0
55	MG	2A	3617	1/1	0.94	0.14	35,35,35,35	0
55	MG	2A	3619	1/1	0.94	0.11	57,57,57,57	0
55	MG	2A	3163	1/1	0.94	0.26	60,60,60,60	0
55	MG	2D	307	1/1	0.94	0.41	60,60,60,60	0
55	MG	1A	3562	1/1	0.94	0.23	52,52,52,52	0
55	MG	2o	3001	1/1	0.94	0.13	57,57,57,57	0
55	MG	1A	3043	1/1	0.94	0.33	13,13,13,13	0
55	MG	2E	304	1/1	0.94	0.15	71,71,71,71	0
55	MG	1A	3775	1/1	0.94	0.06	47,47,47,47	0
55	MG	2A	3168	1/1	0.94	0.27	72,72,72,72	0
55	MG	1A	3274	1/1	0.95	0.29	8,8,8,8	0
55	MG	1A	3008	1/1	0.95	0.26	48,48,48,48	0
55	MG	1A	3415	1/1	0.95	0.11	26,26,26,26	0
55	MG	1a	3202	1/1	0.95	0.07	53,53,53,53	0
55	MG	2A	3467	1/1	0.95	0.16	76,76,76,76	0
55	MG	2A	3096	1/1	0.95	0.34	48,48,48,48	0
55	MG	1A	3828	1/1	0.95	0.19	70,70,70,70	0
55	MG	1A	3362	1/1	0.95	0.29	42,42,42,42	0
55	MG	1A	3184	1/1	0.95	0.72	38,38,38,38	0
55	MG	2A	3100	1/1	0.95	0.33	61,61,61,61	0
55	MG	1A	3097	1/1	0.95	0.36	42,42,42,42	0
55	MG	2A	3676	1/1	0.95	0.36	76,76,76,76	0
55	MG	2A	3677	1/1	0.95	0.17	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3429	1/1	0.95	0.12	41,41,41,41	0
55	MG	2A	3679	1/1	0.95	0.05	71,71,71,71	0
55	MG	1A	3153	1/1	0.95	0.47	36,36,36,36	0
55	MG	1A	3916	1/1	0.95	0.87	49,49,49,49	0
55	MG	2A	3477	1/1	0.95	0.12	81,81,81,81	0
55	MG	2A	3261	1/1	0.95	0.29	52,52,52,52	0
55	MG	2A	3262	1/1	0.95	0.19	71,71,71,71	0
55	MG	1A	3917	1/1	0.95	0.41	38,38,38,38	0
55	MG	2A	3264	1/1	0.95	0.16	61,61,61,61	0
55	MG	2A	3265	1/1	0.95	0.40	69,69,69,69	0
55	MG	2A	3106	1/1	0.95	0.31	67,67,67,67	0
55	MG	2a	1606	1/1	0.95	0.45	57,57,57,57	0
55	MG	1X	8001	1/1	0.95	0.11	27,27,27,27	0
55	MG	2A	3108	1/1	0.95	0.10	65,65,65,65	0
55	MG	2A	3269	1/1	0.95	0.18	38,38,38,38	0
55	MG	1A	3373	1/1	0.95	0.33	53,53,53,53	0
55	MG	2A	3274	1/1	0.95	0.16	51,51,51,51	0
55	MG	1a	3080	1/1	0.95	0.17	67,67,67,67	0
55	MG	1A	3601	1/1	0.95	0.07	38,38,38,38	0
55	MG	1A	3025	1/1	0.95	0.31	32,32,32,32	0
55	MG	1A	3675	1/1	0.95	0.12	65,65,65,65	0
55	MG	10	104	1/1	0.95	0.10	73,73,73,73	0
55	MG	1A	3434	1/1	0.95	0.14	46,46,46,46	0
55	MG	2A	3285	1/1	0.95	0.08	46,46,46,46	0
55	MG	2A	3711	1/1	0.95	0.08	67,67,67,67	0
55	MG	1a	3093	1/1	0.95	0.06	68,68,68,68	0
55	MG	2A	3715	1/1	0.95	0.07	63,63,63,63	0
55	MG	2A	3503	1/1	0.95	0.24	58,58,58,58	0
55	MG	1A	3925	1/1	0.95	0.17	42,42,42,42	0
55	MG	2A	3718	1/1	0.95	0.09	78,78,78,78	0
55	MG	1A	3320	1/1	0.95	0.30	52,52,52,52	0
55	MG	1A	3927	1/1	0.95	0.30	34,34,34,34	0
55	MG	1A	3379	1/1	0.95	0.19	67,67,67,67	0
55	MG	2A	3126	1/1	0.95	0.30	62,62,62,62	0
55	MG	1e	3001	1/1	0.95	0.26	61,61,61,61	0
55	MG	1f	8001	1/1	0.95	0.21	61,61,61,61	0
55	MG	15	201	1/1	0.95	0.57	46,46,46,46	0
55	MG	1A	3099	1/1	0.95	0.29	62,62,62,62	0
55	MG	2a	1640	1/1	0.95	0.52	50,50,50,50	0
55	MG	2A	3304	1/1	0.95	0.23	41,41,41,41	0
55	MG	1h	3002	1/1	0.95	0.12	73,73,73,73	0
55	MG	2A	3314	1/1	0.95	0.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3733	1/1	0.95	0.13	65,65,65,65	0
55	MG	1a	3108	1/1	0.95	0.04	75,75,75,75	0
55	MG	1A	3680	1/1	0.95	0.08	53,53,53,53	0
55	MG	15	205	1/1	0.95	0.09	62,62,62,62	0
55	MG	1A	3754	1/1	0.95	0.11	71,71,71,71	0
55	MG	2A	3738	1/1	0.95	0.07	62,62,62,62	0
55	MG	2A	3137	1/1	0.95	0.40	58,58,58,58	0
55	MG	1A	3846	1/1	0.95	0.14	53,53,53,53	0
55	MG	1A	3681	1/1	0.95	0.24	57,57,57,57	0
55	MG	2A	3003	1/1	0.95	0.08	35,35,35,35	0
55	MG	2A	3530	1/1	0.95	0.13	71,71,71,71	0
55	MG	1A	3325	1/1	0.95	0.19	22,22,22,22	0
55	MG	2a	1656	1/1	0.95	0.06	78,78,78,78	0
55	MG	1A	3060	1/1	0.95	0.26	38,38,38,38	0
55	MG	2A	3143	1/1	0.95	0.20	59,59,59,59	0
55	MG	2A	3007	1/1	0.95	0.25	61,61,61,61	0
55	MG	1A	3610	1/1	0.95	0.10	68,68,68,68	0
55	MG	1A	3852	1/1	0.95	0.21	22,22,22,22	0
55	MG	1A	3447	1/1	0.95	0.18	24,24,24,24	0
55	MG	1A	3448	1/1	0.95	0.17	19,19,19,19	0
55	MG	2A	3012	1/1	0.95	0.18	42,42,42,42	0
55	MG	1A	3616	1/1	0.95	0.08	63,63,63,63	0
55	MG	2A	3014	1/1	0.95	0.74	58,58,58,58	0
55	MG	1A	3763	1/1	0.95	0.10	70,70,70,70	0
55	MG	1A	3691	1/1	0.95	0.09	42,42,42,42	0
55	MG	2a	1673	1/1	0.95	0.16	59,59,59,59	0
55	MG	2A	3345	1/1	0.95	0.07	78,78,78,78	0
55	MG	1a	3008	1/1	0.95	0.21	76,76,76,76	0
55	MG	1A	3858	1/1	0.95	0.12	60,60,60,60	0
55	MG	2A	3020	1/1	0.95	0.10	42,42,42,42	0
55	MG	2A	3351	1/1	0.95	0.06	69,69,69,69	0
55	MG	2a	1680	1/1	0.95	0.10	63,63,63,63	0
55	MG	1A	3449	1/1	0.95	0.10	41,41,41,41	0
55	MG	2A	3770	1/1	0.95	0.04	74,74,74,74	0
55	MG	2A	3022	1/1	0.95	0.14	72,72,72,72	0
55	MG	2A	3023	1/1	0.95	0.53	47,47,47,47	0
