



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:57 PM BST

PDB ID : 4V6M
EMDB ID: : EMD-1858
Title : Structure of the ribosome-SecYE complex in the membrane environment
Authors : Frauenfeld, J.; Gumbart, J.; van der Sluis, E.O.; Funes, S.; Gartmann, M.;
Beatrix, B.; Mielke, T.; Berninghausen, O.; Becker, T.; Schulten, K.; Beck-
mann, R.
Deposited on : 2011-02-08
Resolution : 7.10 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

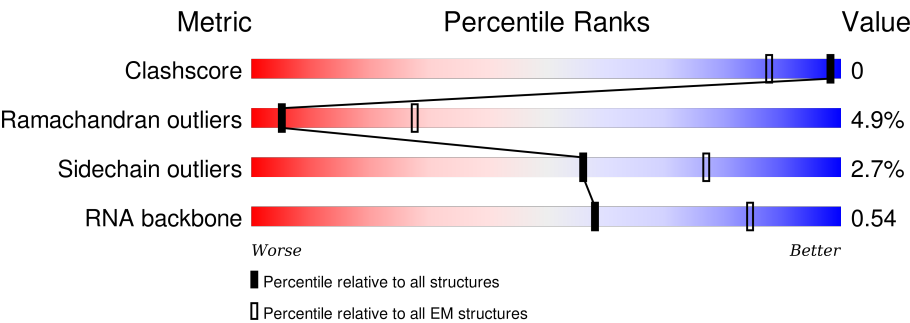
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance i

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

The reported resolution of this entry is 7.10 Å.

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




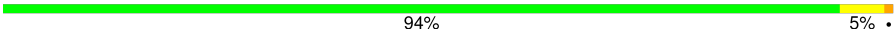

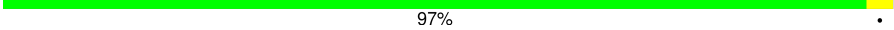
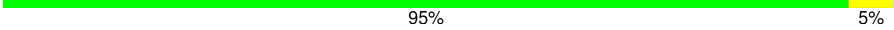


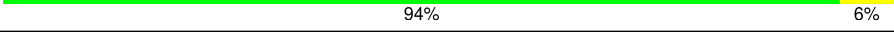
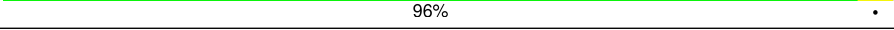


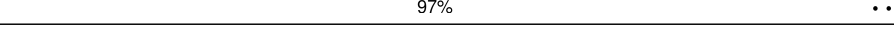
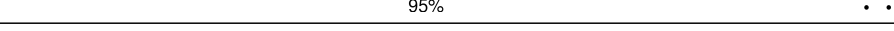


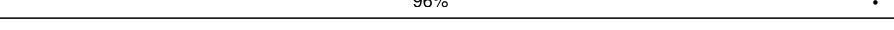
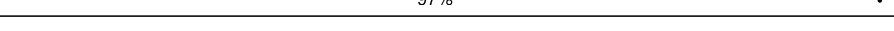
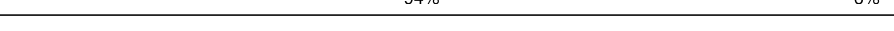

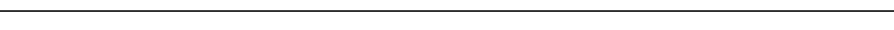

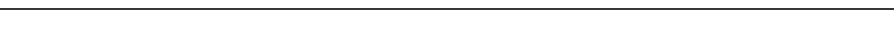
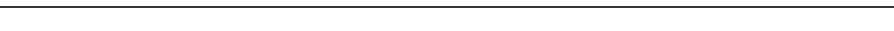


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AA	1542	<div><div></div><div>77%</div><div>20%</div><div></div></div>
2	AX	11	<div><div>9%</div><div>45%</div><div>45%</div><div></div></div>
3	AV	77	<div><div>75%</div><div>25%</div><div></div></div>
4	AZ	98	<div><div>76%</div><div>23%</div><div></div></div>
5	A0	200	<div><div>96%</div><div>5%</div><div></div></div>
5	A1	200	<div><div>95%</div><div>5%</div><div></div></div>
6	AB	240	<div><div>94%</div><div>5%</div><div></div></div>
7	AC	232	<div><div>90%</div><div>9%</div><div></div></div>





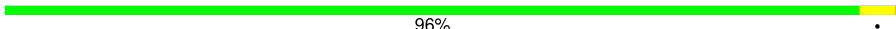


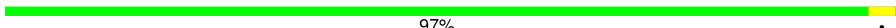


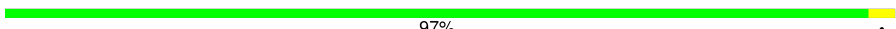





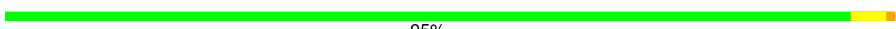
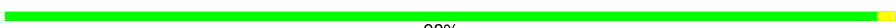
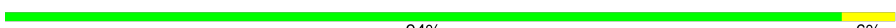

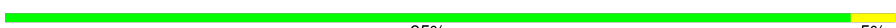

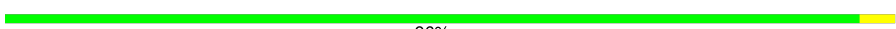


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Mol	Chain	Length	Quality of chain
8	AD	205	 91% 9%
9	AE	166	 94% 5% .
10	AF	135	 93% 7%
11	AG	178	 97% .
12	AH	129	 95% 5%
13	AI	129	 90% 9% .
14	AJ	103	 88% 12%
15	AK	128	 94% 6%
16	AL	123	 96% .
17	AM	117	 92% 7% .
18	AN	100	 88% 12%
19	AO	88	 97% ..
20	AP	82	 95% . .
21	AQ	83	 87% 13%
22	AR	74	 92% 8%
23	AS	91	 96% .
24	AT	86	 97% .
25	AU	70	 94% 6%
26	B7	120	 82% 18% .
27	B8	2904	 80% 18% .
28	BA	435	 80% 16% .
29	BB	116	 89% 10% .
30	B5	234	 95% 5%
31	B6	272	 93% 6% .
32	BD	209	 90% 10%

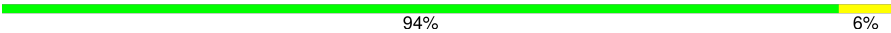

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Mol	Chain	Length	Quality of chain
33	BE	201	 94% 6%
34	BF	178	 90% 9% .
35	BG	176	 93% 7% .
36	BH	149	 88% 11% .
37	BI	141	 96% . .
38	BJ	142	 95% 5%
39	BK	123	 91% 9%
40	BL	144	 97% . .
41	BM	136	 92% 7% .
42	BN	127	 89% 11%
43	BO	117	 97% .
44	BP	114	 91% 9%
45	BQ	117	 94% 6%
46	BR	103	 94% 5% .
47	BS	110	 92% 7% .
48	BT	100	 89% 9% .
49	BU	103	 95% . .
50	BV	94	 98% .
51	BW	84	 94% 6%
52	BX	77	 91% 9%
53	BY	63	 95% 5%
54	BZ	58	 93% 7%
55	B0	56	 96% .
56	B1	54	 94% 6%
57	B2	46	 87% 11% .

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Mol	Chain	Length	Quality of chain
58	B3	64	 94%6%
59	B4	38	 92%8%

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
60	PEV	A0	308	X	-	-	-
60	PEV	A0	314	X	-	-	-
60	PEV	A0	323	X	-	-	-
60	PEV	A1	301	X	-	-	-
60	PEV	A1	305	X	-	-	-
60	PEV	A1	313	X	-	-	-
60	PEV	A1	317	X	-	-	-
60	PEV	AZ	204	X	-	-	-
60	PEV	B8	3001	X	-	-	-
60	PEV	BA	502	X	-	-	-
60	PEV	BA	508	X	-	-	-
60	PEV	BA	526	X	-	-	-
60	PEV	BA	530	X	-	-	-
60	PEV	BA	533	-	-	X	-
60	PEV	BA	535	X	-	-	-
60	PEV	BA	537	X	-	-	-
60	PEV	BA	538	X	-	-	-
60	PEV	BB	202	X	-	-	-
60	PEV	BB	206	X	-	-	-
61	PGV	A0	304	X	-	-	-
61	PGV	A0	305	X	-	-	-
61	PGV	A0	306	X	-	-	-
61	PGV	A0	317	X	-	-	-
61	PGV	A0	318	X	-	-	-
61	PGV	A0	325	X	-	-	-
61	PGV	A0	327	X	-	-	-
61	PGV	A0	328	X	-	-	-
61	PGV	A0	331	X	-	-	-
61	PGV	A0	332	X	-	-	-
61	PGV	A1	303	X	-	-	-
61	PGV	A1	311	X	-	-	-
61	PGV	A1	315	X	-	-	-
61	PGV	A1	318	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	PGV	AZ	205	X	-	-	-
61	PGV	AZ	207	X	-	-	-
61	PGV	B8	3005	X	-	-	-
61	PGV	BA	501	X	-	-	-
61	PGV	BA	505	X	-	-	-
61	PGV	BA	512	X	-	-	-
61	PGV	BA	515	X	-	-	-
61	PGV	BA	516	X	-	-	-
61	PGV	BA	522	X	-	-	-
61	PGV	BA	536	X	-	-	-
61	PGV	BA	540	X	-	-	-
61	PGV	BB	203	X	-	-	-
61	PGV	BB	204	X	-	-	-
61	PGV	BB	205	X	-	-	-
61	PGV	BB	207	X	-	-	-
61	PGV	BB	208	X	-	-	-
61	PGV	BB	213	X	-	-	-
61	PGV	BB	217	X	-	-	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 163040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1542	Total	C	N	O	P	0	0
			33080	14754	6064	10720	1542		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AX	11	Total	C	N	O	P	0	0
			231	103	39	78	11		

- Molecule 3 is a RNA chain called FtsQ nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AV	77	Total	C	N	O	P	0	0
			1649	733	297	542	77		

- Molecule 4 is a protein called Cell division protein FtsQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AZ	98	Total	C	N	O	S	0	0
			779	496	142	138	3		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	104	GLN	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	105	HIS	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	106	ALA	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	107	ARG	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	108	LEU	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	109	ASP	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	110	LYS	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	111	PRO	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	112	GLY	-	EXPRESSION TAG	UNP Q8X9Y5

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Chain	Residue	Modelled	Actual	Comment	Reference
AZ	113	ALA	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	114	ARG	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	115	HIS	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	116	PRO	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	117	CYS	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	118	TRP	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	119	PRO	-	EXPRESSION TAG	UNP Q8X9Y5

- Molecule 5 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A0	200	Total	C	N	O	S	0	0
			1640	1028	290	319	3		
5	A1	200	Total	C	N	O	S	0	0
			1640	1028	290	319	3		

- Molecule 6 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AB	240	Total	C	N	O	S	0	0
			1872	1180	332	352	8		

- Molecule 7 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AC	232	Total	C	N	O	S	0	0
			1822	1149	346	323	4		

- Molecule 8 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 9 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AE	166	Total	C	N	O	S	0	0
			1225	761	232	226	6		

- Molecule 10 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AF	135	Total	C	N	O	S	0	0
			1101	677	198	219	7		

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AG	178	Total	C	N	O	S	0	0
			1400	874	269	253	4		

- Molecule 12 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 13 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AI	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 14 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AJ	103	Total	C	N	O	S	0	0
			825	514	158	151	2		

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AK	128	Total	C	N	O	S	0	0
			965	595	196	171	3		

- Molecule 16 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 17 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AM	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 18 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AN	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 19 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AO	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	79	ARG	GLN	CONFLICT	UNP P0ADZ4

- Molecule 20 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 21 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AQ	83	Total	C	N	O	S	0	0
			672	425	124	120	3		

- Molecule 22 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 23 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AS	91	Total	C	N	O	S	0	0
			727	464	139	122	2		

- Molecule 24 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 25 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AU	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 26 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B7	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 27 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B8	2904	Total	C	N	O	P	0	0
			62341	27810	11469	20158	2904		

- Molecule 28 is a protein called Preprotein translocase secY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BA	435	Total	C	N	O	S	0	0
			3362	2221	553	571	17		

- Molecule 29 is a protein called Preprotein translocase secE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BB	116	Total	C	N	O	S	0	0
			889	587	154	145	3		

- Molecule 30 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 31 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B6	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 33 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 34 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 35 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 36 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BH	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 38 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BJ	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 39 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BK	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 40 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BL	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BN	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 43 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BO	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 44 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BP	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 45 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BQ	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 46 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 47 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BT	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BU	103	Total	C	N	O	S	0	0
			789	498	148	143			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BV	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BW	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 52 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BX	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 54 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BZ	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 55 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 56 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	B1	54	Total	C	N	O	0	0
			441	284	81	76		

- Molecule 57 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

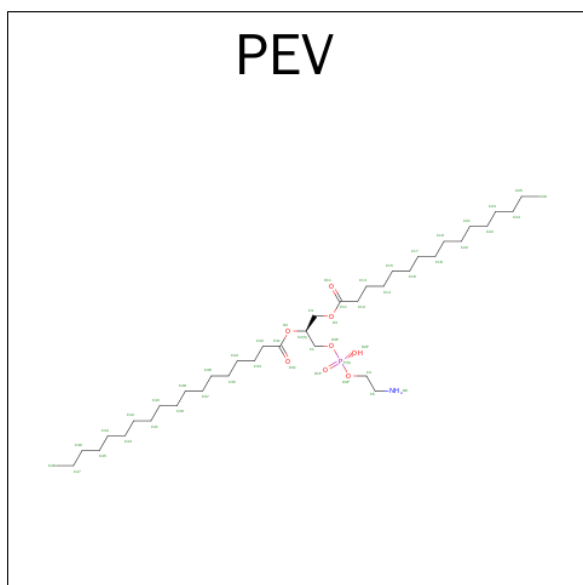
- Molecule 58 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 59 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 60 is (1S)-2-{|(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL}OXY}-1-|(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: C₃₉H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	

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Mol	Chain	Residues	Atoms					AltConf
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	

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Mol	Chain	Residues	Atoms					AltConf
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	

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Mol	Chain	Residues	Atoms					AltConf
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	

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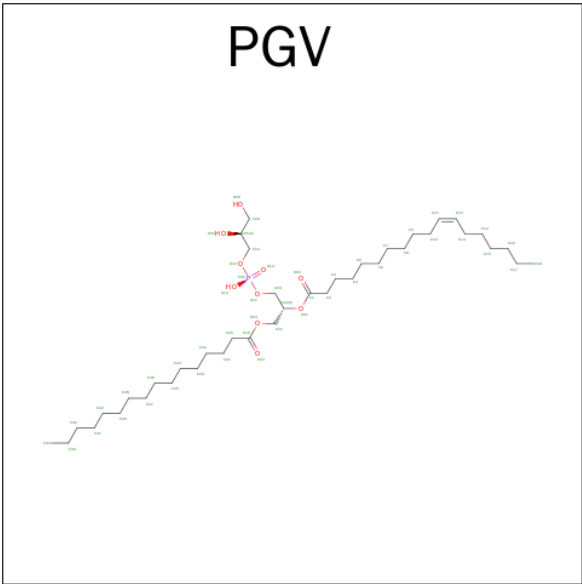
Mol	Chain	Residues	Atoms					AltConf
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	

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Mol	Chain	Residues	Atoms					AltConf
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	

- Molecule 61 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
61	AZ	1	Total	C	O	P	0
			102	80	20	2	
61	AZ	1	Total	C	O	P	0
			102	80	20	2	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	B8	1	Total	C	O	P	0
			51	40	10	1	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	