55	MG	1B	208	1/1	0.95	0.23	68,68,68,68	0
55	MG	1a	3138	1/1	0.95	0.15	66,66,66,66	0
55	MG	1B	209	1/1	0.95	0.23	59,59,59,59	0
55	MG	2A	3361	1/1	0.95	0.15	53,53,53,53	0
55	MG	2a	1692	1/1	0.95	0.23	82,82,82,82	0
55	MG	2A	3781	1/1	0.95	0.12	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3362	1/1	0.95	0.10	56,56,56,56	0
55	MG	1A	3767	1/1	0.95	0.13	52,52,52,52	0
55	MG	2A	3561	1/1	0.95	0.06	82,82,82,82	0
55	MG	1A	3768	1/1	0.95	0.08	58,58,58,58	0
55	MG	2a	1701	1/1	0.95	0.23	85,85,85,85	0
55	MG	2a	1702	1/1	0.95	0.10	72,72,72,72	0
55	MG	2a	1704	1/1	0.95	0.18	76,76,76,76	0
55	MG	2A	3365	1/1	0.95	0.09	81,81,81,81	0
55	MG	2A	3369	1/1	0.95	0.08	81,81,81,81	0
55	MG	2A	3565	1/1	0.95	0.49	70,70,70,70	0
55	MG	2A	3372	1/1	0.95	0.14	54,54,54,54	0
55	MG	1A	3385	1/1	0.95	0.07	69,69,69,69	0
55	MG	1A	3771	1/1	0.95	0.21	38,38,38,38	0
55	MG	2A	3570	1/1	0.95	0.29	54,54,54,54	0
55	MG	2A	3171	1/1	0.95	0.34	45,45,45,45	0
55	MG	2A	3377	1/1	0.95	0.15	54,54,54,54	0
55	MG	2a	1716	1/1	0.95	0.23	75,75,75,75	0
55	MG	1A	3386	1/1	0.95	0.26	49,49,49,49	0
55	MG	1A	3069	1/1	0.95	0.32	34,34,34,34	0
55	MG	1A	3009	1/1	0.95	0.29	32,32,32,32	0
55	MG	2A	3384	1/1	0.95	0.18	37,37,37,37	0
55	MG	2A	3580	1/1	0.95	0.11	71,71,71,71	0
55	MG	1A	3456	1/1	0.95	0.16	49,49,49,49	0
55	MG	2A	3386	1/1	0.95	0.15	63,63,63,63	0
55	MG	2A	3388	1/1	0.95	0.17	47,47,47,47	0
55	MG	1A	3780	1/1	0.95	0.54	34,34,34,34	0
55	MG	2A	3038	1/1	0.95	0.22	54,54,54,54	0
55	MG	1A	3117	1/1	0.95	0.09	61,61,61,61	0
55	MG	1A	3783	1/1	0.95	0.17	44,44,44,44	0
55	MG	1A	3703	1/1	0.95	0.10	42,42,42,42	0
55	MG	1A	3787	1/1	0.95	0.08	48,48,48,48	0
55	MG	1A	3788	1/1	0.95	0.14	28,28,28,28	0
55	MG	1A	3459	1/1	0.95	0.08	65,65,65,65	0
55	MG	2A	3047	1/1	0.95	0.37	45,45,45,45	0
55	MG	2A	3595	1/1	0.95	0.16	52,52,52,52	0
55	MG	1A	3342	1/1	0.95	0.06	29,29,29,29	0
55	MG	2A	3597	1/1	0.95	0.10	47,47,47,47	0
55	MG	1A	3461	1/1	0.95	0.11	27,27,27,27	0
55	MG	2A	3406	1/1	0.95	0.56	81,81,81,81	0
55	MG	1a	3160	1/1	0.95	0.29	67,67,67,67	0
55	MG	2A	3190	1/1	0.95	0.73	66,66,66,66	0
55	MG	2a	1742	1/1	0.95	0.08	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3463	1/1	0.95	0.33	60,60,60,60	0
55	MG	1A	3092	1/1	0.95	0.14	33,33,33,33	0
55	MG	1A	3574	1/1	0.95	0.41	49,49,49,49	0
55	MG	1A	3799	1/1	0.95	0.11	57,57,57,57	0
55	MG	2A	3836	1/1	0.95	0.56	61,61,61,61	0
55	MG	1A	3231	1/1	0.95	0.60	25,25,25,25	0
55	MG	1D	314	1/1	0.95	0.32	77,77,77,77	0
55	MG	1A	3713	1/1	0.95	0.14	75,75,75,75	0
55	MG	1A	3346	1/1	0.95	0.20	69,69,69,69	0
55	MG	2a	1754	1/1	0.95	0.67	78,78,78,78	0
55	MG	2A	3614	1/1	0.95	0.09	56,56,56,56	0
55	MG	1A	3520	1/1	0.95	0.12	33,33,33,33	0
55	MG	2a	1757	1/1	0.95	0.26	66,66,66,66	0
55	MG	2a	1758	1/1	0.95	0.08	74,74,74,74	0
55	MG	1A	3165	1/1	0.95	0.38	41,41,41,41	0
55	MG	2A	3423	1/1	0.95	0.36	51,51,51,51	0
55	MG	2B	3010	1/1	0.95	0.05	73,73,73,73	0
55	MG	2A	3618	1/1	0.95	0.31	68,68,68,68	0
55	MG	1A	3001	1/1	0.95	0.14	38,38,38,38	0
55	MG	1A	3891	1/1	0.95	0.11	84,84,84,84	0
55	MG	2A	3622	1/1	0.95	0.13	52,52,52,52	0
55	MG	1A	3306	1/1	0.95	0.12	43,43,43,43	0
55	MG	2A	3206	1/1	0.95	0.10	64,64,64,64	0
55	MG	1A	3352	1/1	0.95	0.11	34,34,34,34	0
55	MG	2A	3208	1/1	0.95	0.10	80,80,80,80	0
55	MG	2A	3629	1/1	0.95	0.06	73,73,73,73	0
55	MG	2A	3630	1/1	0.95	0.39	56,56,56,56	0
55	MG	1F	306	1/1	0.95	0.20	25,25,25,25	0
55	MG	2A	3067	1/1	0.95	0.42	61,61,61,61	0
55	MG	2D	305	1/1	0.95	0.10	73,73,73,73	0
55	MG	2A	3212	1/1	0.95	0.14	36,36,36,36	0
55	MG	2a	1781	1/1	0.95	0.16	51,51,51,51	0
55	MG	1A	3651	1/1	0.95	0.14	34,34,34,34	0
55	MG	2a	1784	1/1	0.95	0.05	87,87,87,87	0
55	MG	2D	309	1/1	0.95	0.13	57,57,57,57	0
55	MG	1A	3473	1/1	0.95	0.48	32,32,32,32	0
55	MG	2A	3438	1/1	0.95	0.25	66,66,66,66	0
55	MG	2E	303	1/1	0.95	0.18	52,52,52,52	0
55	MG	2A	3215	1/1	0.95	0.31	42,42,42,42	0
55	MG	2A	3217	1/1	0.95	0.10	57,57,57,57	0
55	MG	1A	3896	1/1	0.95	0.48	38,38,38,38	0
55	MG	1A	3271	1/1	0.95	0.34	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3007	1/1	0.95	0.12	38,38,38,38	0
55	MG	2F	306	1/1	0.95	0.39	47,47,47,47	0
55	MG	1G	3003	1/1	0.95	0.09	49,49,49,49	0
55	MG	1A	3309	1/1	0.95	0.14	37,37,37,37	0
55	MG	1a	3187	1/1	0.95	0.07	82,82,82,82	0
55	MG	1A	3901	1/1	0.95	0.47	35,35,35,35	0
55	MG	2A	3081	1/1	0.95	0.32	39,39,39,39	0
55	MG	1A	3822	1/1	0.95	0.10	54,54,54,54	0
55	MG	1a	3190	1/1	0.95	0.07	73,73,73,73	0
55	MG	1a	3061	1/1	0.95	0.26	66,66,66,66	0