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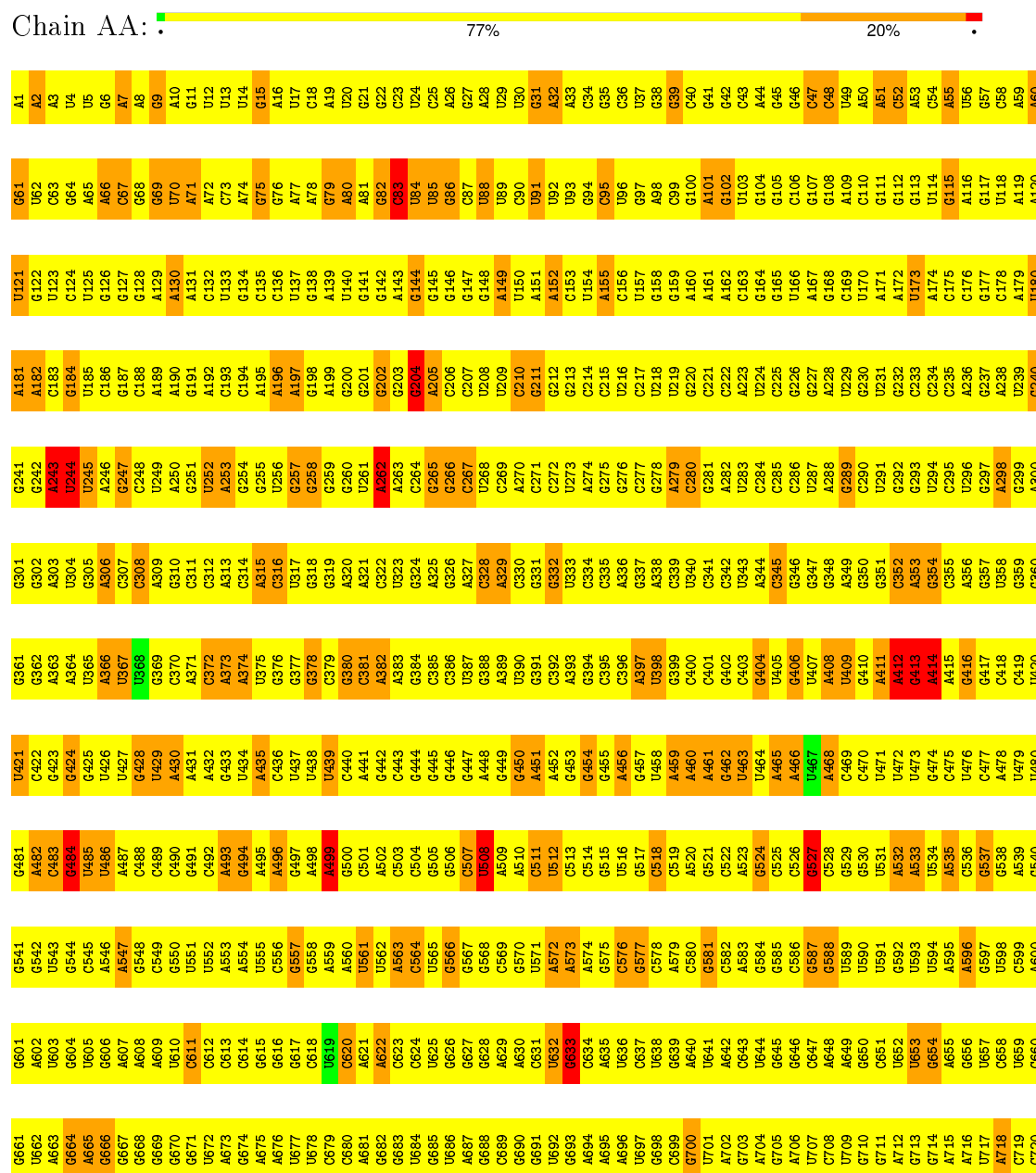
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Mol	Chain	Residues	Atoms				AltConf
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	

3 Residue-property plots

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

• Molecule 1: 16S RIBOSOMAL RNA



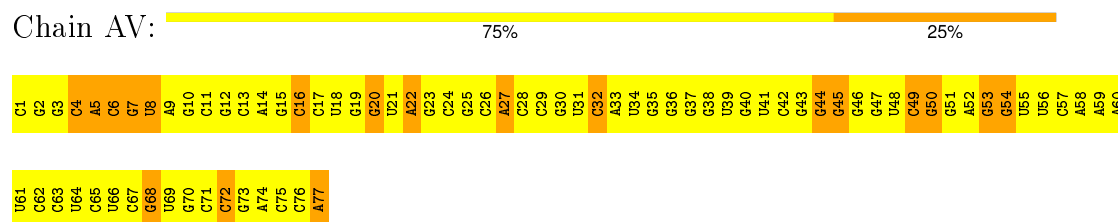
A1502	A1503	G1504	G1505	U1506	A1507	A1508	C1509	U1510	G1511	A1512	G1513	G1514	G1515	G1516	G1517	A1518	A1519	C1520	C1521	U1522	G1523	C1524	G1525	G1526	U1527	U1528	G1529	G1530	A1531	U1532	C1533	A1534	C1535	G1536	U1537	G1538	C1539	U1540	U1541	A1542																				
C1442	C1443	U1444	U1445	U1446	A1447	C1448	C1449	U1450	U1451	C1452	G1453	G1454	G1455	A1456	G1457	G1458	G1459	C1460	G1461	C1462	U1463	U1464	A1465	C1466	C1467	A1468	C1469	U1470	U1471	U1472	C1473	G1474	U1475	A1476	U1477	U1478	C1479	U1480	U1481	G1482	A1483	C1484	U1485	U1486	G1487	G1488	A1489	U1490	G1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499	A1500	C1501	
C1382	C1383	C1384	C1385	G1386	C1387	C1388	C1389	U1390	G1391	G1392	C1393	A1394	U1395	A1396	C1397	G1398	C1399	C1400	C1401	C1402	C1403	C1404	U1405	U1406	C1407	A1408	C1409	A1410	C1411	U1412	C1413	G1414	U1415	G1416	U1417	A1418	C1419	U1420	G1421	G1422	C1423	C1424	U1425	U1426	C1427	A1428	A1429	U1430	A1431	G1432	A1433	U1434	U1435	U1436	G1437	U1438	A1439	U1500	U1501	
C1322	G1323	A1324	C1325	U1326	C1327	C1328	A1329	U1330	G1331	A1332	C1333	A1334	U1335	C1336	G1337	G1338	A1339	C1340	U1341	C1342	C1343	C1344	U1345	U1346	A1347	U1348	C1349	A1350	U1351	C1352	G1353	U1354	G1355	C1356	U1357	U1358	C1359	A1360	G1361	A1362	C1363	U1364	G1365	C1366	C1367	A1368	C1369	G1370	C1371	U1372	C1373	A1374	U1375	U1376	A1377	C1378	A1379	U1380	U1381	
C1262	C1263	U1264	C1265	G1266	C1267	C1268	A1269	C1270	G1271	U1272	C1273	A1274	U1275	G1276	C1277	G1278	C1279	C1280	C1281	G1282	U1283	C1284	U1285	U1286	A1287	U1288	A1289	C1290	U1291	C1292	C1293	U1294	U1295	C1296	U1297	U1298	A1299	G1300	U1301	C1302	C1303	U1304	G1305	A1306	U1307	U1308	C1309	C1310	G1311	U1312	C1313	A1314	U1315	G1316	C1317	A1318	C1319	C1320	U1321	
U1202	C1203	A1204	U1205	U1206	G1207	C1208	C1209	G1210	U1211	U1212	A1213	C1214	G1215	A1216	C1217	C1218	C1219	C1220	G1221	G1222	C1223	U1224	A1225	U1226	C1227	C1228	A1229	C1230	U1231	G1232	C1233	U1234	U1235	C1236	C1237	A1238	A1239	U1240	G1241	G1242	C1243	U1244	G1245	A1246	U1247	A1248	C1249	A1250	A1251	C1252	G1253	U1254	C1255	U1256	C1257	A1258	C1259	G1260	A1261	
G1142	U1143	A1144	U1145	U1146	C1147	C1148	C1149	A1150	A1151	A1152	G1153	G1154	A1155	G1156	C1157	C1158	U1159	C1160	C1161	G1162	C1163	U1164	U1165	G1166	A1167	U1168	U1169	A1170	A1171	C1172	U1173	C1174	G1175	U1176	U1177	U1178	A1179	A1180	G1181	U1182	U1183	U1184	G1185	U1186	G1187	A1188	C1189	U1190	A1191	C1192	G1193	U1194	C1195	A1196	C1197	U1198	U1199	C1200	C1141	
A1082	U1083	G1084	U1085	U1086	C1087	C1088	C1089	U1090	U1091	A1092	G1093	G1094	U1095	C1096	C1097	C1098	G1099	C1100	A1101	A1102	C1103	U1104	C1105	G1106	C1107	C1108	U1109	A1110	A1111	C1112	C1113	C1114	U1115	U1116	U1117	U1118	C1119	C1120	U1121	U1122	C1123	U1124	U1125	U1126	G1127	C1128	C1129	A1130	G1131	C1132	G1133	U1134	C1135	U1136	C1137	A1138	U1139	C1200	A1201	
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• Molecule 2: mRNA

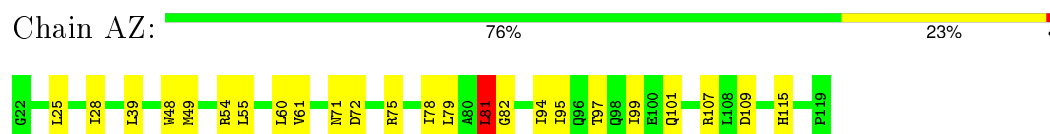
Chain AX: 9% 45% 45%

U12	C13	G14	C15	C16	C17	C18	U19	G20	A21	A22
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

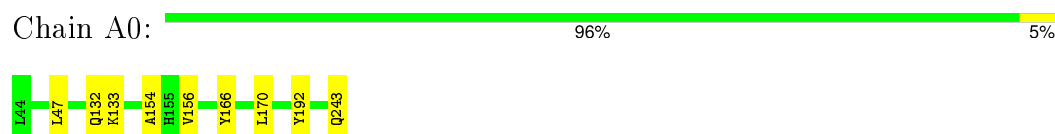
- Molecule 3: FtsQ nascent chain



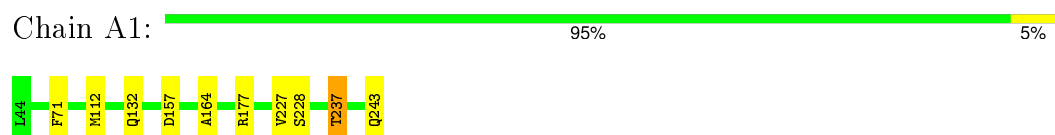
- Molecule 4: Cell division protein FtsQ



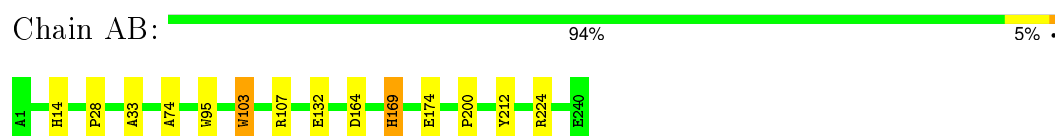
- Molecule 5: Apolipoprotein A-I



- Molecule 5: Apolipoprotein A-I



- Molecule 6: 30S ribosomal protein S2



- Molecule 9: 30S ribosomal protein S5

Chain AE:  94% 5%



- Molecule 10: 30S ribosomal protein S6

Chain AF:  93% 7%



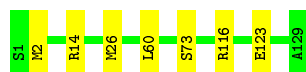
- Molecule 11: 30S ribosomal protein S7

Chain AG:  97%




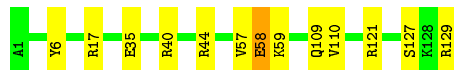
- Molecule 12: 30S ribosomal protein S8

Chain AH:  95% 5%




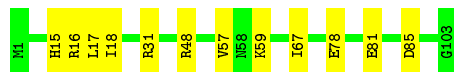
- Molecule 13: 30S ribosomal protein S9

Chain AI:  90% 9%



- Molecule 14: 30S ribosomal protein S10

Chain AJ:  88% 12%



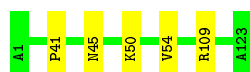
- Molecule 15: 30S ribosomal protein S11

Chain AK:  94% 6%



- Molecule 16: 30S ribosomal protein S12

Chain AL:  96% .



- Molecule 17: 30S ribosomal protein S13

Chain AM:  92% 7% .



- Molecule 18: 30S ribosomal protein S14

Chain AN:  88% 12%



- Molecule 19: 30S ribosomal protein S15

Chain AO:  97% ..




- Molecule 20: 30S ribosomal protein S16

Chain AP:  95% ..



- Molecule 21: 30S ribosomal protein S17

Chain AQ:  87% 13%



- Molecule 22: 30S ribosomal protein S18

Chain AR:  92% 8%



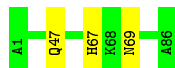
- Molecule 23: 30S ribosomal protein S19

Chain AS:  96% .



- Molecule 24: 30S ribosomal protein S20

Chain AT: 97%



- Molecule 25: 30S ribosomal protein S21

Chain AU: 94%



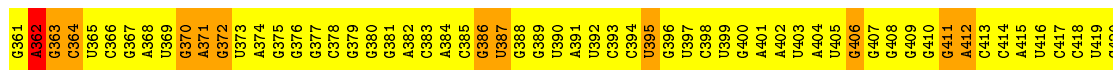
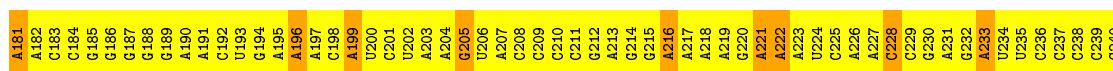
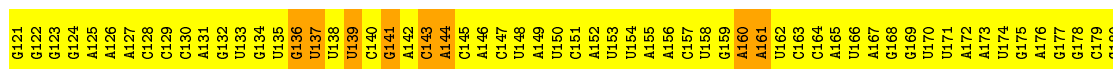
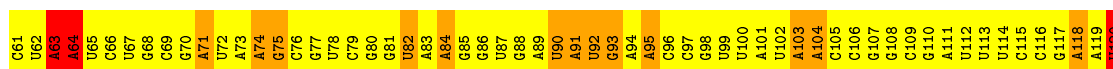
- Molecule 26: 5S RIBOSOMAL RNA

Chain B7: 82%



- Molecule 27: 23S RIBOSOMAL RNA

Chain B8: 80%

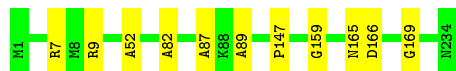


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C1323	G1263	U1203	A1143	U1083	G1023	U963	C903	G843	A783	A723	A663	A603	G543	A483	A423
G1324	A1264	U1204	A1144	A1084	G1024	C964	G904	A844	A784	A724	A664	G604	G544	C484	G424
U1325	A1265	G1205	A1145	A1085	G1025	C965	A905	U845	A785	A725	A665	G605	U545	C485	G425
A1326	G1266	A1206	C1146	A1086	G1026	G966	U906	U846	A786	A726	A666	U606	U546	C486	C426
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A1328	A1268	C1208	A1148	A1088	A1028	C968	C908	A848	A788	A728	A668	A608	G548	C488	A428
U1329	A1269	U1209	G1149	A1089	A1029	G969	A909	A849	A789	G729	A669	A609	G549	C489	A429
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G1331	C1271	C1211	A1151	G1091	G1031	G971	A911	C851	C791	C731	C671	C611	C551	C491	U431
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G2307	G2127	G2067	U2007	G1947	C1887	G1827	C1767	G1707	U1647	G1587	G1527	U1467	G1407
G2308	G2128	C2068	C2008	G1948	G1888	G1828	C1768	C1708	A1648	U1588	A1528	U1468	G1408
A2309	C2129	G2069	A2009	G1949	A1889	A1829	U1769	U1709	G1649	U1589	A1529	A1469	U1409
G2310	U2130	A2070	G2010	G1950	A1890	C1830	G1770	G1710	A1650	A1590	G1530	A1470	G1410
G2311	U2131	A2071	U2011	U1951	G1891	G1831	C1771	U1711	G1651	A1591	C1531	G1471	U1411
U2312	U2132	C2072	U2012	A1952	C1892	G1832	A1772	U1712	A1652	C1592	A1532	C1472	U1412
G2313	G2133	C2073	A2013	G1953	C1893	C1833	A1773	A1713	G1653	A1593	C1533	C1473	A1413
G2314	A2134	U2074	A2014	G1954	C1894	C1834	C1774	U1714	A1654	U1594	U1534	U1474	C1414
G2315	U2135	U2075	A2015	G1955	C1895	G1835	U1775	G1715	A1655	C1595	A1535	U1475	U1415
G2316	G2136	U2076	U2016	U1956	G1896	C1836	G1776	U1716	C1656	A1596	C1536	U1476	G1416
G2317	U2137	A2077	U2017	G1957	G1897	C1837	U1777	A1717	U1657	A1597	G1537	U1477	C1417
G2318	G2138	C2078	G2018	C1958	U1898	U1838	U1778	G1718	C1658	A1598	G1538	G1478	G1418
G2319	U2139	U2079	A2019	G1959	A1899	G1839	U1779	G1719	G1659	U1599	U1539	G1479	A1419
G2320	G2140	A2080	A2020	A1960	A1900	G1840	A1780	U1720	G1660	C1600	G1540	C1480	A1420
U2321	G2141	U2081	C2021	C1961	A1901	U1841	U1781	G1721	G1661	G1601	C1541	U1481	G1421
U2322	A2142	A2082	U2022	C1962	C1902	G1842	U1782	A1722	U1662	U1602	U1542	G1482	G1422
G2323	C2143	G2083	C2023	U1963	G1903	C1843	A1783	G1723	G1663	A1603	G1543	G1483	G1423
G2324	G2144	C2084	G2024	G1964	G1904	C1844	U1784	G1724	A1664	C1604	A1544	U1484	G1424
U2325	C2145	U2085	C2025	C1965	C1905	G1845	A1785	U1725	A1665	C1605	A1545	U1485	G1425
G2326	C2146	U2086	U2026	A1966	G1906	G1846	A1786	C1726	G1666	C1606	G1546	U1486	G1426
A2327	A2147	G2087	G2027	C1967	G1907	A1847	A1787	C1727	G1667	C1607	C1547	U1487	A1427
A2328	G2148	C2088	U2028	G1968	C1908	A1848	C1788	C1728	A1668	A1608	A1548	C1488	C1428
G2329	U2149	C2089	G2029	A1969	C1909	G1849	A1789	U1729	A1669	A1609	A1549	G1489	G1429
G2330	C2150	A2090	A2030	U1970	G1910	G1850	C1790	C1730	C1670	A1610	C1550	A1490	G1430
G2331	U2151	C2091	A2031	U1971	U1911	U1851	A1791	G1731	U1671	C1611	A1551	G1491	A1431
U2332	G2152	U2092	G2032	G1972	A1912	U1852	G1792	C1732	A1672	C1612	A1552	G1492	G1432
A2333	C2153	A2093	A2033	G1973	A1913	A1853	G1793	G1733	G1673	G1613	A1553	C1493	A1433
U2334	A2154	G2094	U2034	C1974	C1914	A1854	A1794	G1734	G1674	A1614	U1554	A1494	A1434
G2335	U2155	G2095	G2035	U1975	U1915	U1855	C1795	A1735	G1675	C1615	G1555	A1495	G1435
G2336	G2156	C2096	C2036	U1976	A1916	U1856	U1796	U1736	A1676	A1616	C1556	A1496	G1436
G2337	G2157	A2097	A2037	A1977	U1917	G1857	G1797	G1737	A1677	C1617	C1557	U1497	C1437
G2338	A2158	U2098	G2038	A1978	A1918	A1858	U1798	G1738	A1678	A1618	C1558	C1498	U1438
G2339	G2159	U2099	U2039	A1979	A1919	A1859	G1799	A1739	A1679	A1619	U1559	C1499	A1439
G2340	C2160	G2100	G2040	G1980	C1920	G1860	C1800	G1740	U1680	G1620	G1560	G1500	U1440

- Molecule 30: 50S ribosomal protein L1

Chain B5:  95% 5%



- Molecule 31: 50S ribosomal protein L2

Chain B6:  93% 6%



- Molecule 32: 50S ribosomal protein L3

Chain BD:  90% 10%



- Molecule 33: 50S ribosomal protein L4

Chain BE:  94% 6%



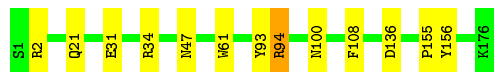
- Molecule 34: 50S ribosomal protein L5

Chain BF:  90% 9%



- Molecule 35: 50S ribosomal protein L6

Chain BG:  93% 7%



- Molecule 36: 50S ribosomal protein L9

Chain BH:  88% 11%



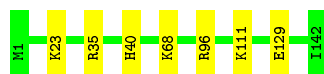
- Molecule 37: 50S ribosomal protein L11

Chain BI:  96% ..



- Molecule 38: 50S ribosomal protein L13

Chain BJ:  95% 5%



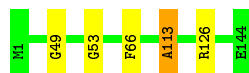
- Molecule 39: 50S ribosomal protein L14

Chain BK:  91% 9%



- Molecule 40: 50S ribosomal protein L15

Chain BL:  97% ..



- Molecule 41: 50S ribosomal protein L16

Chain BM:  92% 7% .




- Molecule 42: 50S ribosomal protein L17

Chain BN:  89% 11%



- Molecule 43: 50S ribosomal protein L18

Chain BO:  97% .



- Molecule 44: 50S ribosomal protein L19

Chain BP:  91% 9%



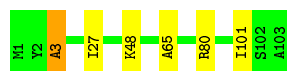
- Molecule 45: 50S ribosomal protein L20

Chain BQ: 94% 6%



- Molecule 46: 50S ribosomal protein L21

Chain BR: 94% 5%



- Molecule 47: 50S ribosomal protein L22

Chain BS: 92% 7%



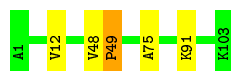
- Molecule 48: 50S ribosomal protein L23

Chain BT: 89% 9%



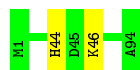
- Molecule 49: 50S ribosomal protein L24

Chain BU: 95% 5%



- Molecule 50: 50S ribosomal protein L25

Chain BV: 98% 2%

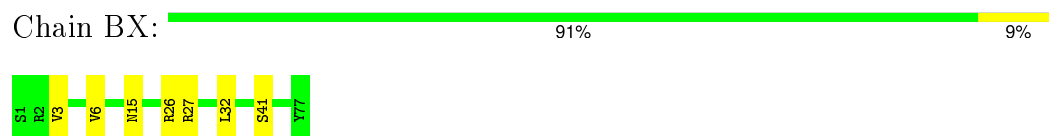


- Molecule 51: 50S ribosomal protein L27

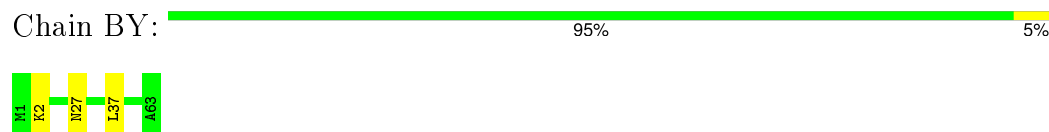
Chain BW: 94% 6%



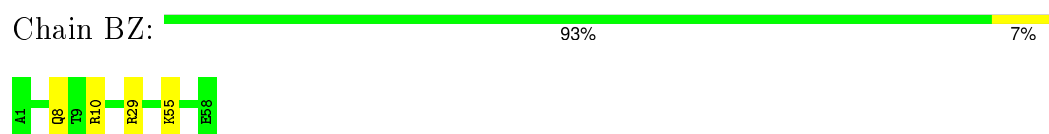
- Molecule 52: 50S ribosomal protein L28



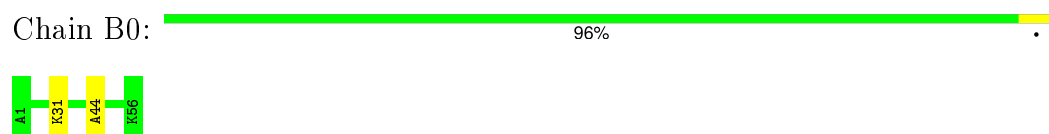
- Molecule 53: 50S ribosomal protein L29



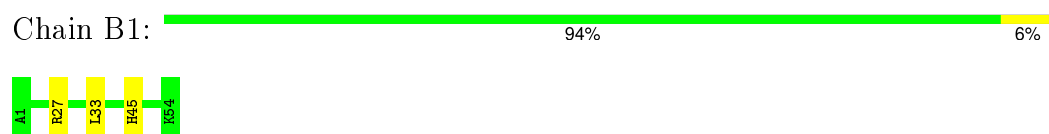
- Molecule 54: 50S ribosomal protein L30



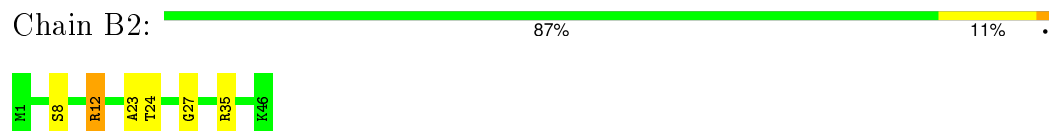
- Molecule 55: 50S ribosomal protein L32



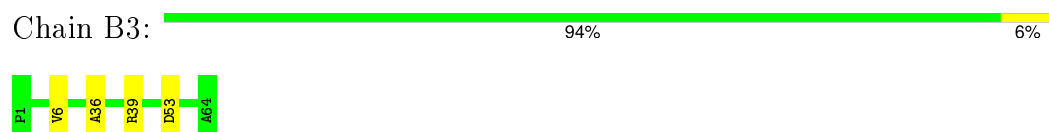
- Molecule 56: 50S ribosomal protein L33



- Molecule 57: 50S ribosomal protein L34



- Molecule 58: 50S ribosomal protein L35



- Molecule 59: 50S ribosomal protein L36





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	85664	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI Polara 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	39000	Depositor
Image detector	Kodak SO163	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, PEV

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	AA	1.60	46/37039 (0.1%)	2.50	4339/57778 (7.5%)
10	AF	0.99	0/1121	1.06	0/1509
11	AG	1.03	0/1422	1.01	2/1908 (0.1%)
12	AH	0.96	0/989	1.01	0/1326
13	AI	1.12	0/1048	1.01	0/1394
14	AJ	1.03	0/835	1.03	0/1127
15	AK	1.05	0/982	1.05	0/1323
16	AL	1.07	0/969	1.01	0/1300
17	AM	1.05	0/919	0.99	1/1226 (0.1%)
18	AN	1.07	0/817	1.05	1/1088 (0.1%)
19	AO	1.06	0/724	0.92	0/966
2	AX	1.56	0/256	2.32	28/394 (7.1%)
20	AP	1.07	0/659	1.03	0/884
21	AQ	0.99	0/681	1.05	0/913
22	AR	1.14	0/637	1.05	2/851 (0.2%)
23	AS	0.96	0/744	0.96	0/995
24	AT	0.96	0/676	0.94	0/895
25	AU	1.18	0/598	0.99	0/792
26	B7	1.59	2/2873 (0.1%)	2.49	325/4478 (7.3%)
27	B8	1.60	100/69822 (0.1%)	2.50	8171/108926 (7.5%)
28	BA	1.68	7/3439 (0.2%)	1.14	15/4662 (0.3%)
29	BB	0.98	1/902 (0.1%)	1.05	1/1228 (0.1%)
3	AV	1.61	1/1842 (0.1%)	2.43	211/2870 (7.4%)
30	B5	0.92	0/1748	0.97	0/2355
31	B6	1.04	0/2131	1.03	1/2863 (0.0%)
32	BD	0.97	0/1586	1.08	4/2134 (0.2%)
33	BE	0.95	0/1571	1.01	2/2113 (0.1%)
34	BF	1.01	0/1444	1.06	1/1937 (0.1%)
35	BG	0.96	0/1343	1.06	4/1816 (0.2%)
36	BH	0.93	0/1122	1.05	0/1515
37	BI	0.86	0/1046	1.00	1/1410 (0.1%)
38	BJ	0.97	0/1152	1.01	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BK	1.03	0/956	1.03	0/1279
4	AZ	0.98	0/795	1.16	0/1082
40	BL	1.04	0/1062	0.98	1/1413 (0.1%)
41	BM	1.03	0/1093	1.06	2/1460 (0.1%)
42	BN	1.10	0/1021	1.03	1/1364 (0.1%)
43	BO	1.07	0/910	0.98	0/1219
44	BP	1.06	0/929	1.03	0/1242
45	BQ	1.09	0/960	1.00	2/1278 (0.2%)
46	BR	1.01	0/829	1.07	1/1107 (0.1%)
47	BS	0.99	0/864	1.04	1/1156 (0.1%)
48	BT	0.98	0/794	1.09	1/1060 (0.1%)
49	BU	0.96	0/797	1.04	0/1062
5	A0	0.96	1/1667 (0.1%)	0.95	3/2240 (0.1%)
5	A1	0.97	1/1667 (0.1%)	0.95	0/2240
50	BV	0.96	0/766	1.02	0/1025
51	BW	1.04	0/642	1.05	0/848
52	BX	1.09	0/635	1.04	0/848
53	BY	1.00	0/510	0.90	0/677
54	BZ	0.99	0/453	0.99	0/605
55	B0	1.05	0/450	0.97	0/599
56	B1	0.93	0/448	1.01	0/594
57	B2	1.25	0/380	1.06	0/498
58	B3	0.98	0/513	0.98	0/676
59	B4	1.20	2/303 (0.7%)	1.03	0/397
6	AB	0.92	0/1904	0.98	1/2565 (0.0%)
7	AC	1.00	0/1852	1.06	1/2490 (0.0%)
8	AD	1.04	0/1665	0.99	0/2227
9	AE	0.97	0/1239	1.03	0/1664
All	All	1.44	161/169241 (0.1%)	2.16	13123/251442 (5.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	72
12	AH	0	1
13	AI	0	1
26	B7	0	2
27	B8	0	100
28	BA	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	AV	0	2
34	BF	0	1
36	BH	0	1
49	BU	0	1
5	A1	0	1
57	B2	0	1
7	AC	0	1
All	All	0	189