55	MG	2A	3235	1/1	0.95	0.08	77,77,77,77	0
55	MG	1N	8002	1/1	0.95	0.21	61,61,61,61	0
56	ZN	1Y	501	1/1	0.95	0.12	61,61,61,61	0
55	MG	2A	3237	1/1	0.95	0.14	45,45,45,45	0
56	ZN	2Y	501	1/1	0.95	0.06	91,91,91,91	0
55	MG	1N	8003	1/1	0.95	0.17	61,61,61,61	0
55	MG	1A	3658	1/1	0.95	0.04	50,50,50,50	0
55	MG	1G	3001	1/1	0.96	0.07	74,74,74,74	0
55	MG	1A	3065	1/1	0.96	0.35	33,33,33,33	0
55	MG	1a	3083	1/1	0.96	0.23	66,66,66,66	0
55	MG	1A	3502	1/1	0.96	0.19	16,16,16,16	0
55	MG	1A	3438	1/1	0.96	0.19	61,61,61,61	0
55	MG	1a	3088	1/1	0.96	0.37	61,61,61,61	0
55	MG	1A	3439	1/1	0.96	0.15	51,51,51,51	0
55	MG	1A	3125	1/1	0.96	0.19	30,30,30,30	0
55	MG	2A	3633	1/1	0.96	0.11	80,80,80,80	0
55	MG	2A	3414	1/1	0.96	0.07	77,77,77,77	0
55	MG	2A	3016	1/1	0.96	0.46	50,50,50,50	0
55	MG	1a	3094	1/1	0.96	0.06	47,47,47,47	0
55	MG	1a	3095	1/1	0.96	0.31	63,63,63,63	0
55	MG	2A	3418	1/1	0.96	0.11	44,44,44,44	0
55	MG	1A	3360	1/1	0.96	0.19	25,25,25,25	0
55	MG	1N	8004	1/1	0.96	0.22	71,71,71,71	0
55	MG	1A	3301	1/1	0.96	0.21	12,12,12,12	0
55	MG	1A	3777	1/1	0.96	0.06	73,73,73,73	0
55	MG	1a	3103	1/1	0.96	0.13	77,77,77,77	0
55	MG	2A	3645	1/1	0.96	0.07	64,64,64,64	0
55	MG	1a	3105	1/1	0.96	0.11	54,54,54,54	0
55	MG	2V	203	1/1	0.96	0.15	73,73,73,73	0
55	MG	1Q	202	1/1	0.96	0.29	51,51,51,51	0
55	MG	2X	101	1/1	0.96	0.30	77,77,77,77	0
55	MG	1A	3778	1/1	0.96	0.12	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3126	1/1	0.96	0.25	23,23,23,23	0
55	MG	1A	3509	1/1	0.96	0.21	31,31,31,31	0
55	MG	1a	3110	1/1	0.96	0.16	54,54,54,54	0
55	MG	1a	3112	1/1	0.96	0.24	85,85,85,85	0
55	MG	2A	3031	1/1	0.96	0.15	64,64,64,64	0
55	MG	2I	101	1/1	0.96	0.12	66,66,66,66	0
55	MG	2A	3654	1/1	0.96	0.05	34,34,34,34	0
55	MG	2A	3433	1/1	0.96	0.19	81,81,81,81	0
55	MG	1A	3066	1/1	0.96	0.28	39,39,39,39	0
55	MG	1A	3785	1/1	0.96	0.17	24,24,24,24	0
55	MG	2A	3659	1/1	0.96	0.07	73,73,73,73	0
55	MG	1A	3513	1/1	0.96	0.16	53,53,53,53	0
55	MG	1A	3589	1/1	0.96	0.10	28,28,28,28	0
55	MG	2A	3205	1/1	0.96	0.15	44,44,44,44	0
55	MG	2A	3036	1/1	0.96	0.52	38,38,38,38	0
55	MG	1A	3023	1/1	0.96	0.15	21,21,21,21	0
55	MG	2A	3442	1/1	0.96	0.09	62,62,62,62	0
55	MG	1V	201	1/1	0.96	0.10	67,67,67,67	0
55	MG	2A	3039	1/1	0.96	0.23	25,25,25,25	0
55	MG	2A	3210	1/1	0.96	0.15	44,44,44,44	0
55	MG	1A	3591	1/1	0.96	0.08	26,26,26,26	0
55	MG	1A	3684	1/1	0.96	0.23	59,59,59,59	0
55	MG	1A	3040	1/1	0.96	0.19	40,40,40,40	0
55	MG	2a	1611	1/1	0.96	0.36	76,76,76,76	0
55	MG	1a	3128	1/1	0.96	0.20	75,75,75,75	0
55	MG	1A	3210	1/1	0.96	0.52	42,42,42,42	0
55	MG	1A	3451	1/1	0.96	0.16	23,23,23,23	0
55	MG	1A	3189	1/1	0.96	0.11	69,69,69,69	0
55	MG	1A	3795	1/1	0.96	0.13	48,48,48,48	0
55	MG	1A	3797	1/1	0.96	0.13	50,50,50,50	0
55	MG	2A	3224	1/1	0.96	0.15	55,55,55,55	0
55	MG	1A	3377	1/1	0.96	0.14	47,47,47,47	0
55	MG	2A	3226	1/1	0.96	0.12	70,70,70,70	0
55	MG	1A	3266	1/1	0.96	0.19	34,34,34,34	0
55	MG	1A	3908	1/1	0.96	0.24	40,40,40,40	0
55	MG	2a	1623	1/1	0.96	0.65	60,60,60,60	0
55	MG	1a	3137	1/1	0.96	0.29	63,63,63,63	0
55	MG	2a	1625	1/1	0.96	0.28	49,49,49,49	0
55	MG	1A	3313	1/1	0.96	0.22	39,39,39,39	0
55	MG	2a	1627	1/1	0.96	0.17	54,54,54,54	0
55	MG	1A	3694	1/1	0.96	0.24	46,46,46,46	0
55	MG	2A	3692	1/1	0.96	0.06	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3314	1/1	0.96	0.09	53,53,53,53	0
55	MG	2a	1632	1/1	0.96	0.46	73,73,73,73	0
55	MG	1A	3212	1/1	0.96	0.45	39,39,39,39	0
55	MG	1A	3027	1/1	0.96	0.17	31,31,31,31	0
55	MG	2A	3697	1/1	0.96	0.05	53,53,53,53	0
55	MG	1A	3808	1/1	0.96	0.23	19,19,19,19	0
55	MG	1A	3149	1/1	0.96	0.18	49,49,49,49	0
55	MG	17	102	1/1	0.96	0.15	55,55,55,55	0
55	MG	2A	3703	1/1	0.96	0.25	91,91,91,91	0
55	MG	1A	3918	1/1	0.96	0.22	28,28,28,28	0
55	MG	2A	3241	1/1	0.96	0.33	44,44,44,44	0
55	MG	1A	3810	1/1	0.96	0.06	63,63,63,63	0
55	MG	2A	3064	1/1	0.96	0.61	54,54,54,54	0
55	MG	2A	3708	1/1	0.96	0.12	69,69,69,69	0
55	MG	1A	3811	1/1	0.96	0.11	35,35,35,35	0
55	MG	2A	3710	1/1	0.96	0.14	62,62,62,62	0
55	MG	2A	3246	1/1	0.96	0.03	71,71,71,71	0
55	MG	2A	3247	1/1	0.96	0.20	38,38,38,38	0
55	MG	2A	3714	1/1	0.96	0.11	52,52,52,52	0
55	MG	19	101	1/1	0.96	0.39	52,52,52,52	0
55	MG	1A	3462	1/1	0.96	0.58	33,33,33,33	0
55	MG	2A	3069	1/1	0.96	0.23	54,54,54,54	0
55	MG	1A	3702	1/1	0.96	0.19	31,31,31,31	0
55	MG	2A	3071	1/1	0.96	0.28	38,38,38,38	0
55	MG	1A	3272	1/1	0.96	0.20	23,23,23,23	0
55	MG	1A	3464	1/1	0.96	0.22	61,61,61,61	0
55	MG	2a	1658	1/1	0.96	0.14	58,58,58,58	0