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BA	416	PHE	CG-CD2	41.52	2.01	1.38
28	BA	416	PHE	CG-CD1	39.62	1.98	1.38
28	BA	416	PHE	CE2-CZ	30.78	1.95	1.37
28	BA	416	PHE	CE1-CZ	30.54	1.95	1.37
28	BA	416	PHE	CD2-CE2	27.89	1.95	1.39
28	BA	416	PHE	CD1-CE1	26.46	1.92	1.39
27	B8	2860	A	N7-C5	-7.97	1.34	1.39
27	B8	2378	A	N7-C5	-7.45	1.34	1.39
1	AA	1016	A	N7-C5	-7.37	1.34	1.39
27	B8	2111	U	C2-N3	7.37	1.43	1.37
5	A0	243	GLN	C-OXT	7.34	1.37	1.23
28	BA	442	GLY	C-OXT	7.34	1.37	1.23
5	A1	243	GLN	C-OXT	7.32	1.37	1.23
29	BB	127	PHE	C-OXT	7.29	1.37	1.23
27	B8	1571	A	N7-C5	-7.16	1.34	1.39
27	B8	1213	A	N7-C5	-7.09	1.34	1.39
1	AA	190	A	N7-C5	-7.09	1.34	1.39
1	AA	162	A	N7-C5	-6.95	1.35	1.39
27	B8	633	A	N7-C5	-6.93	1.35	1.39
1	AA	487	A	N7-C5	-6.92	1.35	1.39
27	B8	1641	A	N7-C5	-6.54	1.35	1.39
1	AA	1005	A	N7-C5	-6.34	1.35	1.39
27	B8	705	A	N7-C5	-6.32	1.35	1.39
1	AA	1339	A	N7-C5	-6.25	1.35	1.39
1	AA	1468	A	N7-C5	-6.24	1.35	1.39
26	B7	73	A	N7-C5	-6.23	1.35	1.39
27	B8	1608	A	N7-C5	-6.18	1.35	1.39
27	B8	402	A	N7-C5	-6.18	1.35	1.39
27	B8	216	A	N7-C5	-6.17	1.35	1.39
27	B8	471	A	N7-C5	-6.08	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B8	2225	A	N7-C5	-6.08	1.35	1.39
1	AA	495	A	N7-C5	-6.06	1.35	1.39
1	AA	119	A	N7-C5	-6.05	1.35	1.39
27	B8	820	A	N7-C5	-6.03	1.35	1.39
1	AA	1014	A	O3'-P	-6.01	1.53	1.61
27	B8	2412	A	N7-C5	-6.00	1.35	1.39
27	B8	1469	A	N7-C5	-5.99	1.35	1.39
27	B8	1722	A	N7-C5	-5.95	1.35	1.39
27	B8	2366	A	N7-C5	-5.95	1.35	1.39
27	B8	1029	A	N7-C5	-5.94	1.35	1.39
27	B8	374	A	N7-C5	-5.85	1.35	1.39
27	B8	2082	A	N7-C5	-5.84	1.35	1.39
27	B8	1001	A	N7-C5	-5.83	1.35	1.39
27	B8	877	A	N7-C5	-5.82	1.35	1.39
27	B8	2352	A	N7-C5	-5.82	1.35	1.39
27	B8	310	A	N7-C5	-5.82	1.35	1.39
27	B8	1866	A	N7-C5	-5.79	1.35	1.39
27	B8	513	A	N7-C5	-5.78	1.35	1.39
27	B8	52	A	N7-C5	-5.78	1.35	1.39
27	B8	1572	A	N7-C5	-5.75	1.35	1.39
27	B8	1744	A	N7-C5	-5.75	1.35	1.39
1	AA	533	A	N7-C5	-5.74	1.35	1.39
27	B8	2435	A	N7-C5	-5.70	1.35	1.39
1	AA	327	A	N7-C5	-5.69	1.35	1.39
1	AA	1375	A	N7-C5	-5.68	1.35	1.39
27	B8	2587	A	N7-C5	-5.67	1.35	1.39
27	B8	371	A	N7-C5	-5.66	1.35	1.39
1	AA	909	A	N7-C5	-5.64	1.35	1.39
1	AA	151	A	N7-C5	-5.63	1.35	1.39
27	B8	2013	A	N7-C5	-5.61	1.35	1.39
27	B8	2335	A	N7-C5	-5.60	1.35	1.39
27	B8	2662	A	N7-C5	-5.59	1.35	1.39
1	AA	1170	A	N7-C5	-5.58	1.35	1.39
59	B4	27	CYS	CB-SG	5.56	1.91	1.82
27	B8	1286	A	N7-C5	-5.55	1.35	1.39
27	B8	1477	A	N7-C5	-5.52	1.35	1.39
27	B8	340	A	N7-C5	-5.52	1.35	1.39
27	B8	190	A	N7-C5	-5.50	1.35	1.39
27	B8	2268	A	N7-C5	-5.50	1.35	1.39
27	B8	1021	A	N7-C5	-5.48	1.35	1.39
27	B8	256	A	N7-C5	-5.46	1.35	1.39
27	B8	1872	A	N7-C5	-5.46	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	B4	11	CYS	CB-SG	5.45	1.91	1.82
1	AA	873	A	N7-C5	-5.45	1.35	1.39
27	B8	191	A	N7-C5	-5.45	1.35	1.39
27	B8	251	A	N7-C5	-5.42	1.35	1.39
27	B8	2430	A	N7-C5	-5.42	1.35	1.39
27	B8	1373	A	N7-C5	-5.41	1.36	1.39
1	AA	468	A	N7-C5	-5.41	1.36	1.39
1	AA	1055	A	N7-C5	-5.41	1.36	1.39
1	AA	383	A	N7-C5	-5.39	1.36	1.39
27	B8	973	A	N7-C5	-5.39	1.36	1.39
27	B8	1717	A	N7-C5	-5.39	1.36	1.39
27	B8	609	A	N7-C5	-5.38	1.36	1.39
1	AA	919	A	N7-C5	-5.38	1.36	1.39
27	B8	278	A	N7-C5	-5.38	1.36	1.39
1	AA	781	A	N7-C5	-5.36	1.36	1.39
27	B8	1802	A	N7-C5	-5.36	1.36	1.39
27	B8	1378	A	N7-C5	-5.34	1.36	1.39
27	B8	918	A	N7-C5	-5.34	1.36	1.39
27	B8	447	A	N7-C5	-5.32	1.36	1.39
27	B8	1970	A	N7-C5	-5.32	1.36	1.39
1	AA	171	A	N7-C5	-5.31	1.36	1.39
27	B8	556	A	N7-C5	-5.30	1.36	1.39
27	B8	2297	A	N7-C5	-5.29	1.36	1.39
27	B8	279	A	N7-C5	-5.28	1.36	1.39
1	AA	908	A	N7-C5	-5.27	1.36	1.39
1	AA	439	U	C2-N3	5.26	1.41	1.37
27	B8	138	U	C2-N3	5.26	1.41	1.37
27	B8	266	G	C2-N3	5.26	1.36	1.32
27	B8	1439	A	N7-C5	-5.26	1.36	1.39
27	B8	1890	A	N7-C5	-5.26	1.36	1.39
27	B8	412	A	N7-C5	-5.25	1.36	1.39
27	B8	49	A	N7-C5	-5.25	1.36	1.39
27	B8	1470	A	N7-C5	-5.25	1.36	1.39
1	AA	55	A	N7-C5	-5.25	1.36	1.39
27	B8	917	A	N7-C5	-5.24	1.36	1.39
26	B7	99	A	N7-C5	-5.24	1.36	1.39
27	B8	1354	A	N7-C5	-5.24	1.36	1.39
27	B8	1237	A	N7-C5	-5.23	1.36	1.39
27	B8	428	A	N7-C5	-5.22	1.36	1.39
27	B8	2903	U	C2-N3	5.22	1.41	1.37
1	AA	262	A	N7-C5	-5.21	1.36	1.39
27	B8	975	A	N7-C5	-5.21	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	498	A	N7-C5	-5.21	1.36	1.39
1	AA	1401	G	C2-N3	5.20	1.36	1.32
1	AA	1306	A	N7-C5	-5.17	1.36	1.39
27	B8	879	G	C2-N3	5.17	1.36	1.32
27	B8	1419	A	N7-C5	-5.17	1.36	1.39
27	B8	1580	A	N7-C5	-5.16	1.36	1.39
27	B8	1254	A	N7-C5	-5.16	1.36	1.39
1	AA	696	A	N7-C5	-5.15	1.36	1.39
27	B8	1340	U	C2-N3	5.15	1.41	1.37
27	B8	2741	A	N7-C5	-5.14	1.36	1.39
1	AA	860	A	N7-C5	-5.14	1.36	1.39
27	B8	470	A	N7-C5	-5.13	1.36	1.39
1	AA	759	A	N7-C5	-5.13	1.36	1.39
27	B8	713	G	C2-N3	5.13	1.36	1.32
1	AA	69	G	N1-C2	5.13	1.41	1.37
1	AA	1483	A	N7-C5	-5.12	1.36	1.39
1	AA	753	A	N7-C5	-5.12	1.36	1.39
27	B8	2029	G	C2-N3	5.12	1.36	1.32
1	AA	653	U	C2-N3	5.12	1.41	1.37
1	AA	115	G	C2-N3	5.12	1.36	1.32
27	B8	1	G	C2-N3	5.12	1.36	1.32
27	B8	699	A	N7-C5	-5.11	1.36	1.39
27	B8	2748	A	N7-C5	-5.10	1.36	1.39
1	AA	1261	A	N7-C5	-5.10	1.36	1.39
27	B8	2171	A	N7-C5	-5.10	1.36	1.39
27	B8	2077	A	N7-C5	-5.10	1.36	1.39
1	AA	116	A	N7-C5	-5.09	1.36	1.39
27	B8	1690	A	N7-C5	-5.09	1.36	1.39
1	AA	1077	G	N1-C2	5.08	1.41	1.37
1	AA	1288	A	N7-C5	-5.08	1.36	1.39
27	B8	1395	A	N7-C5	-5.07	1.36	1.39
27	B8	1932	A	N7-C5	-5.07	1.36	1.39
1	AA	1255	G	C2-N3	5.07	1.36	1.32
27	B8	2511	U	C2-N3	5.06	1.41	1.37
1	AA	282	A	N7-C5	-5.06	1.36	1.39
27	B8	1634	A	N7-C5	-5.06	1.36	1.39
27	B8	1848	A	N7-C5	-5.05	1.36	1.39
1	AA	1316	G	C2-N3	5.05	1.36	1.32
27	B8	1027	A	N7-C5	-5.04	1.36	1.39
27	B8	2199	A	N7-C5	-5.03	1.36	1.39
27	B8	1803	A	N7-C5	-5.03	1.36	1.39
1	AA	1365	G	C2-N3	5.03	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B8	2566	A	N7-C5	-5.02	1.36	1.39
27	B8	2033	A	N7-C5	-5.01	1.36	1.39
3	AV	40	G	N1-C2	5.01	1.41	1.37
27	B8	2405	G	C2-N3	5.00	1.36	1.32
27	B8	2592	G	C2-N3	5.00	1.36	1.32