55	MG	1A	3818	1/1	0.96	0.09	52,52,52,52	0
55	MG	2A	3491	1/1	0.96	0.13	49,49,49,49	0
55	MG	1A	3819	1/1	0.96	0.52	45,45,45,45	0
55	MG	1A	3242	1/1	0.96	0.65	46,46,46,46	0
55	MG	1A	3324	1/1	0.96	0.17	24,24,24,24	0
55	MG	2A	3497	1/1	0.96	0.13	39,39,39,39	0
55	MG	1A	3070	1/1	0.96	0.22	37,37,37,37	0
55	MG	2A	3079	1/1	0.96	0.31	60,60,60,60	0
55	MG	1A	3708	1/1	0.96	0.23	51,51,51,51	0
55	MG	1A	3533	1/1	0.96	0.17	41,41,41,41	0
55	MG	2A	3082	1/1	0.96	0.30	60,60,60,60	0
55	MG	1a	3011	1/1	0.96	0.15	74,74,74,74	0
55	MG	2A	3504	1/1	0.96	0.24	58,58,58,58	0
55	MG	1A	3614	1/1	0.96	0.03	50,50,50,50	0
55	MG	2A	3739	1/1	0.96	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3936	1/1	0.96	0.28	55,55,55,55	0
55	MG	2A	3507	1/1	0.96	0.57	62,62,62,62	0
55	MG	1a	3167	1/1	0.96	0.09	79,79,79,79	0
55	MG	1A	3327	1/1	0.96	0.10	43,43,43,43	0
55	MG	1A	3005	1/1	0.96	0.16	22,22,22,22	0
55	MG	1A	3939	1/1	0.96	0.62	39,39,39,39	0
55	MG	2a	1684	1/1	0.96	0.19	64,64,64,64	0
55	MG	1a	3171	1/1	0.96	0.11	54,54,54,54	0
55	MG	2A	3093	1/1	0.96	0.50	56,56,56,56	0
55	MG	2a	1687	1/1	0.96	0.30	58,58,58,58	0
55	MG	2A	3280	1/1	0.96	0.15	35,35,35,35	0
55	MG	2a	1689	1/1	0.96	0.16	63,63,63,63	0
55	MG	2A	3515	1/1	0.96	0.09	50,50,50,50	0
55	MG	1A	3829	1/1	0.96	0.34	67,67,67,67	0
55	MG	1A	3134	1/1	0.96	0.12	40,40,40,40	0
55	MG	1A	3619	1/1	0.96	0.20	44,44,44,44	0
55	MG	1A	3943	1/1	0.96	0.30	37,37,37,37	0
55	MG	1A	3059	1/1	0.96	0.20	58,58,58,58	0
55	MG	1a	3178	1/1	0.96	0.07	70,70,70,70	0
55	MG	1A	3336	1/1	0.96	0.17	19,19,19,19	0
55	MG	1a	3025	1/1	0.96	0.08	51,51,51,51	0
55	MG	1B	202	1/1	0.96	0.21	60,60,60,60	0
55	MG	2a	1703	1/1	0.96	0.09	60,60,60,60	0
55	MG	1A	3338	1/1	0.96	0.14	24,24,24,24	0
55	MG	2a	1705	1/1	0.96	0.20	75,75,75,75	0
55	MG	2A	3298	1/1	0.96	0.17	37,37,37,37	0
55	MG	1A	3544	1/1	0.96	0.27	30,30,30,30	0
55	MG	2A	3767	1/1	0.96	0.06	69,69,69,69	0
55	MG	2A	3301	1/1	0.96	0.08	85,85,85,85	0
55	MG	1A	3627	1/1	0.96	0.15	49,49,49,49	0
55	MG	1A	3475	1/1	0.96	0.08	25,25,25,25	0
55	MG	1A	3339	1/1	0.96	0.12	23,23,23,23	0
55	MG	1A	3630	1/1	0.96	0.10	60,60,60,60	0
55	MG	2A	3306	1/1	0.96	0.33	62,62,62,62	0
55	MG	2A	3312	1/1	0.96	0.14	62,62,62,62	0
55	MG	2A	3313	1/1	0.96	0.20	65,65,65,65	0
55	MG	2A	3778	1/1	0.96	0.24	51,51,51,51	0
55	MG	2A	3779	1/1	0.96	0.15	36,36,36,36	0
55	MG	1A	3631	1/1	0.96	0.26	81,81,81,81	0
55	MG	1A	3727	1/1	0.96	0.09	48,48,48,48	0
55	MG	1A	3403	1/1	0.96	0.14	48,48,48,48	0
55	MG	2A	3317	1/1	0.96	0.05	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3543	1/1	0.96	0.04	85,85,85,85	0
55	MG	1a	3192	1/1	0.96	0.15	64,64,64,64	0
55	MG	1B	214	1/1	0.96	0.11	50,50,50,50	0
55	MG	2A	3788	1/1	0.96	0.19	66,66,66,66	0
55	MG	1A	3155	1/1	0.96	0.74	60,60,60,60	0
55	MG	2A	3323	1/1	0.96	0.11	59,59,59,59	0
55	MG	1a	3195	1/1	0.96	0.14	68,68,68,68	0
55	MG	2A	3116	1/1	0.96	0.21	56,56,56,56	0
55	MG	1A	3279	1/1	0.96	0.12	55,55,55,55	0
55	MG	1B	218	1/1	0.96	0.08	49,49,49,49	0
55	MG	2A	3331	1/1	0.96	0.18	45,45,45,45	0
55	MG	1A	3343	1/1	0.96	0.26	54,54,54,54	0
55	MG	2A	3120	1/1	0.96	0.07	75,75,75,75	0
55	MG	2A	3121	1/1	0.96	0.23	46,46,46,46	0
55	MG	1A	3637	1/1	0.96	0.14	45,45,45,45	0
55	MG	2a	1739	1/1	0.96	0.13	81,81,81,81	0
55	MG	1A	3407	1/1	0.96	0.12	58,58,58,58	0
55	MG	1B	223	1/1	0.96	0.32	61,61,61,61	0
55	MG	2A	3560	1/1	0.96	0.08	66,66,66,66	0
55	MG	2a	1743	1/1	0.96	0.32	65,65,65,65	0
55	MG	1a	3203	1/1	0.96	0.16	64,64,64,64	0
55	MG	2A	3339	1/1	0.96	0.17	37,37,37,37	0
55	MG	1a	3045	1/1	0.96	0.33	63,63,63,63	0
55	MG	1A	3249	1/1	0.96	0.23	10,10,10,10	0
55	MG	1A	3640	1/1	0.96	0.44	37,37,37,37	0
55	MG	1a	3209	1/1	0.96	0.14	56,56,56,56	0
55	MG	1A	3641	1/1	0.96	0.13	41,41,41,41	0
55	MG	2A	3817	1/1	0.96	1.18	56,56,56,56	0
55	MG	1a	3211	1/1	0.96	0.28	65,65,65,65	0
55	MG	2A	3346	1/1	0.96	0.05	77,77,77,77	0
55	MG	2A	3820	1/1	0.96	0.56	51,51,51,51	0
55	MG	1a	3212	1/1	0.96	0.05	56,56,56,56	0
55	MG	1A	3197	1/1	0.96	0.41	31,31,31,31	0
55	MG	2A	3349	1/1	0.96	0.14	80,80,80,80	0
55	MG	2A	3575	1/1	0.96	0.16	52,52,52,52	0
55	MG	1A	3411	1/1	0.96	0.04	48,48,48,48	0
55	MG	2a	1761	1/1	0.96	0.15	68,68,68,68	0
55	MG	2A	3826	1/1	0.96	1.08	56,56,56,56	0
55	MG	1A	3743	1/1	0.96	0.04	58,58,58,58	0
55	MG	2A	3828	1/1	0.96	0.69	65,65,65,65	0
55	MG	2A	3352	1/1	0.96	0.20	29,29,29,29	0
55	MG	2a	1766	1/1	0.96	0.25	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3555	1/1	0.96	0.12	28,28,28,28	0
55	MG	1A	3646	1/1	0.96	0.16	49,49,49,49	0