All (13123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	85	U	P-O3'-C3'	19.51	143.11	119.70
27	B8	670	A	P-O3'-C3'	17.35	140.52	119.70
27	B8	2076	U	P-O3'-C3'	15.69	138.53	119.70
27	B8	6	A	N1-C6-N6	14.72	127.43	118.60
1	AA	1252	A	N1-C6-N6	14.43	127.26	118.60
27	B8	449	A	N1-C6-N6	14.43	127.26	118.60
1	AA	328	C	P-O3'-C3'	14.42	137.00	119.70
27	B8	2766	A	N1-C6-N6	14.36	127.21	118.60
27	B8	677	A	N1-C6-N6	14.21	127.12	118.60
27	B8	890	C	P-O3'-C3'	14.20	136.75	119.70
1	AA	1036	A	N1-C6-N6	14.12	127.07	118.60
27	B8	1977	A	N1-C6-N6	14.11	127.07	118.60
27	B8	2899	A	N1-C6-N6	14.10	127.06	118.60
27	B8	863	A	N1-C6-N6	14.04	127.02	118.60
1	AA	262	A	N1-C6-N6	14.02	127.01	118.60
1	AA	937	A	N1-C6-N6	14.01	127.01	118.60
27	B8	1745	A	N1-C6-N6	13.97	126.98	118.60
1	AA	1014	A	P-O3'-C3'	13.90	136.38	119.70
27	B8	880	G	P-O3'-C3'	13.88	136.36	119.70
27	B8	1784	A	N1-C6-N6	13.85	126.91	118.60
1	AA	174	A	N1-C6-N6	13.84	126.91	118.60
26	B7	66	A	N1-C6-N6	13.79	126.88	118.60
1	AA	780	A	N1-C6-N6	13.79	126.87	118.60
1	AA	16	A	N1-C6-N6	13.75	126.85	118.60
1	AA	181	A	N1-C6-N6	13.74	126.84	118.60
26	B7	109	A	N1-C6-N6	13.73	126.84	118.60
27	B8	959	A	N1-C6-N6	13.71	126.83	118.60
27	B8	1713	A	N1-C6-N6	13.71	126.82	118.60
27	B8	330	A	N1-C6-N6	13.68	126.81	118.60
1	AA	906	A	N1-C6-N6	13.66	126.80	118.60
27	B8	5	A	N1-C6-N6	13.64	126.78	118.60
27	B8	2171	A	N1-C6-N6	13.64	126.78	118.60
1	AA	1465	A	N1-C6-N6	13.62	126.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1500	A	N1-C6-N6	13.62	126.77	118.60
1	AA	1035	A	N1-C6-N6	13.61	126.77	118.60
27	B8	2662	A	N1-C6-N6	13.54	126.72	118.60
1	AA	1111	A	N1-C6-N6	13.54	126.72	118.60
27	B8	1598	A	N1-C6-N6	13.51	126.71	118.60
1	AA	71	A	N1-C6-N6	13.47	126.68	118.60
1	AA	288	A	N1-C6-N6	13.46	126.68	118.60
27	B8	689	A	N1-C6-N6	13.46	126.67	118.60
1	AA	901	A	N1-C6-N6	13.44	126.66	118.60
1	AA	1492	A	N1-C6-N6	13.44	126.66	118.60
1	AA	192	A	N1-C6-N6	13.43	126.66	118.60
27	B8	2163	A	N1-C6-N6	13.41	126.65	118.60
27	B8	2826	A	N1-C6-N6	13.39	126.64	118.60
1	AA	923	A	N1-C6-N6	13.38	126.63	118.60
27	B8	1205	A	P-O3'-C3'	13.38	135.75	119.70
27	B8	1899	A	N1-C6-N6	13.38	126.63	118.60
27	B8	2090	A	N1-C6-N6	13.37	126.62	118.60
27	B8	219	A	N1-C6-N6	13.36	126.61	118.60
26	B7	108	A	N1-C6-N6	13.34	126.60	118.60
27	B8	928	A	N1-C6-N6	13.33	126.60	118.60
27	B8	718	A	N1-C6-N6	13.32	126.59	118.60
27	B8	794	A	N1-C6-N6	13.32	126.59	118.60
27	B8	443	A	N1-C6-N6	13.31	126.59	118.60
27	B8	1532	A	N1-C6-N6	13.31	126.58	118.60
27	B8	1127	A	N1-C6-N6	13.29	126.57	118.60
27	B8	56	A	N1-C6-N6	13.28	126.57	118.60
1	AA	199	A	N1-C6-N6	13.26	126.56	118.60
27	B8	233	A	N1-C6-N6	13.25	126.55	118.60
3	AV	9	A	N1-C6-N6	13.24	126.54	118.60
27	B8	911	A	N1-C6-N6	13.24	126.54	118.60
1	AA	1437	A	N1-C6-N6	13.22	126.53	118.60
1	AA	595	A	N1-C6-N6	13.22	126.53	118.60
27	B8	734	A	N1-C6-N6	13.20	126.52	118.60
27	B8	2734	A	N1-C6-N6	13.20	126.52	118.60
1	AA	1236	A	N1-C6-N6	13.18	126.51	118.60
1	AA	996	A	N1-C6-N6	13.17	126.50	118.60
1	AA	1226	C	P-O3'-C3'	13.17	135.51	119.70
1	AA	1513	A	N1-C6-N6	13.17	126.50	118.60
27	B8	947	A	N1-C6-N6	13.16	126.50	118.60
1	AA	746	A	N1-C6-N6	13.16	126.50	118.60
1	AA	155	A	N1-C6-N6	13.13	126.48	118.60
27	B8	1027	A	N1-C6-N6	13.12	126.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	814	A	N1-C6-N6	13.11	126.47	118.60
27	B8	213	A	N1-C6-N6	13.11	126.47	118.60
1	AA	1360	A	N1-C6-N6	13.10	126.46	118.60
27	B8	19	A	N1-C6-N6	13.07	126.44	118.60
27	B8	2154	A	N1-C6-N6	13.07	126.44	118.60
1	AA	1014	A	N1-C6-N6	13.06	126.44	118.60
27	B8	1791	A	N1-C6-N6	13.06	126.44	118.60
27	B8	13	A	N1-C6-N6	13.06	126.43	118.60
27	B8	1431	A	N1-C6-N6	13.04	126.42	118.60
27	B8	1787	A	N1-C6-N6	13.03	126.42	118.60
27	B8	2051	A	N1-C6-N6	13.03	126.42	118.60
1	AA	1080	A	N1-C6-N6	13.03	126.42	118.60
27	B8	104	A	N1-C6-N6	13.03	126.42	118.60
27	B8	2453	A	N1-C6-N6	13.01	126.41	118.60
1	AA	1398	A	N1-C6-N6	13.01	126.41	118.60
27	B8	2879	A	N1-C6-N6	13.00	126.40	118.60
27	B8	2284	A	N1-C6-N6	13.00	126.40	118.60
27	B8	1144	A	N1-C6-N6	12.99	126.39	118.60
1	AA	1197	A	N1-C6-N6	12.99	126.39	118.60
27	B8	199	A	N1-C6-N6	12.98	126.39	118.60
27	B8	1700	A	N1-C6-N6	12.98	126.39	118.60
27	B8	1084	A	N1-C6-N6	12.97	126.38	118.60
27	B8	1603	A	N1-C6-N6	12.97	126.38	118.60
27	B8	1918	A	N1-C6-N6	12.97	126.38	118.60
27	B8	685	A	N1-C6-N6	12.96	126.38	118.60
27	B8	756	A	N1-C6-N6	12.95	126.37	118.60
1	AA	502	A	N1-C6-N6	12.95	126.37	118.60
27	B8	28	A	N1-C6-N6	12.95	126.37	118.60
27	B8	849	A	N1-C6-N6	12.94	126.37	118.60
26	B7	101	A	N1-C6-N6	12.94	126.36	118.60
27	B8	1590	A	N1-C6-N6	12.93	126.36	118.60
27	B8	599	A	N1-C6-N6	12.93	126.36	118.60
1	AA	451	A	N1-C6-N6	12.90	126.34	118.60
27	B8	152	A	N1-C6-N6	12.90	126.34	118.60
27	B8	1095	A	N1-C6-N6	12.89	126.33	118.60
27	B8	1927	A	N1-C6-N6	12.88	126.33	118.60
27	B8	322	A	N1-C6-N6	12.87	126.32	118.60
1	AA	563	A	N1-C6-N6	12.87	126.32	118.60
27	B8	2800	A	N1-C6-N6	12.84	126.30	118.60
27	B8	1269	A	N1-C6-N6	12.84	126.30	118.60
27	B8	1354	A	N1-C6-N6	12.83	126.30	118.60
27	B8	1061	U	P-O3'-C3'	12.82	135.09	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	503	A	N1-C6-N6	12.81	126.29	118.60
27	B8	582	A	N1-C6-N6	12.80	126.28	118.60
27	B8	221	A	N1-C6-N6	12.77	126.26	118.60
1	AA	1044	A	N1-C6-N6	12.77	126.26	118.60
27	B8	1677	A	N1-C6-N6	12.76	126.25	118.60
27	B8	2184	A	N1-C6-N6	12.75	126.25	118.60
1	AA	673	A	N1-C6-N6	12.75	126.25	118.60
27	B8	515	A	N1-C6-N6	12.75	126.25	118.60
27	B8	502	A	N1-C6-N6	12.74	126.25	118.60
27	B8	1275	A	N1-C6-N6	12.74	126.25	118.60
27	B8	2873	A	N1-C6-N6	12.74	126.25	118.60
27	B8	899	A	N1-C6-N6	12.74	126.24	118.60
1	AA	915	A	N1-C6-N6	12.73	126.24	118.60
27	B8	1433	A	N1-C6-N6	12.72	126.23	118.60
1	AA	320	A	N1-C6-N6	12.72	126.23	118.60
27	B8	1936	A	N1-C6-N6	12.72	126.23	118.60
27	B8	155	A	N1-C6-N6	12.71	126.23	118.60
27	B8	1496	A	N1-C6-N6	12.71	126.22	118.60
27	B8	429	A	N1-C6-N6	12.71	126.22	118.60
1	AA	81	A	N1-C6-N6	12.70	126.22	118.60
1	AA	1229	A	N1-C6-N6	12.70	126.22	118.60
27	B8	878	A	N1-C6-N6	12.69	126.22	118.60
1	AA	77	A	N1-C6-N6	12.69	126.22	118.60
27	B8	1634	A	N1-C6-N6	12.69	126.21	118.60
1	AA	478	A	N1-C6-N6	12.68	126.21	118.60
27	B8	1264	A	N1-C6-N6	12.68	126.21	118.60
1	AA	371	A	N1-C6-N6	12.67	126.20	118.60
27	B8	2430	A	N1-C6-N6	12.67	126.20	118.60
27	B8	262	A	N1-C6-N6	12.67	126.20	118.60
27	B8	182	A	N1-C6-N6	12.65	126.19	118.60
27	B8	226	A	N1-C6-N6	12.65	126.19	118.60
1	AA	98	A	N1-C6-N6	12.65	126.19	118.60
27	B8	522	A	N1-C6-N6	12.65	126.19	118.60
27	B8	2037	A	N1-C6-N6	12.65	126.19	118.60
27	B8	2042	A	N1-C6-N6	12.65	126.19	118.60
27	B8	2352	A	N1-C6-N6	12.65	126.19	118.60
27	B8	693	A	N1-C6-N6	12.65	126.19	118.60
1	AA	1269	A	N1-C6-N6	12.64	126.19	118.60
27	B8	532	A	N1-C6-N6	12.64	126.19	118.60
27	B8	255	A	N1-C6-N6	12.64	126.18	118.60
1	AA	10	A	N1-C6-N6	12.64	126.18	118.60
1	AA	1219	A	N1-C6-N6	12.64	126.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B7	58	A	N1-C6-N6	12.63	126.18	118.60
1	AA	162	A	N1-C6-N6	12.63	126.18	118.60
1	AA	336	A	N1-C6-N6	12.63	126.17	118.60
1	AA	964	A	N1-C6-N6	12.62	126.17	118.60
27	B8	342	A	N1-C6-N6	12.62	126.17	118.60
1	AA	456	A	N1-C6-N6	12.62	126.17	118.60
27	B8	1244	A	N1-C6-N6	12.61	126.17	118.60
27	B8	2281	A	N1-C6-N6	12.61	126.17	118.60
3	AV	27	A	N1-C6-N6	12.61	126.17	118.60
27	B8	190	A	N1-C6-N6	12.61	126.17	118.60
27	B8	666	A	N1-C6-N6	12.61	126.16	118.60
26	B7	29	A	N1-C6-N6	12.60	126.16	118.60
27	B8	2267	A	N1-C6-N6	12.60	126.16	118.60
1	AA	1306	A	N1-C6-N6	12.60	126.16	118.60
1	AA	309	A	N1-C6-N6	12.60	126.16	118.60
27	B8	1773	A	N1-C6-N6	12.60	126.16	118.60
27	B8	2013	A	N1-C6-N6	12.60	126.16	118.60
27	B8	761	A	N1-C6-N6	12.59	126.16	118.60
27	B8	2369	A	N1-C6-N6	12.59	126.16	118.60
27	B8	347	A	N1-C6-N6	12.59	126.16	118.60
27	B8	655	A	N1-C6-N6	12.58	126.15	118.60
27	B8	1260	A	N1-C6-N6	12.58	126.15	118.60
1	AA	675	A	N1-C6-N6	12.58	126.15	118.60
27	B8	195	A	N1-C6-N6	12.58	126.15	118.60
27	B8	2600	A	N1-C6-N6	12.58	126.15	118.60
1	AA	139	A	N1-C6-N6	12.57	126.14	118.60
1	AA	205	A	N1-C6-N6	12.57	126.14	118.60
1	AA	1016	A	N1-C6-N6	12.57	126.14	118.60
26	B7	39	A	N1-C6-N6	12.57	126.14	118.60
27	B8	2336	A	P-O3'-C3'	12.57	134.78	119.70
27	B8	2412	A	N1-C6-N6	12.57	126.14	118.60
1	AA	974	A	N1-C6-N6	12.56	126.14	118.60
27	B8	1039	A	N1-C6-N6	12.56	126.14	118.60
27	B8	730	A	N1-C6-N6	12.56	126.14	118.60
1	AA	1167	A	N1-C6-N6	12.56	126.14	118.60
27	B8	83	A	N1-C6-N6	12.56	126.14	118.60
27	B8	592	A	N1-C6-N6	12.56	126.14	118.60
27	B8	637	A	N1-C6-N6	12.56	126.14	118.60
27	B8	2516	A	N1-C6-N6	12.56	126.14	118.60
27	B8	2278	A	N1-C6-N6	12.56	126.14	118.60
27	B8	1637	A	N1-C6-N6	12.56	126.13	118.60
27	B8	721	A	N1-C6-N6	12.54	126.13	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	33	A	N1-C6-N6	12.54	126.12	118.60
1	AA	300	A	N1-C6-N6	12.54	126.12	118.60
1	AA	1110	A	N1-C6-N6	12.54	126.13	118.60
1	AA	1151	A	N1-C6-N6	12.54	126.12	118.60
27	B8	492	A	N1-C6-N6	12.54	126.12	118.60
27	B8	1387	A	N1-C6-N6	12.54	126.12	118.60
27	B8	743	A	N1-C6-N6	12.54	126.12	118.60
27	B8	2311	A	N1-C6-N6	12.54	126.12	118.60
27	B8	749	A	N1-C6-N6	12.53	126.12	118.60
27	B8	1213	A	N1-C6-N6	12.53	126.12	118.60
1	AA	1000	A	N1-C6-N6	12.53	126.11	118.60
27	B8	497	A	N1-C6-N6	12.53	126.12	118.60
27	B8	2381	A	N1-C6-N6	12.52	126.11	118.60
27	B8	95	A	N1-C6-N6	12.52	126.11	118.60
1	AA	238	A	N1-C6-N6	12.52	126.11	118.60
1	AA	1081	A	N1-C6-N6	12.51	126.11	118.60
27	B8	2317	A	N1-C6-N6	12.51	126.10	118.60
27	B8	2333	A	N1-C6-N6	12.51	126.10	118.60
27	B8	2541	A	N1-C6-N6	12.51	126.10	118.60
27	B8	2274	A	N1-C6-N6	12.50	126.10	118.60
27	B8	2860	A	N1-C6-N6	12.50	126.10	118.60
27	B8	1551	A	N1-C6-N6	12.49	126.10	118.60
1	AA	655	A	N1-C6-N6	12.49	126.09	118.60
1	AA	468	A	N1-C6-N6	12.48	126.09	118.60
27	B8	644	A	N1-C6-N6	12.48	126.09	118.60
27	B8	2378	A	N1-C6-N6	12.48	126.09	118.60
27	B8	265	A	N1-C6-N6	12.48	126.09	118.60
27	B8	1204	A	N1-C6-N6	12.48	126.09	118.60
27	B8	1810	A	N1-C6-N6	12.48	126.09	118.60
27	B8	575	A	N1-C6-N6	12.48	126.08	118.60
27	B8	742	A	N1-C6-N6	12.47	126.08	118.60
1	AA	716	A	N1-C6-N6	12.47	126.08	118.60
1	AA	263	A	N1-C6-N6	12.47	126.08	118.60
1	AA	865	A	N1-C6-N6	12.47	126.08	118.60
1	AA	1171	A	N1-C6-N6	12.47	126.08	118.60
1	AA	53	A	N1-C6-N6	12.46	126.08	118.60
27	B8	2727	A	N1-C6-N6	12.46	126.08	118.60
1	AA	1357	A	N1-C6-N6	12.46	126.08	118.60
27	B8	2386	A	N1-C6-N6	12.46	126.08	118.60
1	AA	1434	A	N1-C6-N6	12.46	126.07	118.60
27	B8	1143	A	N1-C6-N6	12.46	126.07	118.60
1	AA	228	A	N1-C6-N6	12.45	126.07	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B7	115	A	N1-C6-N6	12.45	126.07	118.60
27	B8	705	A	N1-C6-N6	12.45	126.07	118.60