55	MG	2a	1770	1/1	0.96	0.06	61,61,61,61	0
55	MG	1A	3284	1/1	0.96	0.11	64,64,64,64	0
55	MG	1A	3559	1/1	0.96	0.18	56,56,56,56	0
55	MG	1a	3221	1/1	0.96	0.44	79,79,79,79	0
55	MG	1A	3107	1/1	0.96	0.23	25,25,25,25	0
55	MG	2A	3145	1/1	0.96	0.13	75,75,75,75	0
55	MG	1A	3158	1/1	0.96	0.13	31,31,31,31	0
55	MG	1D	311	1/1	0.96	0.09	61,61,61,61	0
55	MG	1a	3059	1/1	0.96	0.16	78,78,78,78	0
55	MG	1A	3349	1/1	0.96	0.38	62,62,62,62	0
55	MG	2A	3592	1/1	0.96	0.10	80,80,80,80	0
55	MG	2B	3006	1/1	0.96	0.44	80,80,80,80	0
55	MG	2a	1783	1/1	0.96	0.07	59,59,59,59	0
55	MG	1b	3001	1/1	0.96	0.07	71,71,71,71	0
55	MG	1A	3753	1/1	0.96	0.05	50,50,50,50	0
55	MG	1a	3062	1/1	0.96	0.62	81,81,81,81	0
55	MG	1A	3563	1/1	0.96	0.15	29,29,29,29	0
55	MG	1A	3564	1/1	0.96	0.13	28,28,28,28	0
55	MG	2A	3156	1/1	0.96	0.27	58,58,58,58	0
55	MG	1E	302	1/1	0.96	0.19	26,26,26,26	0
55	MG	2A	3600	1/1	0.96	0.38	53,53,53,53	0
55	MG	2a	1793	1/1	0.96	0.14	56,56,56,56	0
55	MG	2a	1794	1/1	0.96	0.06	74,74,74,74	0
55	MG	2a	1795	1/1	0.96	0.37	80,80,80,80	0
55	MG	2a	1796	1/1	0.96	0.12	58,58,58,58	0
55	MG	1A	3428	1/1	0.96	0.14	18,18,18,18	0
55	MG	1A	3867	1/1	0.96	0.34	45,45,45,45	0
55	MG	1A	3868	1/1	0.96	0.12	27,27,27,27	0
55	MG	2e	201	1/1	0.96	0.15	71,71,71,71	0
55	MG	1A	3656	1/1	0.96	0.11	57,57,57,57	0
55	MG	1A	3108	1/1	0.96	0.21	32,32,32,32	0
55	MG	2A	3387	1/1	0.96	0.08	58,58,58,58	0
55	MG	1A	3494	1/1	0.96	0.09	48,48,48,48	0
55	MG	1A	3082	1/1	0.96	0.76	47,47,47,47	0
55	MG	2A	3392	1/1	0.96	0.13	55,55,55,55	0
55	MG	1A	3291	1/1	0.96	0.10	72,72,72,72	0
55	MG	2A	3394	1/1	0.96	0.15	49,49,49,49	0
55	MG	1A	3762	1/1	0.96	0.17	19,19,19,19	0
55	MG	1a	3075	1/1	0.96	0.23	57,57,57,57	0
55	MG	1A	3096	1/1	0.96	0.35	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3181	1/1	0.96	0.42	43,43,43,43	0
56	ZN	1n	501	1/1	0.96	0.13	85,85,85,85	0
55	MG	1A	3573	1/1	0.96	0.19	21,21,21,21	0
55	MG	1A	3435	1/1	0.96	0.09	44,44,44,44	0
56	ZN	2n	501	1/1	0.96	0.06	94,94,94,94	0
55	MG	1F	312	1/1	0.96	0.11	47,47,47,47	0
55	MG	1A	3484	1/1	0.97	0.20	69,69,69,69	0
55	MG	2A	3353	1/1	0.97	0.06	70,70,70,70	0
55	MG	2A	3806	1/1	0.97	0.26	47,47,47,47	0
55	MG	2A	3807	1/1	0.97	0.43	57,57,57,57	0
55	MG	2A	3218	1/1	0.97	0.34	23,23,23,23	0
55	MG	1A	3230	1/1	0.97	0.67	35,35,35,35	0
55	MG	2A	3220	1/1	0.97	0.31	49,49,49,49	0
55	MG	1A	3157	1/1	0.97	0.20	33,33,33,33	0
55	MG	1A	3715	1/1	0.97	0.06	51,51,51,51	0
55	MG	1A	3716	1/1	0.97	0.12	31,31,31,31	0
55	MG	1A	3539	1/1	0.97	0.52	35,35,35,35	0
55	MG	1A	3389	1/1	0.97	0.18	21,21,21,21	0
55	MG	1A	3350	1/1	0.97	0.13	26,26,26,26	0
55	MG	2a	1664	1/1	0.97	0.34	68,68,68,68	0
55	MG	1A	3321	1/1	0.97	0.25	49,49,49,49	0
55	MG	1A	3597	1/1	0.97	0.05	49,49,49,49	0
55	MG	2A	3366	1/1	0.97	0.20	35,35,35,35	0
55	MG	2A	3230	1/1	0.97	0.18	44,44,44,44	0
55	MG	2a	1669	1/1	0.97	0.07	49,49,49,49	0
55	MG	2a	1670	1/1	0.97	0.10	49,49,49,49	0
55	MG	1A	3491	1/1	0.97	0.15	42,42,42,42	0
55	MG	1A	3075	1/1	0.97	0.47	33,33,33,33	0
55	MG	2A	3122	1/1	0.97	0.28	46,46,46,46	0
55	MG	2a	1674	1/1	0.97	0.19	71,71,71,71	0
55	MG	2A	3517	1/1	0.97	0.13	80,80,80,80	0
55	MG	2A	3123	1/1	0.97	0.22	52,52,52,52	0
55	MG	1A	3446	1/1	0.97	0.16	24,24,24,24	0
55	MG	1B	205	1/1	0.97	0.10	54,54,54,54	0
55	MG	1A	3798	1/1	0.97	0.14	46,46,46,46	0
55	MG	2A	3667	1/1	0.97	0.15	64,64,64,64	0
55	MG	1A	3323	1/1	0.97	0.07	29,29,29,29	0
55	MG	2A	3670	1/1	0.97	0.04	76,76,76,76	0
55	MG	2A	3381	1/1	0.97	0.11	66,66,66,66	0
55	MG	2A	3382	1/1	0.97	0.21	61,61,61,61	0
55	MG	2A	3383	1/1	0.97	0.14	66,66,66,66	0
55	MG	11	101	1/1	0.97	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3527	1/1	0.97	0.20	37,37,37,37	0
55	MG	1A	3020	1/1	0.97	0.42	38,38,38,38	0
55	MG	1A	3664	1/1	0.97	0.25	48,48,48,48	0
55	MG	1A	3356	1/1	0.97	0.14	23,23,23,23	0
55	MG	2B	3004	1/1	0.97	0.12	78,78,78,78	0
55	MG	1A	3666	1/1	0.97	0.23	53,53,53,53	0
55	MG	2a	1693	1/1	0.97	0.33	60,60,60,60	0
55	MG	2A	3389	1/1	0.97	0.18	51,51,51,51	0
55	MG	1B	212	1/1	0.97	0.18	56,56,56,56	0
55	MG	1A	3604	1/1	0.97	0.05	59,59,59,59	0
55	MG	2A	3248	1/1	0.97	0.07	28,28,28,28	0
55	MG	2a	1698	1/1	0.97	0.65	61,61,61,61	0
55	MG	1A	3398	1/1	0.97	0.24	66,66,66,66	0
55	MG	1A	3300	1/1	0.97	0.11	43,43,43,43	0
55	MG	1A	3452	1/1	0.97	0.07	55,55,55,55	0
55	MG	2A	3688	1/1	0.97	0.17	73,73,73,73	0
55	MG	1A	3261	1/1	0.97	0.19	17,17,17,17	0
55	MG	1A	3304	1/1	0.97	0.12	14,14,14,14	0
55	MG	1A	3738	1/1	0.97	0.17	23,23,23,23	0
55	MG	1B	221	1/1	0.97	0.35	79,79,79,79	0
55	MG	1a	3085	1/1	0.97	0.33	66,66,66,66	0
55	MG	1a	3086	1/1	0.97	0.45	64,64,64,64	0
55	MG	2A	3259	1/1	0.97	0.12	89,89,89,89	0
55	MG	2A	3044	1/1	0.97	0.38	38,38,38,38	0
55	MG	2A	3698	1/1	0.97	0.17	40,40,40,40	0
55	MG	2A	3699	1/1	0.97	0.15	37,37,37,37	0
55	MG	1A	3028	1/1	0.97	0.29	37,37,37,37	0
55	MG	2a	1715	1/1	0.97	0.17	81,81,81,81	0
55	MG	1a	3191	1/1	0.97	0.12	49,49,49,49	0
55	MG	2D	308	1/1	0.97	0.25	28,28,28,28	0
55	MG	1A	3815	1/1	0.97	0.16	25,25,25,25	0
55	MG	1A	3331	1/1	0.97	0.19	23,23,23,23	0
55	MG	1A	3365	1/1	0.97	0.22	30,30,30,30	0
55	MG	2A	3413	1/1	0.97	0.13	70,70,70,70	0
55	MG	1A	3368	1/1	0.97	0.11	47,47,47,47	0
55	MG	1A	3121	1/1	0.97	0.43	31,31,31,31	0
55	MG	1A	3370	1/1	0.97	0.21	26,26,26,26	0
55	MG	1a	3198	1/1	0.97	0.08	57,57,57,57	0
55	MG	2F	304	1/1	0.97	0.34	62,62,62,62	0
55	MG	1A	3223	1/1	0.97	0.08	72,72,72,72	0
55	MG	2A	3272	1/1	0.97	0.07	60,60,60,60	0
55	MG	1A	3620	1/1	0.97	0.09	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1D	305	1/1	0.97	0.35	42,42,42,42	0
55	MG	1A	3748	1/1	0.97	0.07	39,39,39,39	0
55	MG	1A	3510	1/1	0.97	0.40	44,44,44,44	0
55	MG	1A	3897	1/1	0.97	0.22	11,11,11,11	0
55	MG	1A	3337	1/1	0.97	0.18	18,18,18,18	0
55	MG	2A	3566	1/1	0.97	0.34	55,55,55,55	0
55	MG	1a	3206	1/1	0.97	0.04	74,74,74,74	0
55	MG	2A	3282	1/1	0.97	0.12	42,42,42,42	0
55	MG	2A	3164	1/1	0.97	0.29	41,41,41,41	0
55	MG	2A	3429	1/1	0.97	0.20	76,76,76,76	0
55	MG	1A	3224	1/1	0.97	0.14	35,35,35,35	0
55	MG	1A	3827	1/1	0.97	0.09	69,69,69,69	0
55	MG	2A	3726	1/1	0.97	0.11	38,38,38,38	0
55	MG	2R	8002	1/1	0.97	0.25	45,45,45,45	0
55	MG	2A	3290	1/1	0.97	0.22	71,71,71,71	0
55	MG	2A	3728	1/1	0.97	0.12	46,46,46,46	0
55	MG	1A	3413	1/1	0.97	0.09	28,28,28,28	0
55	MG	2V	201	1/1	0.97	0.72	54,54,54,54	0
55	MG	2A	3730	1/1	0.97	0.14	51,51,51,51	0
55	MG	1A	3686	1/1	0.97	0.29	55,55,55,55	0
55	MG	1A	3625	1/1	0.97	0.45	44,44,44,44	0
55	MG	2A	3578	1/1	0.97	0.09	61,61,61,61	0
55	MG	2A	3294	1/1	0.97	0.14	45,45,45,45	0
55	MG	1A	3466	1/1	0.97	0.11	53,53,53,53	0
55	MG	2A	3068	1/1	0.97	0.11	65,65,65,65	0
55	MG	1A	3414	1/1	0.97	0.15	31,31,31,31	0
55	MG	1a	3023	1/1	0.97	0.48	53,53,53,53	0
55	MG	1A	3283	1/1	0.97	0.23	40,40,40,40	0
55	MG	1A	3416	1/1	0.97	0.20	31,31,31,31	0
55	MG	1A	3417	1/1	0.97	0.16	37,37,37,37	0
55	MG	1a	3121	1/1	0.97	0.71	72,72,72,72	0
55	MG	1A	3187	1/1	0.97	0.56	35,35,35,35	0
55	MG	2A	3745	1/1	0.97	0.10	65,65,65,65	0
55	MG	1A	3910	1/1	0.97	0.38	36,36,36,36	0
55	MG	1A	3422	1/1	0.97	0.07	68,68,68,68	0
55	MG	2A	3307	1/1	0.97	0.16	63,63,63,63	0
55	MG	2A	3308	1/1	0.97	0.15	58,58,58,58	0
55	MG	2a	1768	1/1	0.97	0.21	74,74,74,74	0
55	MG	2A	3182	1/1	0.97	0.09	80,80,80,80	0
55	MG	1A	3696	1/1	0.97	0.16	25,25,25,25	0
55	MG	1A	3376	1/1	0.97	0.13	13,13,13,13	0
55	MG	1A	3765	1/1	0.97	0.05	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3635	1/1	0.97	0.08	29,29,29,29	0
55	MG	1A	3699	1/1	0.97	0.15	27,27,27,27	0
55	MG	1A	3102	1/1	0.97	0.34	34,34,34,34	0
55	MG	2A	3319	1/1	0.97	0.20	30,30,30,30	0
55	MG	2A	3084	1/1	0.97	0.30	49,49,49,49	0
55	MG	2a	1778	1/1	0.97	0.09	64,64,64,64	0
55	MG	2A	3761	1/1	0.97	0.17	38,38,38,38	0
55	MG	2A	3321	1/1	0.97	0.04	65,65,65,65	0
55	MG	1A	3844	1/1	0.97	0.09	25,25,25,25	0
55	MG	1a	3037	1/1	0.97	0.16	70,70,70,70	0
55	MG	2A	3087	1/1	0.97	0.17	61,61,61,61	0
55	MG	1A	3378	1/1	0.97	0.16	47,47,47,47	0
55	MG	1A	3269	1/1	0.97	0.09	26,26,26,26	0
55	MG	1A	3380	1/1	0.97	0.14	49,49,49,49	0
55	MG	2A	3330	1/1	0.97	0.13	45,45,45,45	0
55	MG	1A	3923	1/1	0.97	0.14	17,17,17,17	0
55	MG	1A	3581	1/1	0.97	0.22	39,39,39,39	0
55	MG	1a	3142	1/1	0.97	0.15	86,86,86,86	0
55	MG	1k	201	1/1	0.97	0.23	50,50,50,50	0
55	MG	1A	3381	1/1	0.97	0.17	23,23,23,23	0
55	MG	2A	3775	1/1	0.97	0.12	63,63,63,63	0
55	MG	1A	3850	1/1	0.97	0.12	23,23,23,23	0
55	MG	2A	3620	1/1	0.97	0.12	40,40,40,40	0
55	MG	2a	1797	1/1	0.97	0.09	75,75,75,75	0
55	MG	1A	3003	1/1	0.97	0.10	20,20,20,20	0
55	MG	1A	3776	1/1	0.97	0.06	43,43,43,43	0
55	MG	2A	3204	1/1	0.97	0.71	58,58,58,58	0
55	MG	2A	3482	1/1	0.97	0.66	56,56,56,56	0
55	MG	1a	3147	1/1	0.97	0.13	73,73,73,73	0
55	MG	2A	3784	1/1	0.97	0.16	64,64,64,64	0
55	MG	1A	3015	1/1	0.97	0.29	30,30,30,30	0
55	MG	2A	3628	1/1	0.97	0.22	57,57,57,57	0
55	MG	1A	3229	1/1	0.97	0.15	41,41,41,41	0
55	MG	1Q	201	1/1	0.97	0.12	51,51,51,51	0
55	MG	1A	3779	1/1	0.97	0.04	57,57,57,57	0
55	MG	2A	3006	1/1	0.97	0.13	40,40,40,40	0