27	B8	1794	A	N1-C6-N6	12.44	126.07	118.60
27	B8	127	A	N1-C6-N6	12.44	126.06	118.60
1	AA	629	A	N1-C6-N6	12.44	126.06	118.60
27	B8	2753	A	N1-C6-N6	12.44	126.06	118.60
1	AA	1065	U	P-O3'-C3'	12.43	134.62	119.70
27	B8	149	A	N1-C6-N6	12.43	126.06	118.60
27	B8	2482	A	N1-C6-N6	12.43	126.06	118.60
1	AA	482	A	N1-C6-N6	12.43	126.06	118.60
27	B8	299	A	N1-C6-N6	12.43	126.06	118.60
27	B8	382	A	N1-C6-N6	12.43	126.06	118.60
27	B8	300	A	N1-C6-N6	12.43	126.06	118.60
27	B8	466	A	N1-C6-N6	12.43	126.06	118.60
1	AA	270	A	N1-C6-N6	12.42	126.06	118.60
27	B8	633	A	N1-C6-N6	12.42	126.05	118.60
27	B8	2670	A	N1-C6-N6	12.42	126.05	118.60
27	B8	2598	A	N1-C6-N6	12.42	126.05	118.60
1	AA	223	A	N1-C6-N6	12.41	126.05	118.60
1	AA	1418	A	N1-C6-N6	12.41	126.05	118.60
1	AA	459	A	N1-C6-N6	12.41	126.05	118.60
27	B8	2094	A	N1-C6-N6	12.41	126.05	118.60
27	B8	415	A	N1-C6-N6	12.41	126.05	118.60
27	B8	1285	A	N1-C6-N6	12.41	126.05	118.60
27	B8	1654	A	N1-C6-N6	12.41	126.05	118.60
1	AA	960	U	P-O3'-C3'	12.40	134.59	119.70
27	B8	1664	A	N1-C6-N6	12.40	126.04	118.60
27	B8	89	A	N1-C6-N6	12.40	126.04	118.60
27	B8	2147	A	N1-C6-N6	12.40	126.04	118.60
1	AA	695	A	N1-C6-N6	12.40	126.04	118.60
1	AA	253	A	N1-C6-N6	12.39	126.04	118.60
27	B8	1579	A	N1-C6-N6	12.39	126.04	118.60
27	B8	84	A	N1-C6-N6	12.39	126.03	118.60
27	B8	2088	A	N1-C6-N6	12.38	126.03	118.60
1	AA	80	A	N1-C6-N6	12.38	126.03	118.60
1	AA	694	A	N1-C6-N6	12.38	126.03	118.60
1	AA	1155	A	N1-C6-N6	12.38	126.03	118.60
27	B8	1755	A	N1-C6-N6	12.38	126.03	118.60
27	B8	1194	A	N1-C6-N6	12.38	126.03	118.60
27	B8	2781	A	N1-C6-N6	12.38	126.03	118.60
1	AA	28	A	N1-C6-N6	12.38	126.03	118.60
26	B7	94	A	N1-C6-N6	12.38	126.03	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2711	A	N1-C6-N6	12.38	126.03	118.60
1	AA	959	A	N1-C6-N6	12.37	126.02	118.60
27	B8	2031	A	N1-C6-N6	12.37	126.02	118.60
27	B8	943	A	N1-C6-N6	12.37	126.02	118.60
27	B8	1384	A	N1-C6-N6	12.37	126.02	118.60
26	B7	50	A	N1-C6-N6	12.36	126.02	118.60
27	B8	2900	A	N1-C6-N6	12.37	126.02	118.60
27	B8	368	A	N1-C6-N6	12.36	126.02	118.60
27	B8	513	A	N1-C6-N6	12.36	126.02	118.60
27	B8	1502	A	N1-C6-N6	12.36	126.02	118.60
1	AA	600	A	N1-C6-N6	12.36	126.02	118.60
27	B8	1640	A	N1-C6-N6	12.36	126.02	118.60
27	B8	2211	A	N1-C6-N6	12.36	126.02	118.60
27	B8	1253	A	N1-C6-N6	12.36	126.01	118.60
1	AA	768	A	N1-C6-N6	12.35	126.01	118.60
27	B8	111	A	N1-C6-N6	12.35	126.01	118.60
27	B8	1528	A	N1-C6-N6	12.35	126.01	118.60
1	AA	1105	A	N1-C6-N6	12.34	126.00	118.60
27	B8	227	A	N1-C6-N6	12.34	126.00	118.60
27	B8	1928	A	N1-C6-N6	12.34	126.00	118.60
1	AA	460	A	N1-C6-N6	12.34	126.00	118.60
1	AA	676	A	N1-C6-N6	12.34	126.00	118.60
27	B8	1366	A	N1-C6-N6	12.34	126.00	118.60
1	AA	994	A	N1-C6-N6	12.34	126.00	118.60
27	B8	2700	A	N1-C6-N6	12.34	126.00	118.60
27	B8	2411	A	N1-C6-N6	12.33	126.00	118.60
27	B8	626	A	N1-C6-N6	12.33	126.00	118.60
27	B8	1548	A	N1-C6-N6	12.33	126.00	118.60
27	B8	1705	A	N1-C6-N6	12.33	126.00	118.60
27	B8	2170	A	N1-C6-N6	12.32	125.99	118.60
27	B8	2665	A	N1-C6-N6	12.32	126.00	118.60
27	B8	716	A	N1-C6-N6	12.32	125.99	118.60
27	B8	1998	A	N1-C6-N6	12.32	125.99	118.60
27	B8	1525	A	N1-C6-N6	12.32	125.99	118.60
1	AA	236	A	N1-C6-N6	12.31	125.99	118.60
1	AA	573	A	N1-C6-N6	12.31	125.99	118.60
27	B8	1490	A	N1-C6-N6	12.31	125.99	118.60
27	B8	38	A	N1-C6-N6	12.31	125.99	118.60
27	B8	1969	A	N1-C6-N6	12.31	125.99	118.60
27	B8	2198	A	N1-C6-N6	12.31	125.98	118.60
27	B8	2434	A	N1-C6-N6	12.31	125.98	118.60
1	AA	1377	A	N1-C6-N6	12.30	125.98	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	251	A	N1-C6-N6	12.30	125.98	118.60
27	B8	1586	A	N1-C6-N6	12.30	125.98	118.60
27	B8	1757	A	N1-C6-N6	12.30	125.98	118.60
1	AA	784	A	N1-C6-N6	12.30	125.98	118.60
27	B8	167	A	N1-C6-N6	12.30	125.98	118.60
27	B8	1913	A	N1-C6-N6	12.30	125.98	118.60
1	AA	831	A	N1-C6-N6	12.30	125.98	118.60
27	B8	2589	A	N1-C6-N6	12.30	125.98	118.60
1	AA	8	A	N1-C6-N6	12.30	125.98	118.60
1	AA	32	A	N1-C6-N6	12.30	125.98	118.60
27	B8	2632	A	N1-C6-N6	12.30	125.98	118.60
27	B8	1669	A	N1-C6-N6	12.29	125.98	118.60
27	B8	1591	A	N1-C6-N6	12.29	125.97	118.60
1	AA	131	A	N1-C6-N6	12.29	125.97	118.60
1	AA	1004	A	N1-C6-N6	12.28	125.97	118.60
1	AA	1188	A	N1-C6-N6	12.28	125.97	118.60
27	B8	1077	A	N1-C6-N6	12.28	125.97	118.60
1	AA	1280	A	N1-C6-N6	12.28	125.97	118.60
27	B8	1650	A	N1-C6-N6	12.28	125.97	118.60
27	B8	1286	A	N1-C6-N6	12.28	125.97	118.60
27	B8	2887	A	N1-C6-N6	12.28	125.97	118.60
1	AA	935	A	N1-C6-N6	12.27	125.96	118.60
27	B8	1413	A	N1-C6-N6	12.27	125.96	118.60
1	AA	983	A	N1-C6-N6	12.27	125.96	118.60
27	B8	2183	A	N1-C6-N6	12.27	125.96	118.60
1	AA	574	A	N1-C6-N6	12.27	125.96	118.60
27	B8	2158	A	N1-C6-N6	12.27	125.96	118.60
1	AA	1287	A	N1-C6-N6	12.27	125.96	118.60
27	B8	782	A	N1-C6-N6	12.26	125.96	118.60
27	B8	632	A	N1-C6-N6	12.26	125.96	118.60
27	B8	1952	A	N1-C6-N6	12.26	125.96	118.60
1	AA	559	A	N1-C6-N6	12.26	125.95	118.60
1	AA	706	A	N1-C6-N6	12.26	125.95	118.60
1	AA	1374	A	N1-C6-N6	12.26	125.95	118.60
3	AV	22	A	N1-C6-N6	12.25	125.95	118.60
1	AA	182	A	N1-C6-N6	12.25	125.95	118.60
27	B8	1274	A	N1-C6-N6	12.25	125.95	118.60
27	B8	1819	A	N1-C6-N6	12.25	125.95	118.60
27	B8	2503	A	N1-C6-N6	12.25	125.95	118.60
1	AA	66	A	N1-C6-N6	12.25	125.95	118.60
3	AV	77	A	N1-C6-N6	12.24	125.95	118.60
27	B8	845	A	N1-C6-N6	12.24	125.95	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2679	A	N1-C6-N6	12.24	125.95	118.60
27	B8	1226	A	N1-C6-N6	12.24	125.94	118.60
1	AA	907	A	N1-C6-N6	12.24	125.94	118.60
1	AA	1250	A	N1-C6-N6	12.24	125.94	118.60
27	B8	1735	A	N1-C6-N6	12.24	125.94	118.60
1	AA	3	A	N1-C6-N6	12.24	125.94	118.60
1	AA	1251	A	N1-C6-N6	12.24	125.94	118.60
27	B8	2439	A	N1-C6-N6	12.24	125.94	118.60
27	B8	1009	A	N1-C6-N6	12.23	125.94	118.60
27	B8	608	A	N1-C6-N6	12.23	125.94	118.60
27	B8	2328	A	N1-C6-N6	12.23	125.94	118.60
27	B8	203	A	N1-C6-N6	12.22	125.93	118.60
27	B8	996	A	N1-C6-N6	12.22	125.93	118.60
27	B8	2340	A	N1-C6-N6	12.22	125.93	118.60
27	B8	2660	A	N1-C6-N6	12.22	125.93	118.60
27	B8	1367	A	N1-C6-N6	12.22	125.93	118.60
27	B8	2837	A	N1-C6-N6	12.22	125.93	118.60
27	B8	354	A	N1-C6-N6	12.21	125.93	118.60
1	AA	190	A	N1-C6-N6	12.21	125.92	118.60
1	AA	787	A	N1-C6-N6	12.21	125.92	118.60
27	B8	2675	A	N1-C6-N6	12.21	125.92	118.60
3	AV	5	A	N1-C6-N6	12.21	125.92	118.60
27	B8	2738	A	N1-C6-N6	12.20	125.92	118.60
27	B8	91	A	N1-C6-N6	12.20	125.92	118.60
27	B8	892	A	N1-C6-N6	12.20	125.92	118.60
27	B8	925	A	N1-C6-N6	12.20	125.92	118.60
27	B8	2376	A	N1-C6-N6	12.20	125.92	118.60
27	B8	2406	A	N1-C6-N6	12.20	125.92	118.60
1	AA	919	A	N1-C6-N6	12.20	125.92	118.60
26	B7	119	A	N1-C6-N6	12.20	125.92	118.60
1	AA	383	A	N1-C6-N6	12.19	125.92	118.60
1	AA	1152	A	N1-C6-N6	12.19	125.92	118.60
1	AA	1447	A	N1-C6-N6	12.19	125.92	118.60
27	B8	2821	A	N1-C6-N6	12.19	125.92	118.60
1	AA	143	A	N1-C6-N6	12.19	125.91	118.60
27	B8	294	A	N1-C6-N6	12.19	125.91	118.60
27	B8	1618	A	N1-C6-N6	12.19	125.91	118.60
27	B8	2126	A	N1-C6-N6	12.19	125.91	118.60
1	AA	560	A	N1-C6-N6	12.18	125.91	118.60
27	B8	602	A	N1-C6-N6	12.18	125.91	118.60
27	B8	1134	A	N1-C6-N6	12.18	125.91	118.60
27	B8	2358	A	N1-C6-N6	12.18	125.91	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	120	A	N1-C6-N6	12.18	125.91	118.60
1	AA	1456	A	N1-C6-N6	12.18	125.91	118.60
27	B8	1866	A	N1-C6-N6	12.18	125.91	118.60
27	B8	1829	A	N1-C6-N6	12.18	125.91	118.60
1	AA	59	A	N1-C6-N6	12.18	125.91	118.60
27	B8	2314	A	N1-C6-N6	12.18	125.91	118.60
1	AA	648	A	N1-C6-N6	12.17	125.91	118.60
1	AA	1519	A	N1-C6-N6	12.17	125.90	118.60
27	B8	2893	A	N1-C6-N6	12.17	125.90	118.60
1	AA	1196	A	N1-C6-N6	12.16	125.90	118.60
27	B8	423	A	N1-C6-N6	12.16	125.90	118.60
27	B8	430	A	N1-C6-N6	12.16	125.90	118.60
27	B8	482	A	N1-C6-N6	12.16	125.90	118.60
1	AA	1396	A	N1-C6-N6	12.16	125.90	118.60
27	B8	53	A	N1-C6-N6	12.16	125.90	118.60
27	B8	1495	A	N1-C6-N6	12.16	125.89	118.60
1	AA	303	A	N1-C6-N6	12.15	125.89	118.60
27	B8	1953	A	N1-C6-N6	12.15	125.89	118.60
1	AA	366	A	N1-C6-N6	12.15	125.89	118.60
1	AA	546	A	N1-C6-N6	12.15	125.89	118.60
27	B8	332	A	N1-C6-N6	12.14	125.89	118.60
27	B8	789	A	N1-C6-N6	12.14	125.88	118.60
1	AA	630	A	N1-C6-N6	12.13	125.88	118.60
27	B8	1420	A	N1-C6-N6	12.13	125.88	118.60
27	B8	1609	A	N1-C6-N6	12.13	125.88	118.60
27	B8	1987	A	N1-C6-N6	12.13	125.88	118.60
27	B8	981	A	N1-C6-N6	12.13	125.88	118.60
27	B8	2792	A	N1-C6-N6	12.13	125.88	118.60
27	B8	2471	A	N1-C6-N6	12.13	125.88	118.60
27	B8	217	A	N1-C6-N6	12.13	125.88	118.60
1	AA	1201	A	N1-C6-N6	12.12	125.87	118.60
1	AA	149	A	N1-C6-N6	12.12	125.87	118.60
27	B8	14	A	N1-C6-N6	12.12	125.87	118.60
1	AA	349	A	N1-C6-N6	12.12	125.87	118.60
1	AA	635	A	N1-C6-N6	12.12	125.87	118.60
1	AA	1170	A	N1-C6-N6	12.12	125.87	118.60
1	AA	815	A	N1-C6-N6	12.12	125.87	118.60
1	AA	900	A	N1-C6-N6	12.12	125.87	118.60
27	B8	320	A	N1-C6-N6	12.12	125.87	118.60
1	AA	539	A	N1-C6-N6	12.12	125.87	118.60
1	AA	1507	A	N1-C6-N6	12.12	125.87	118.60
27	B8	2810	A	N1-C6-N6	12.11	125.87	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1324	A	N1-C6-N6	12.11	125.87	118.60
27	B8	146	A	N1-C6-N6	12.11	125.86	118.60
27	B8	2706	A	N1-C6-N6	12.11	125.86	118.60
1	AA	493	A	N1-C6-N6	12.10	125.86	118.60
1	AA	1274	A	N1-C6-N6	12.10	125.86	118.60
27	B8	1762	A	N1-C6-N6	12.10	125.86	118.60
27	B8	272	A	N1-C6-N6	12.10	125.86	118.60
27	B8	802	A	N1-C6-N6	12.10	125.86	118.60
27	B8	945	A	N1-C6-N6	12.10	125.86	118.60
1	AA	510	A	N1-C6-N6	12.10	125.86	118.60
1	AA	1169	A	N1-C6-N6	12.10	125.86	118.60
27	B8	352	A	N1-C6-N6	12.10	125.86	118.60
27	B8	1073	A	N1-C6-N6	12.10	125.86	118.60
27	B8	2518	A	N1-C6-N6	12.10	125.86	118.60
27	B8	2572	A	N1-C6-N6	12.10	125.86	118.60
1	AA	119	A	N1-C6-N6	12.09	125.86	118.60
27	B8	2823	A	N1-C6-N6	12.09	125.86	118.60
1	AA	873	A	N1-C6-N6	12.09	125.86	118.60
27	B8	833	A	N1-C6-N6	12.09	125.85	118.60
1	AA	499	A	N1-C6-N6	12.09	125.85	118.60
27	B8	2101	A	N1-C6-N6	12.09	125.85	118.60
27	B8	2191	A	N1-C6-N6	12.09	125.85	118.60
27	B8	2461	A	N1-C6-N6	12.09	125.85	118.60
27	B8	792	A	N1-C6-N6	12.09	125.85	118.60
1	AA	465	A	N1-C6-N6	12.09	125.85	118.60
27	B8	819	A	N1-C6-N6	12.09	125.85	118.60
27	B8	1085	A	N1-C6-N6	12.09	125.85	118.60
27	B8	1593	A	N1-C6-N6	12.09	125.85	118.60
1	AA	44	A	N1-C6-N6	12.08	125.85	118.60
27	B8	1978	A	N1-C6-N6	12.08	125.85	118.60
27	B8	160	A	N1-C6-N6	12.08	125.85	118.60
27	B8	1096	A	N1-C6-N6	12.08	125.85	118.60
27	B8	1877	A	N1-C6-N6	12.08	125.85	118.60
27	B8	2432	A	N1-C6-N6	12.08	125.85	118.60
27	B8	2682	A	N1-C6-N6	12.08	125.85	118.60
1	AA	1163	A	N1-C6-N6	12.07	125.84	118.60
27	B8	706	A	N1-C6-N6	12.07	125.84	118.60
27	B8	2377	A	N1-C6-N6	12.07	125.84	118.60
27	B8	1805	A	N1-C6-N6	12.07	125.84	118.60
27	B8	627	A	N1-C6-N6	12.06	125.84	118.60