55	MG	1A	3318	1/1	0.97	0.14	70,70,70,70	0
55	MG	1A	3933	1/1	0.97	0.15	28,28,28,28	0
55	MG	1A	3437	1/1	0.97	0.09	66,66,66,66	0
55	MG	1A	3935	1/1	0.97	0.14	27,27,27,27	0
55	MG	2A	3494	1/1	0.97	0.09	59,59,59,59	0
55	MG	2A	3495	1/1	0.97	0.16	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3639	1/1	0.97	0.19	79,79,79,79	0
56	ZN	25	103	1/1	0.97	0.08	64,64,64,64	0
55	MG	1a	3156	1/1	0.97	0.14	70,70,70,70	0
55	MG	2A	3216	1/1	0.97	0.14	37,37,37,37	0
55	MG	1a	3100	1/1	0.98	0.38	62,62,62,62	0
55	MG	1A	3731	1/1	0.98	0.09	25,25,25,25	0
55	MG	2A	3758	1/1	0.98	0.06	78,78,78,78	0
55	MG	1A	3796	1/1	0.98	0.08	33,33,33,33	0
55	MG	2A	3760	1/1	0.98	0.07	42,42,42,42	0
55	MG	1A	3303	1/1	0.98	0.20	16,16,16,16	0
55	MG	1a	3104	1/1	0.98	0.24	80,80,80,80	0
55	MG	1A	3618	1/1	0.98	0.07	51,51,51,51	0
55	MG	2a	1700	1/1	0.98	0.15	68,68,68,68	0
55	MG	1A	3154	1/1	0.98	0.39	31,31,31,31	0
55	MG	2A	3311	1/1	0.98	0.12	48,48,48,48	0
55	MG	1G	3002	1/1	0.98	0.09	67,67,67,67	0
55	MG	1A	3305	1/1	0.98	0.06	68,68,68,68	0
55	MG	1A	3801	1/1	0.98	0.16	32,32,32,32	0
55	MG	1A	3736	1/1	0.98	0.09	20,20,20,20	0
55	MG	1A	3569	1/1	0.98	0.45	48,48,48,48	0
55	MG	1A	3445	1/1	0.98	0.21	24,24,24,24	0
55	MG	1A	3129	1/1	0.98	0.26	33,33,33,33	0
55	MG	1A	3871	1/1	0.98	0.12	16,16,16,16	0
55	MG	1A	3525	1/1	0.98	0.13	27,27,27,27	0
55	MG	1A	3807	1/1	0.98	0.07	17,17,17,17	0
55	MG	2A	3776	1/1	0.98	0.07	44,44,44,44	0
55	MG	1a	3118	1/1	0.98	0.06	68,68,68,68	0
55	MG	2A	3222	1/1	0.98	0.16	56,56,56,56	0
55	MG	1A	3288	1/1	0.98	0.09	62,62,62,62	0
55	MG	1A	3626	1/1	0.98	0.06	42,42,42,42	0
55	MG	1a	3207	1/1	0.98	0.17	77,77,77,77	0
55	MG	2A	3663	1/1	0.98	0.12	53,53,53,53	0
55	MG	2A	3328	1/1	0.98	0.19	63,63,63,63	0
55	MG	1A	3326	1/1	0.98	0.11	28,28,28,28	0
55	MG	1a	3122	1/1	0.98	0.28	67,67,67,67	0
55	MG	1a	3123	1/1	0.98	0.23	79,79,79,79	0
55	MG	2A	3551	1/1	0.98	0.10	62,62,62,62	0
55	MG	1A	3487	1/1	0.98	0.10	32,32,32,32	0
55	MG	1a	3125	1/1	0.98	0.34	78,78,78,78	0
55	MG	2A	3790	1/1	0.98	0.12	39,39,39,39	0
55	MG	1B	201	1/1	0.98	0.70	48,48,48,48	0
55	MG	1A	3141	1/1	0.98	0.54	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3793	1/1	0.98	0.21	53,53,53,53	0
55	MG	1A	3879	1/1	0.98	0.11	47,47,47,47	0
55	MG	2a	1605	1/1	0.98	0.09	53,53,53,53	0
55	MG	1A	3813	1/1	0.98	0.12	22,22,22,22	0
55	MG	2A	3796	1/1	0.98	0.15	78,78,78,78	0
55	MG	1A	3410	1/1	0.98	0.18	8,8,8,8	0
55	MG	1A	3687	1/1	0.98	0.15	25,25,25,25	0
55	MG	1A	3086	1/1	0.98	0.10	55,55,55,55	0
55	MG	2A	3449	1/1	0.98	0.18	34,34,34,34	0
55	MG	2A	3238	1/1	0.98	0.17	46,46,46,46	0
55	MG	1A	3412	1/1	0.98	0.21	22,22,22,22	0
55	MG	1A	3751	1/1	0.98	0.08	24,24,24,24	0
55	MG	1A	3106	1/1	0.98	0.32	34,34,34,34	0
55	MG	1A	3354	1/1	0.98	0.14	26,26,26,26	0
55	MG	1A	3535	1/1	0.98	0.28	38,38,38,38	0
55	MG	2a	1745	1/1	0.98	0.04	77,77,77,77	0
55	MG	1A	3175	1/1	0.98	0.17	47,47,47,47	0
55	MG	2A	3459	1/1	0.98	0.06	64,64,64,64	0
55	MG	2A	3245	1/1	0.98	0.30	35,35,35,35	0
55	MG	1A	3495	1/1	0.98	0.23	66,66,66,66	0
55	MG	1A	3538	1/1	0.98	0.18	22,22,22,22	0
55	MG	1A	3332	1/1	0.98	0.19	23,23,23,23	0
55	MG	1A	3293	1/1	0.98	0.14	19,19,19,19	0
55	MG	1A	3418	1/1	0.98	0.12	34,34,34,34	0
55	MG	1A	3542	1/1	0.98	0.16	37,37,37,37	0
55	MG	2A	3696	1/1	0.98	0.05	61,61,61,61	0
55	MG	1A	3643	1/1	0.98	0.14	22,22,22,22	0
55	MG	1A	3419	1/1	0.98	0.17	28,28,28,28	0
55	MG	2A	3357	1/1	0.98	0.11	53,53,53,53	0
55	MG	13	101	1/1	0.98	0.30	42,42,42,42	0
55	MG	1A	3334	1/1	0.98	0.16	27,27,27,27	0
55	MG	1A	3421	1/1	0.98	0.16	23,23,23,23	0
55	MG	1A	3268	1/1	0.98	0.16	22,22,22,22	0
55	MG	1A	3423	1/1	0.98	0.18	23,23,23,23	0
55	MG	1A	3295	1/1	0.98	0.19	11,11,11,11	0
55	MG	1A	3769	1/1	0.98	0.16	31,31,31,31	0
55	MG	2a	1639	1/1	0.98	0.15	74,74,74,74	0
55	MG	1A	3361	1/1	0.98	0.10	28,28,28,28	0
55	MG	1A	3391	1/1	0.98	0.12	62,62,62,62	0
55	MG	2A	3367	1/1	0.98	0.09	46,46,46,46	0
55	MG	1A	3248	1/1	0.98	0.12	21,21,21,21	0
55	MG	2A	3371	1/1	0.98	0.18	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3363	1/1	0.98	0.15	39,39,39,39	0
55	MG	2A	3713	1/1	0.98	0.04	79,79,79,79	0
55	MG	2A	3176	1/1	0.98	0.61	43,43,43,43	0
55	MG	1A	3654	1/1	0.98	0.15	40,40,40,40	0
55	MG	1A	3364	1/1	0.98	0.12	26,26,26,26	0
55	MG	2B	3001	1/1	0.98	0.21	64,64,64,64	0
55	MG	1A	3137	1/1	0.98	0.22	43,43,43,43	0
55	MG	2A	3270	1/1	0.98	0.10	45,45,45,45	0
55	MG	1A	3911	1/1	0.98	0.21	33,33,33,33	0
55	MG	2A	3490	1/1	0.98	0.11	56,56,56,56	0