27	B8	2142	A	N1-C6-N6	12.06	125.84	118.60
27	B8	2241	A	N1-C6-N6	12.06	125.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2407	A	N1-C6-N6	12.06	125.84	118.60
1	AA	435	A	N1-C6-N6	12.06	125.84	118.60
1	AA	1022	A	N1-C6-N6	12.06	125.84	118.60
1	AA	496	A	N1-C6-N6	12.06	125.83	118.60
1	AA	1254	A	N1-C6-N6	12.06	125.84	118.60
27	B8	979	A	N1-C6-N6	12.06	125.84	118.60
27	B8	1069	A	N1-C6-N6	12.06	125.83	118.60
27	B8	1566	A	N1-C6-N6	12.06	125.83	118.60
27	B8	1403	A	N1-C6-N6	12.06	125.83	118.60
27	B8	1503	A	N1-C6-N6	12.06	125.83	118.60
27	B8	2560	A	N1-C6-N6	12.06	125.83	118.60
3	AV	14	A	N1-C6-N6	12.05	125.83	118.60
27	B8	1090	A	N1-C6-N6	12.05	125.83	118.60
1	AA	743	A	N1-C6-N6	12.05	125.83	118.60
27	B8	1676	A	N1-C6-N6	12.05	125.83	118.60
27	B8	2814	A	N1-C6-N6	12.05	125.83	118.60
1	AA	938	A	N1-C6-N6	12.05	125.83	118.60
27	B8	1050	A	N1-C6-N6	12.05	125.83	118.60
27	B8	1570	A	N1-C6-N6	12.04	125.83	118.60
27	B8	2602	A	N1-C6-N6	12.04	125.83	118.60
27	B8	1230	A	N1-C6-N6	12.04	125.83	118.60
27	B8	2850	A	N1-C6-N6	12.04	125.83	118.60
27	B8	590	A	N1-C6-N6	12.04	125.82	118.60
27	B8	804	A	N1-C6-N6	12.04	125.82	118.60
27	B8	1678	A	N1-C6-N6	12.04	125.82	118.60
27	B8	10	A	N1-C6-N6	12.03	125.82	118.60
27	B8	2005	A	N1-C6-N6	12.03	125.82	118.60
1	AA	321	A	N1-C6-N6	12.03	125.82	118.60
26	B7	46	A	N1-C6-N6	12.03	125.82	118.60
27	B8	1722	A	N1-C6-N6	12.03	125.82	118.60
1	AA	553	A	N1-C6-N6	12.03	125.82	118.60
27	B8	480	A	N1-C6-N6	12.03	125.81	118.60
27	B8	2388	A	N1-C6-N6	12.03	125.82	118.60
27	B8	1938	A	N1-C6-N6	12.02	125.81	118.60
1	AA	1311	A	N1-C6-N6	12.02	125.81	118.60
1	AA	306	A	N1-C6-N6	12.02	125.81	118.60
27	B8	1353	A	N1-C6-N6	12.02	125.81	118.60
27	B8	1014	A	N1-C6-N6	12.01	125.81	118.60
27	B8	2080	A	N1-C6-N6	12.01	125.81	118.60
27	B8	2346	A	N1-C6-N6	12.01	125.81	118.60
27	B8	2309	A	N1-C6-N6	12.01	125.80	118.60
27	B8	223	A	N1-C6-N6	12.00	125.80	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1020	A	N1-C6-N6	12.00	125.80	118.60
27	B8	2448	A	N1-C6-N6	12.00	125.80	118.60
27	B8	764	A	N1-C6-N6	12.00	125.80	118.60
1	AA	958	A	N1-C6-N6	12.00	125.80	118.60
27	B8	2097	A	N1-C6-N6	12.00	125.80	118.60
1	AA	189	A	N1-C6-N6	12.00	125.80	118.60
1	AA	1350	A	N1-C6-N6	12.00	125.80	118.60
27	B8	563	A	N1-C6-N6	12.00	125.80	118.60
1	AA	579	A	N1-C6-N6	11.99	125.80	118.60
1	AA	363	A	N1-C6-N6	11.99	125.80	118.60
1	AA	1021	A	N1-C6-N6	11.99	125.80	118.60
27	B8	1008	A	N1-C6-N6	11.99	125.80	118.60
27	B8	1057	A	N1-C6-N6	11.99	125.80	118.60
27	B8	472	A	N1-C6-N6	11.99	125.79	118.60
27	B8	1970	A	N1-C6-N6	11.99	125.79	118.60
27	B8	2288	A	N1-C6-N6	11.99	125.79	118.60
27	B8	1754	A	N1-C6-N6	11.99	125.79	118.60
27	B8	2425	A	N1-C6-N6	11.98	125.79	118.60
1	AA	532	A	N1-C6-N6	11.98	125.79	118.60
27	B8	1029	A	N1-C6-N6	11.98	125.79	118.60
27	B8	1048	A	N1-C6-N6	11.98	125.79	118.60
27	B8	1241	A	N1-C6-N6	11.98	125.79	118.60
1	AA	1180	A	N1-C6-N6	11.98	125.79	118.60
27	B8	668	A	N1-C6-N6	11.98	125.79	118.60
27	B8	2019	A	N1-C6-N6	11.98	125.79	118.60
27	B8	311	A	N1-C6-N6	11.97	125.78	118.60
27	B8	345	A	N1-C6-N6	11.97	125.78	118.60
27	B8	1169	A	N1-C6-N6	11.97	125.78	118.60
27	B8	1665	A	N1-C6-N6	11.97	125.78	118.60
1	AA	1092	A	N1-C6-N6	11.97	125.78	118.60
27	B8	1246	A	N1-C6-N6	11.97	125.78	118.60
27	B8	1597	A	N1-C6-N6	11.97	125.78	118.60
27	B8	1802	A	N1-C6-N6	11.97	125.78	118.60
1	AA	728	A	N1-C6-N6	11.97	125.78	118.60
1	AA	1542	A	N1-C6-N6	11.97	125.78	118.60
27	B8	603	A	N1-C6-N6	11.96	125.78	118.60
27	B8	1262	A	N1-C6-N6	11.96	125.78	118.60
1	AA	781	A	N1-C6-N6	11.96	125.78	118.60
3	AV	52	A	N1-C6-N6	11.96	125.78	118.60
27	B8	2776	A	N1-C6-N6	11.96	125.78	118.60
27	B8	52	A	N1-C6-N6	11.96	125.78	118.60
27	B8	218	A	N1-C6-N6	11.96	125.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1672	A	N1-C6-N6	11.96	125.77	118.60
27	B8	2426	A	N1-C6-N6	11.96	125.77	118.60
27	B8	2809	A	N1-C6-N6	11.96	125.77	118.60
27	B8	1327	A	N1-C6-N6	11.95	125.77	118.60
27	B8	1383	A	N1-C6-N6	11.95	125.77	118.60
27	B8	1385	A	N1-C6-N6	11.95	125.77	118.60
27	B8	1871	A	N1-C6-N6	11.95	125.77	118.60
1	AA	1493	A	N1-C6-N6	11.95	125.77	118.60
27	B8	980	A	N1-C6-N6	11.95	125.77	118.60
27	B8	1847	A	N1-C6-N6	11.95	125.77	118.60
27	B8	2740	A	N1-C6-N6	11.95	125.77	118.60
1	AA	101	A	N1-C6-N6	11.94	125.77	118.60
1	AA	816	A	N1-C6-N6	11.94	125.77	118.60
27	B8	2531	A	N1-C6-N6	11.94	125.77	118.60
27	B8	1046	A	N1-C6-N6	11.94	125.76	118.60
1	AA	602	A	N1-C6-N6	11.94	125.76	118.60
27	B8	905	A	N1-C6-N6	11.94	125.76	118.60
1	AA	621	A	N1-C6-N6	11.94	125.76	118.60
1	AA	1431	A	N1-C6-N6	11.94	125.76	118.60
27	B8	631	A	N1-C6-N6	11.94	125.76	118.60
1	AA	807	A	N1-C6-N6	11.93	125.76	118.60
27	B8	191	A	N1-C6-N6	11.93	125.76	118.60
27	B8	348	A	N1-C6-N6	11.93	125.76	118.60
27	B8	2205	A	N1-C6-N6	11.93	125.76	118.60
1	AA	1117	A	N1-C6-N6	11.93	125.76	118.60
1	AA	1271	A	N1-C6-N6	11.93	125.76	118.60
1	AA	1480	A	N1-C6-N6	11.93	125.76	118.60
27	B8	2247	A	N1-C6-N6	11.93	125.76	118.60
1	AA	338	A	N1-C6-N6	11.93	125.76	118.60
1	AA	596	A	N1-C6-N6	11.93	125.76	118.60
1	AA	946	A	N1-C6-N6	11.93	125.76	118.60
27	B8	572	A	N1-C6-N6	11.92	125.75	118.60
1	AA	1257	A	N1-C6-N6	11.92	125.75	118.60
27	B8	793	A	N1-C6-N6	11.92	125.75	118.60
27	B8	983	A	N1-C6-N6	11.92	125.75	118.60
27	B8	1966	A	N1-C6-N6	11.92	125.75	118.60
1	AA	1019	A	N1-C6-N6	11.91	125.75	118.60
27	B8	752	A	N1-C6-N6	11.91	125.75	118.60
27	B8	172	A	N1-C6-N6	11.91	125.75	118.60
1	AA	715	A	N1-C6-N6	11.91	125.75	118.60
27	B8	1759	A	N1-C6-N6	11.91	125.75	118.60
27	B8	739	A	N1-C6-N6	11.91	125.74	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2071	A	N1-C6-N6	11.91	125.75	118.60
27	B8	2058	A	N1-C6-N6	11.91	125.74	118.60
1	AA	51	A	N1-C6-N6	11.90	125.74	118.60
1	AA	1067	A	N1-C6-N6	11.90	125.74	118.60
1	AA	1468	A	N1-C6-N6	11.90	125.74	118.60
27	B8	1504	A	N1-C6-N6	11.90	125.74	118.60
27	B8	1392	A	N1-C6-N6	11.90	125.74	118.60
1	AA	1093	A	N1-C6-N6	11.89	125.74	118.60
27	B8	173	A	N1-C6-N6	11.89	125.74	118.60
27	B8	1000	A	N1-C6-N6	11.89	125.74	118.60
27	B8	2565	A	N1-C6-N6	11.89	125.73	118.60
27	B8	2799	A	N1-C6-N6	11.89	125.73	118.60
1	AA	1394	A	N1-C6-N6	11.88	125.73	118.60
1	AA	1446	A	N1-C6-N6	11.88	125.73	118.60
27	B8	44	A	N1-C6-N6	11.88	125.73	118.60
27	B8	216	A	N1-C6-N6	11.88	125.73	118.60
27	B8	270	A	N1-C6-N6	11.88	125.73	118.60
27	B8	2322	A	N1-C6-N6	11.88	125.73	118.60
1	AA	1082	A	N1-C6-N6	11.88	125.73	118.60
1	AA	1430	A	N1-C6-N6	11.88	125.73	118.60
27	B8	1129	A	N1-C6-N6	11.88	125.73	118.60
27	B8	1470	A	N1-C6-N6	11.88	125.73	118.60
2	AX	21	A	N1-C6-N6	11.87	125.72	118.60
27	B8	125	A	N1-C6-N6	11.87	125.72	118.60
1	AA	918	A	N1-C6-N6	11.87	125.72	118.60
27	B8	2758	A	N1-C6-N6	11.87	125.72	118.60
1	AA	344	A	N1-C6-N6	11.87	125.72	118.60
1	AA	749	A	N1-C6-N6	11.87	125.72	118.60
27	B8	936	A	N1-C6-N6	11.87	125.72	118.60
27	B8	2003	A	N1-C6-N6	11.87	125.72	118.60
1	AA	1213	A	N1-C6-N6	11.87	125.72	118.60
1	AA	19	A	N1-C6-N6	11.86	125.72	118.60
1	AA	1499	A	N1-C6-N6	11.86	125.72	118.60
27	B8	788	A	N1-C6-N6	11.87	125.72	118.60
27	B8	960	A	N1-C6-N6	11.86	125.72	118.60
27	B8	984	A	N1-C6-N6	11.86	125.72	118.60
27	B8	877	A	N1-C6-N6	11.86	125.71	118.60
27	B8	861	A	N1-C6-N6	11.86	125.71	118.60
27	B8	197	A	N1-C6-N6	11.85	125.71	118.60
27	B8	1302	A	N1-C6-N6	11.85	125.71	118.60
27	B8	1151	A	N1-C6-N6	11.85	125.71	118.60
27	B8	2634	A	N1-C6-N6	11.85	125.71	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	572	A	N1-C6-N6	11.85	125.71	118.60
3	AV	59	A	N1-C6-N6	11.85	125.71	118.60
27	B8	1900	A	N1-C6-N6	11.85	125.71	118.60
1	AA	607	A	N1-C6-N6	11.84	125.71	118.60
1	AA	389	A	N1-C6-N6	11.84	125.70	118.60
27	B8	309	A	N1-C6-N6	11.84	125.70	118.60
27	B8	1549	A	N1-C6-N6	11.84	125.70	118.60
27	B8	1981	A	N1-C6-N6	11.84	125.70	118.60
27	B8	2459	A	N1-C6-N6	11.84	125.70	118.60
1	AA	1	A	N1-C6-N6	11.84	125.70	118.60
1	AA	161	A	N1-C6-N6	11.84	125.70	118.60
27	B8	1347	A	N1-C6-N6	11.84	125.70	118.60
1	AA	1476	A	N1-C6-N6	11.83	125.70	118.60
27	B8	1626	A	N1-C6-N6	11.83	125.70	118.60
27	B8	504	A	N1-C6-N6	11.83	125.70	118.60
27	B8	2547	A	N1-C6-N6	11.82	125.69	118.60
1	AA	851	G	N1-C6-O6	11.82	126.99	119.90
1	AA	1046	A	N1-C6-N6	11.82	125.69	118.60
27	B8	101	A	N1-C6-N6	11.82	125.69	118.60
27	B8	231	A	N1-C6-N6	11.82	125.69	118.60
27	B8	2813	A	N1-C6-N6	11.82	125.69	118.60
27	B8	49	A	N1-C6-N6	11.82	125.69	118.60
27	B8	384	A	N1-C6-N6	11.82	125.69	118.60
1	AA	197	A	N1-C6-N6	11.82	125.69	118.60
1	AA	2	A	N1-C6-N6	11.82	125.69	118.60
1	AA	415	A	N1-C6-N6	11.82	125.69	118.60
27	B8	844	A	N1-C6-N6	11.82	125.69	118.60
27	B8	1808	A	N1-C6-N6	11.81	125.69	118.60
1	AA	315	A	N1-C6-N6	11.81	125.69	118.60
1	AA	356	A	N1-C6-N6	11.81	125.69	118.60
27	B8	917	A	N1-C6-N6	11.81	125.69	118.60
2	AX	22	A	N1-C6-N6	11.80	125.68	118.60
27	B8	470	A	N1-C6-N6	11.80	125.68	118.60
1	AA	777	A	N1-C6-N6	11.80	125.68	118.60
26	B7	104	A	N1-C6-N6	11.80	125.68	118.60
27	B8	422	A	N1-C6-N6	11.80	125.68	118.60
1	AA	1216	A	N1-C6-N6	11.80	125.68	118.60
27	B8	1789	A	N1-C6-N6	11.80	125.68	118.60
27	B8	196	A	N1-C6-N6	11.80	125.68	118.60
27	B8	1328	A	N1-C6-N6	11.80	125.68	118.60
1	AA	466	A	N1-C6-N6	11.79	125.68	118.60
1	AA	1102	A	N1-C6-N6	11.79	125.68	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	A	N1-C6-N6	11.79	125.67	118.60
27	B8	1156	A	N1-C6-N6	11.79	125.67	118.60
27	B8	2009	A	N1-C6-N6	11.79	125.67	118.60
27	B8	1508	A	N1-C6-N6	11.79	125.67	118.60
27	B8	1632	A	N1-C6-N6	11.79	125.67	118.60
1	AA	495	A	N1-C6-N6	11.78	125.67	118.60
1	AA	1227	A	N1-C6-N6	11.78	125.67	118.60
27	B8	1175	A	N1-C6-N6	11.78	125.67	118.60
1	AA	767	A	N1-C6-N6	11.78	125.67	118.60
27	B8	507	A	N1-C6-N6	11.78	125.67	118.60
27	B8	972	A	N1-C6-N6	11.78	125.67	118.60
27	B8	1571	A	N1-C6-N6	11.78	125.67	118.60
27	B8	1505	A	N1-C6-N6	11.78	125.67	118.60
1	AA	640	A	N1-C6-N6	11.77	125.66	118.60
27	B8	344	A	N1-C6-N6	11.77	125.66	118.60
27	B8	439	A	N1-C6-N6	11.77	125.66	118.60
27	B8	1801	A	N1-C6-N6	11.77	125.66	118.60
27	B8	2270	A	N1-C6-N6	11.77	125.66	118.60
27	B8	2736	A	N1-C6-N6	11.77	125.66	118.60
1	AA	1503	A	N1-C6-N6	11.76	125.66	118.60
1	AA	712	A	N1-C6-N6	11.76	125.66	118.60
27	B8	1322	A	N1-C6-N6	11.76	125.66	118.60
27	B8	1821	A	N1-C6-N6	11.76	125.66	118.60
1	AA	1483	A	N1-C6-N6	11.76	125.66	118.60
27	B8	1635	A	N1-C6-N6	11.76	125.66	118.60
27	B8	1477	A	N1-C6-N6	11.76	125.66	118.60
1	AA	1375	A	N1-C6-N6	11.76	125.65	118.60
1	AA	622	A	N1-C6-N6	11.75	125.65	118.60
27	B8	156	A	N1-C6-N6	11.75	125.65	118.60
27	B8	1744	A	N1-C6-N6	11.75	125.65	118.60
1	AA	397	A	N1-C6-N6	11.75	125.65	118.60
1	AA	968	A	N1-C6-N6	11.75	125.65	118.60
27	B8	722	A	N1-C6-N6	11.74	125.64	118.60
27	B8	1054	A	N1-C6-N6	11.74	125.64	118.60
27	B8	1509	A	N1-C6-N6	11.74	125.64	118.60