55	MG	1A	3511	1/1	0.98	0.12	25,25,25,25	0
55	MG	2A	3273	1/1	0.98	0.13	44,44,44,44	0
55	MG	1A	3556	1/1	0.98	0.13	32,32,32,32	0
55	MG	2A	3275	1/1	0.98	0.25	35,35,35,35	0
55	MG	1A	3557	1/1	0.98	0.23	29,29,29,29	0
55	MG	2a	1787	1/1	0.98	0.05	78,78,78,78	0
55	MG	2A	3607	1/1	0.98	0.06	74,74,74,74	0
55	MG	1A	3660	1/1	0.98	0.12	35,35,35,35	0
55	MG	1A	3366	1/1	0.98	0.25	31,31,31,31	0
55	MG	1A	3662	1/1	0.98	0.09	22,22,22,22	0
55	MG	1A	3397	1/1	0.98	0.26	17,17,17,17	0
55	MG	1A	3340	1/1	0.98	0.11	25,25,25,25	0
55	MG	1E	305	1/1	0.98	0.17	57,57,57,57	0
55	MG	2A	3391	1/1	0.98	0.22	38,38,38,38	0
55	MG	1A	3317	1/1	0.98	0.28	38,38,38,38	0
55	MG	1A	3611	1/1	0.98	0.05	81,81,81,81	0
55	MG	2A	3286	1/1	0.98	0.07	37,37,37,37	0
55	MG	2d	502	1/1	0.98	0.10	70,70,70,70	0
55	MG	1a	3015	1/1	0.98	0.29	71,71,71,71	0
55	MG	2A	3289	1/1	0.98	0.17	40,40,40,40	0
55	MG	1a	3089	1/1	0.98	0.09	52,52,52,52	0
55	MG	1a	3090	1/1	0.98	0.07	39,39,39,39	0
55	MG	2A	3741	1/1	0.98	0.05	70,70,70,70	0
55	MG	2A	3399	1/1	0.98	0.18	51,51,51,51	0
55	MG	1a	3091	1/1	0.98	0.11	40,40,40,40	0
55	MG	2A	3401	1/1	0.98	0.14	40,40,40,40	0
55	MG	2E	302	1/1	0.98	0.15	39,39,39,39	0
55	MG	1A	3091	1/1	0.98	0.32	17,17,17,17	0
55	MG	1A	3613	1/1	0.98	0.14	23,23,23,23	0
55	MG	1A	3083	1/1	0.98	0.06	50,50,50,50	0
55	MG	2A	3516	1/1	0.98	0.10	59,59,59,59	0
55	MG	1A	3440	1/1	0.98	0.10	54,54,54,54	0

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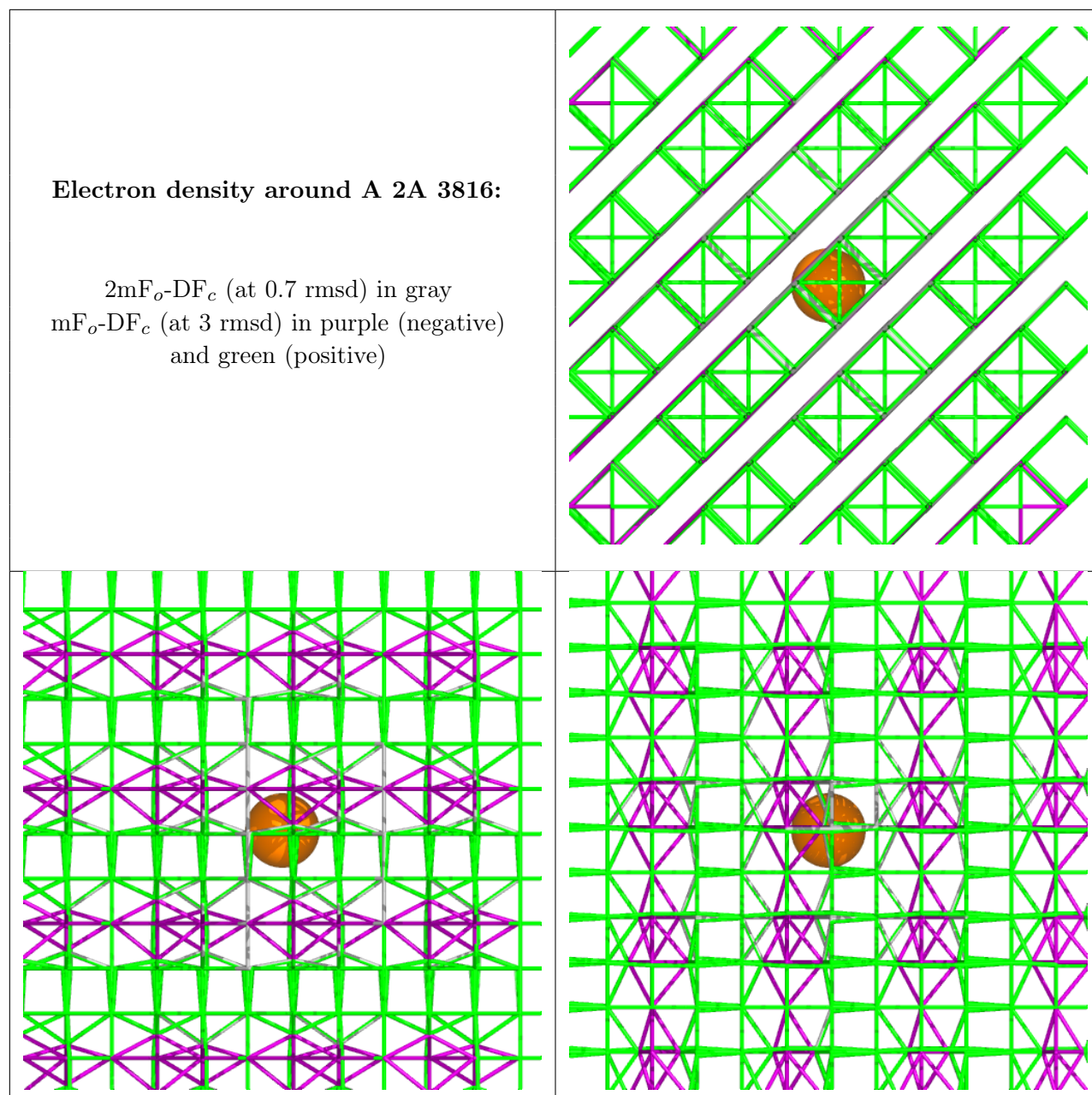
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3302	1/1	0.98	0.12	51,51,51,51	0
56	ZN	16	101	1/1	0.98	0.12	62,62,62,62	0
56	ZN	19	102	1/1	0.98	0.13	68,68,68,68	0
55	MG	1A	3672	1/1	0.98	0.18	35,35,35,35	0
55	MG	1a	3098	1/1	0.98	0.24	59,59,59,59	0
55	MG	2A	3300	1/1	0.98	0.14	42,42,42,42	0
55	MG	2F	308	1/1	0.98	0.38	57,57,57,57	0
56	ZN	29	501	1/1	0.98	0.10	77,77,77,77	0
55	MG	2A	3410	1/1	0.98	0.11	59,59,59,59	0
55	MG	1a	3099	1/1	0.98	0.17	64,64,64,64	0
55	MG	1A	3582	1/1	0.99	0.11	40,40,40,40	0
55	MG	1a	3126	1/1	0.99	0.18	74,74,74,74	0
55	MG	1A	3784	1/1	0.99	0.15	32,32,32,32	0
55	MG	2A	3435	1/1	0.99	0.06	71,71,71,71	0
55	MG	1A	3298	1/1	0.99	0.10	49,49,49,49	0
55	MG	1A	3282	1/1	0.99	0.15	50,50,50,50	0
55	MG	1A	3585	1/1	0.99	0.10	49,49,49,49	0
55	MG	1a	3177	1/1	0.99	0.06	75,75,75,75	0
55	MG	2A	3135	1/1	0.99	0.21	71,71,71,71	0
55	MG	2Q	205	1/1	0.99	0.12	57,57,57,57	0
55	MG	2A	3368	1/1	0.99	0.13	63,63,63,63	0
55	MG	1A	3458	1/1	0.99	0.16	20,20,20,20	0
55	MG	2a	1628	1/1	0.99	0.22	80,80,80,80	0
55	MG	2A	3370	1/1	0.99	0.18	36,36,36,36	0
55	MG	1A	3432	1/1	0.99	0.18	14,14,14,14	0
55	MG	1A	3330	1/1	0.99	0.13	31,31,31,31	0
55	MG	1a	3111	1/1	0.99	0.15	55,55,55,55	0
55	MG	2A	3609	1/1	0.99	0.11	36,36,36,36	0
55	MG	1A	3286	1/1	0.99	0.17	25,25,25,25	0
55	MG	2A	3800	1/1	0.99	0.27	27,27,27,27	0
55	MG	2A	3656	1/1	0.99	0.11	45,45,45,45	0
55	MG	2A	3375	1/1	0.99	0.17	31,31,31,31	0
55	MG	1A	3024	1/1	0.99	0.30	34,34,34,34	0
55	MG	2A	3613	1/1	0.99	0.10	57,57,57,57	0
55	MG	2A	3450	1/1	0.99	0.33	62,62,62,62	0
55	MG	2A	3571	1/1	0.99	0.13	47,47,47,47	0
55	MG	20	104	1/1	0.99	0.07	68,68,68,68	0
55	MG	2A	3451	1/1	0.99	0.07	55,55,55,55	0
55	MG	1A	3296	1/1	0.99	0.20	31,31,31,31	0
55	MG	2A	3309	1/1	0.99	0.17	44,44,44,44	0
55	MG	2A	3310	1/1	0.99	0.21	46,46,46,46	0
55	MG	2A	3251	1/1	0.99	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3424	1/1	0.99	0.10	22,22,22,22	0
55	MG	1A	3739	1/1	0.99	0.08	19,19,19,19	0
55	MG	2A	3669	1/1	0.99	0.14	45,45,45,45	0
55	MG	1A	3085	1/1	0.99	0.22	38,38,38,38	0
55	MG	1A	3367	1/1	0.99	0.09	14,14,14,14	0
55	MG	2A	3625	1/1	0.99	0.06	67,67,67,67	0
55	MG	2A	3284	1/1	0.99	0.10	36,36,36,36	0
55	MG	1A	3427	1/1	0.99	0.14	27,27,27,27	0
55	MG	1a	3214	1/1	0.99	0.06	73,73,73,73	0
55	MG	2A	3287	1/1	0.99	0.21	57,57,57,57	0
55	MG	1A	3335	1/1	0.99	0.14	42,42,42,42	0
56	ZN	15	204	1/1	0.99	0.10	53,53,53,53	0
55	MG	2A	3465	1/1	0.99	0.18	34,34,34,34	0
55	MG	1B	215	1/1	0.99	0.15	50,50,50,50	0
55	MG	1A	3387	1/1	0.99	0.23	47,47,47,47	0
55	MG	1A	3781	1/1	0.99	0.08	36,36,36,36	0
55	MG	2A	3324	1/1	0.99	0.15	37,37,37,37	0
55	MG	2A	3591	1/1	0.99	0.18	56,56,56,56	0
56	ZN	26	101	1/1	0.99	0.12	66,66,66,66	0
55	MG	2A	3153	1/1	0.99	0.16	51,51,51,51	0
55	MG	2A	3685	1/1	0.99	0.34	55,55,55,55	0
57	SF4	1d	501	8/8	0.99	0.12	65,73,78,86	0
57	SF4	2d	501	8/8	0.99	0.09	67,72,87,89	0
55	MG	1A	3710	1/1	0.99	0.23	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.