27	B8	478	A	N1-C6-N6	11.74	125.64	118.60
27	B8	896	A	N1-C6-N6	11.74	125.64	118.60
1	AA	790	A	N1-C6-N6	11.74	125.64	118.60
27	B8	2266	A	N1-C6-N6	11.74	125.64	118.60
27	B8	1535	A	N1-C6-N6	11.73	125.64	118.60
1	AA	975	A	N1-C6-N6	11.73	125.64	118.60
1	AA	1179	A	N1-C6-N6	11.73	125.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1248	A	N1-C6-N6	11.73	125.64	118.60
27	B8	1080	A	N1-C6-N6	11.73	125.64	118.60
1	AA	729	A	N1-C6-N6	11.73	125.64	118.60
3	AV	58	A	N1-C6-N6	11.73	125.64	118.60
27	B8	975	A	N1-C6-N6	11.72	125.63	118.60
27	B8	1960	A	N1-C6-N6	11.72	125.63	118.60
27	B8	2577	A	N1-C6-N6	11.72	125.63	118.60
1	AA	243	A	N1-C6-N6	11.72	125.63	118.60
1	AA	250	A	N1-C6-N6	11.72	125.63	118.60
27	B8	715	A	N1-C6-N6	11.72	125.63	118.60
1	AA	74	A	N1-C6-N6	11.71	125.63	118.60
27	B8	1889	A	N1-C6-N6	11.71	125.63	118.60
27	B8	2614	A	N1-C6-N6	11.71	125.63	118.60
1	AA	845	A	N1-C6-N6	11.71	125.63	118.60
27	B8	176	A	N1-C6-N6	11.71	125.63	118.60
27	B8	1010	A	N1-C6-N6	11.71	125.63	118.60
27	B8	2327	A	N1-C6-N6	11.71	125.63	118.60
1	AA	1130	A	N1-C6-N6	11.71	125.62	118.60
27	B8	2820	A	N1-C6-N6	11.71	125.62	118.60
27	B8	282	A	N1-C6-N6	11.71	125.62	118.60
1	AA	484	G	P-O3'-C3'	11.70	133.74	119.70
27	B8	547	A	N1-C6-N6	11.70	125.62	118.60
1	AA	909	A	N1-C6-N6	11.70	125.62	118.60
1	AA	1408	A	N1-C6-N6	11.70	125.62	118.60
1	AA	1502	A	N1-C6-N6	11.70	125.62	118.60
27	B8	1419	A	N1-C6-N6	11.70	125.62	118.60
27	B8	2070	A	N1-C6-N6	11.70	125.62	118.60
27	B8	2534	A	N1-C6-N6	11.70	125.62	118.60
1	AA	78	A	N1-C6-N6	11.69	125.62	118.60
27	B8	1746	A	N1-C6-N6	11.69	125.62	118.60
27	B8	508	A	N1-C6-N6	11.69	125.62	118.60
27	B8	910	A	N1-C6-N6	11.69	125.62	118.60
1	AA	663	A	N1-C6-N6	11.69	125.61	118.60
1	AA	130	A	N1-C6-N6	11.69	125.61	118.60
27	B8	918	A	N1-C6-N6	11.69	125.61	118.60
27	B8	2433	A	N1-C6-N6	11.69	125.61	118.60
1	AA	167	A	N1-C6-N6	11.69	125.61	118.60
27	B8	1365	A	N1-C6-N6	11.69	125.61	118.60
1	AA	1363	A	N1-C6-N6	11.68	125.61	118.60
27	B8	1359	A	N1-C6-N6	11.68	125.61	118.60
27	B8	1772	A	N1-C6-N6	11.68	125.61	118.60
27	B8	2117	A	N1-C6-N6	11.68	125.61	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2497	A	N1-C6-N6	11.68	125.61	118.60
27	B8	432	A	N1-C6-N6	11.68	125.61	118.60
27	B8	1608	A	N1-C6-N6	11.68	125.61	118.60
27	B8	310	A	N1-C6-N6	11.68	125.61	118.60
1	AA	461	A	N1-C6-N6	11.68	125.61	118.60
27	B8	73	A	N1-C6-N6	11.68	125.61	118.60
27	B8	661	A	N1-C6-N6	11.68	125.61	118.60
27	B8	2468	A	N1-C6-N6	11.68	125.61	118.60
1	AA	412	A	N1-C6-N6	11.67	125.60	118.60
1	AA	681	A	N1-C6-N6	11.67	125.60	118.60
1	AA	704	A	N1-C6-N6	11.67	125.60	118.60
1	AA	298	A	N1-C6-N6	11.67	125.60	118.60
27	B8	643	A	N1-C6-N6	11.67	125.60	118.60
27	B8	1284	A	N1-C6-N6	11.67	125.60	118.60
27	B8	2082	A	N1-C6-N6	11.67	125.60	118.60
27	B8	1572	A	N1-C6-N6	11.66	125.60	118.60
1	AA	747	A	N1-C6-N6	11.66	125.60	118.60
27	B8	866	A	N1-C6-N6	11.66	125.60	118.60
1	AA	1340	A	N1-C6-N6	11.66	125.59	118.60
27	B8	404	A	N1-C6-N6	11.66	125.59	118.60
27	B8	1912	A	N1-C6-N6	11.65	125.59	118.60
27	B8	2476	A	N1-C6-N6	11.65	125.59	118.60
27	B8	391	A	N1-C6-N6	11.65	125.59	118.60
27	B8	1089	A	N1-C6-N6	11.65	125.59	118.60
1	AA	1145	A	N1-C6-N6	11.64	125.59	118.60
27	B8	753	A	N1-C6-N6	11.64	125.58	118.60
26	B7	53	A	N1-C6-N6	11.64	125.58	118.60
27	B8	2513	A	N1-C6-N6	11.64	125.58	118.60
27	B8	2062	A	N1-C6-N6	11.63	125.58	118.60
1	AA	1410	A	N1-C6-N6	11.63	125.58	118.60
1	AA	1534	A	N1-C6-N6	11.63	125.58	118.60
27	B8	1916	A	N1-C6-N6	11.63	125.58	118.60
27	B8	2059	A	N1-C6-N6	11.63	125.58	118.60
27	B8	2590	A	N1-C6-N6	11.63	125.58	118.60
27	B8	2705	A	N1-C6-N6	11.63	125.58	118.60
27	B8	1749	A	N1-C6-N6	11.63	125.58	118.60
27	B8	144	A	N1-C6-N6	11.62	125.57	118.60
1	AA	374	A	N1-C6-N6	11.62	125.57	118.60
1	AA	977	A	N1-C6-N6	11.62	125.57	118.60
1	AA	1318	A	N1-C6-N6	11.62	125.57	118.60
1	AA	393	A	N1-C6-N6	11.62	125.57	118.60
27	B8	278	A	N1-C6-N6	11.61	125.57	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	408	A	N1-C6-N6	11.61	125.56	118.60
27	B8	131	A	N1-C6-N6	11.61	125.57	118.60
27	B8	1614	A	N1-C6-N6	11.60	125.56	118.60
27	B8	1265	A	N1-C6-N6	11.60	125.56	118.60
27	B8	1544	A	N1-C6-N6	11.60	125.56	118.60
1	AA	7	A	N1-C6-N6	11.60	125.56	118.60
1	AA	1042	A	N1-C6-N6	11.60	125.56	118.60
27	B8	2883	A	N1-C6-N6	11.60	125.56	118.60
27	B8	2418	A	N1-C6-N6	11.59	125.56	118.60
27	B8	2886	A	N1-C6-N6	11.59	125.55	118.60
27	B8	1247	A	N1-C6-N6	11.59	125.55	118.60
27	B8	1304	A	N1-C6-N6	11.59	125.55	118.60
1	AA	327	A	N1-C6-N6	11.58	125.55	118.60
27	B8	1254	A	N1-C6-N6	11.58	125.55	118.60
27	B8	1919	A	N1-C6-N6	11.58	125.55	118.60
27	B8	2287	A	N1-C6-N6	11.58	125.55	118.60
1	AA	50	A	N1-C6-N6	11.58	125.55	118.60
27	B8	71	A	N1-C6-N6	11.58	125.55	118.60
27	B8	165	A	N1-C6-N6	11.58	125.55	118.60
1	AA	72	A	N1-C6-N6	11.57	125.55	118.60
27	B8	1040	A	N1-C6-N6	11.57	125.54	118.60
27	B8	2114	A	N1-C6-N6	11.57	125.54	118.60
27	B8	2765	A	N1-C6-N6	11.57	125.54	118.60
1	AA	913	A	N1-C6-N6	11.57	125.54	118.60
27	B8	2176	A	N1-C6-N6	11.57	125.54	118.60
27	B8	2721	A	N1-C6-N6	11.57	125.54	118.60
1	AA	1246	A	N1-C6-N6	11.57	125.54	118.60
1	AA	1339	A	N1-C6-N6	11.56	125.54	118.60
27	B8	750	A	N1-C6-N6	11.56	125.54	118.60
27	B8	1336	A	N1-C6-N6	11.56	125.54	118.60
27	B8	2664	G	N1-C6-O6	11.56	126.84	119.90
27	B8	1133	A	N1-C6-N6	11.56	125.53	118.60
27	B8	2077	A	N1-C6-N6	11.56	125.53	118.60
1	AA	702	A	N1-C6-N6	11.55	125.53	118.60
1	AA	1531	A	N1-C6-N6	11.55	125.53	118.60
1	AA	452	A	N1-C6-N6	11.55	125.53	118.60
27	B8	1569	A	N1-C6-N6	11.55	125.53	118.60
27	B8	614	A	N1-C6-N6	11.54	125.53	118.60
27	B8	1711	A	N1-C6-N6	11.54	125.53	118.60
27	B8	1276	A	N1-C6-N6	11.54	125.53	118.60
27	B8	1434	A	N1-C6-N6	11.54	125.52	118.60
27	B8	2835	A	N1-C6-N6	11.54	125.52	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	160	A	N1-C6-N6	11.53	125.52	118.60
1	AA	411	A	N1-C6-N6	11.53	125.52	118.60
1	AA	1204	A	N1-C6-N6	11.53	125.52	118.60
27	B8	2733	A	N1-C6-N6	11.53	125.52	118.60
1	AA	523	A	N1-C6-N6	11.52	125.51	118.60
27	B8	2199	A	N1-C6-N6	11.52	125.51	118.60
27	B8	2566	A	N1-C6-N6	11.51	125.51	118.60
27	B8	2882	A	N1-C6-N6	11.51	125.51	118.60
1	AA	609	A	N1-C6-N6	11.51	125.51	118.60
27	B8	2095	A	N1-C6-N6	11.51	125.50	118.60
27	B8	1272	A	N1-C6-N6	11.51	125.50	118.60
27	B8	1583	A	N1-C6-N6	11.51	125.50	118.60
27	B8	74	A	N1-C6-N6	11.50	125.50	118.60
27	B8	1616	A	N1-C6-N6	11.50	125.50	118.60
1	AA	364	A	N1-C6-N6	11.50	125.50	118.60
27	B8	21	A	N1-C6-N6	11.50	125.50	118.60
27	B8	2030	A	N1-C6-N6	11.50	125.50	118.60
1	AA	1428	A	N1-C6-N6	11.49	125.50	118.60
27	B8	988	A	N1-C6-N6	11.49	125.50	118.60
1	AA	649	A	N1-C6-N6	11.48	125.49	118.60
27	B8	2530	A	N1-C6-N6	11.48	125.49	118.60
27	B8	920	A	N1-C6-N6	11.48	125.49	118.60
27	B8	927	A	N1-C6-N6	11.48	125.49	118.60
1	AA	313	A	N1-C6-N6	11.48	125.49	118.60
1	AA	819	A	N1-C6-N6	11.48	125.49	118.60
1	AA	1413	A	N1-C6-N6	11.47	125.48	118.60
1	AA	535	A	N1-C6-N6	11.47	125.48	118.60
1	AA	949	A	N1-C6-N6	11.47	125.48	118.60
27	B8	126	A	N1-C6-N6	11.47	125.48	118.60
27	B8	453	A	N1-C6-N6	11.47	125.48	118.60
27	B8	1067	A	N1-C6-N6	11.47	125.48	118.60
1	AA	382	A	N1-C6-N6	11.47	125.48	118.60
1	AA	449	G	N1-C6-O6	11.47	126.78	119.90
27	B8	2134	A	N1-C6-N6	11.46	125.48	118.60
1	AA	1225	A	N1-C6-N6	11.46	125.48	118.60
27	B8	2336	A	N1-C6-N6	11.46	125.48	118.60
1	AA	969	A	N1-C6-N6	11.46	125.47	118.60
1	AA	792	A	N1-C6-N6	11.46	125.47	118.60
1	AA	441	A	N1-C6-N6	11.45	125.47	118.60
27	B8	1321	A	N1-C6-N6	11.45	125.47	118.60
27	B8	1910	G	N1-C6-O6	11.45	126.77	119.90
1	AA	1256	A	N1-C6-N6	11.45	125.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	64	A	N1-C6-N6	11.44	125.47	118.60
27	B8	1395	A	N1-C6-N6	11.44	125.46	118.60
27	B8	2635	A	N1-C6-N6	11.44	125.46	118.60
1	AA	1508	A	N1-C6-N6	11.44	125.46	118.60
1	AA	547	A	N1-C6-N6	11.44	125.46	118.60
1	AA	878	A	N1-C6-N6	11.43	125.46	118.60
1	AA	1429	A	N1-C6-N6	11.43	125.46	118.60
27	B8	1510	G	N1-C6-O6	11.42	126.75	119.90
27	B8	2726	A	N1-C6-N6	11.42	125.45	118.60
27	B8	1147	A	N1-C6-N6	11.42	125.45	118.60
1	AA	1368	A	N1-C6-N6	11.42	125.45	118.60
3	AV	33	A	N1-C6-N6	11.42	125.45	118.60
27	B8	1469	A	N1-C6-N6	11.42	125.45	118.60
27	B8	340	A	N1-C6-N6	11.41	125.45	118.60
27	B8	613	A	N1-C6-N6	11.41	125.45	118.60
1	AA	1012	A	N1-C6-N6	11.41	125.45	118.60
27	B8	2020	A	N1-C6-N6	11.41	125.44	118.60
27	B8	526	A	N1-C6-N6	11.41	125.44	118.60
27	B8	781	A	N1-C6-N6	11.41	125.44	118.60
27	B8	2542	A	N1-C6-N6	11.41	125.44	118.60
1	AA	665	A	N1-C6-N6	11.40	125.44	118.60
27	B8	1103	A	N1-C6-N6	11.40	125.44	118.60
27	B8	751	A	N1-C6-N6	11.40	125.44	118.60
27	B8	1165	A	N1-C6-N6	11.40	125.44	118.60
3	AV	74	A	N1-C6-N6	11.40	125.44	118.60
27	B8	1237	A	N1-C6-N6	11.40	125.44	118.60
27	B8	2108	A	N1-C6-N6	11.40	125.44	118.60
26	B7	99	A	N1-C6-N6	11.39	125.44	118.60
27	B8	1142	A	N1-C6-N6	11.39	125.44	118.60
27	B8	1596	A	N1-C6-N6	11.39	125.44	118.60
1	AA	325	A	N1-C6-N6	11.39	125.43	118.60
27	B8	142	A	N1-C6-N6	11.39	125.43	118.60
27	B8	800	A	N1-C6-N6	11.39	125.43	118.60
27	B8	1373	A	N1-C6-N6	11.39	125.43	118.60
27	B8	42	A	N1-C6-N6	11.39	125.43	118.60
26	B7	52	A	N1-C6-N6	11.38	125.43	118.60
27	B8	1786	A	N1-C6-N6	11.38	125.43	118.60
1	AA	1332	A	N1-C6-N6	11.37	125.42	118.60
27	B8	2872	A	N1-C6-N6	11.37	125.42	118.60
26	B7	59	A	N1-C6-N6	11.36	125.42	118.60
27	B8	529	A	N1-C6-N6	11.36	125.42	118.60
27	B8	1494	A	N1-C6-N6	11.36	125.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	222	A	N1-C6-N6	11.35	125.41	118.60
1	AA	1346	A	N1-C6-N6	11.35	125.41	118.60
1	AA	825	A	N1-C6-N6	11.35	125.41	118.60
27	B8	783	A	N1-C6-N6	11.35	125.41	118.60
27	B8	1848	A	N1-C6-N6	11.34	125.41	118.60
27	B8	2425	A	P-O3'-C3'	11.34	133.31	119.70
3	AV	60	A	N1-C6-N6	11.34	125.40	118.60
27	B8	1086	A	N1-C6-N6	11.34	125.40	118.60
27	B8	1111	A	N1-C6-N6	11.34	125.40	118.60
27	B8	541	A	N1-C6-N6	11.33	125.40	118.60
1	AA	864	A	N1-C6-N6	11.33	125.40	118.60
27	B8	2029	G	N1-C6-O6	11.33	126.70	119.90
27	B8	941	A	N1-C6-N6	11.32	125.39	118.60
27	B8	2060	A	N1-C6-N6	11.31	125.39	118.60
27	B8	2451	A	N1-C6-N6	11.31	125.38	118.60
26	B7	73	A	N1-C6-N6	11.30	125.38	118.60
27	B8	2761	A	N1-C6-N6	11.31	125.38	118.60
1	AA	432	A	N1-C6-N6	11.30	125.38	118.60
27	B8	1189	A	N1-C6-N6	11.30	125.38	118.60
27	B8	479	A	N1-C6-N6	11.28	125.37	118.60
27	B8	63	A	N1-C6-N6	11.28	125.37	118.60
27	B8	362	A	N1-C6-N6	11.28	125.37	118.60
1	AA	794	A	N1-C6-N6	11.28	125.37	118.60
27	B8	1088	A	N1-C6-N6	11.28	125.37	118.60
27	B8	621	A	N1-C6-N6	11.27	125.36	118.60
27	B8	1580	A	N1-C6-N6	11.27	125.36	118.60
27	B8	886	A	N1-C6-N6	11.27	125.36	118.60
1	AA	60	A	P-O3'-C3'	11.27	133.22	119.70
27	B8	477	A	N1-C6-N6	11.27	125.36	118.60
1	AA	1362	A	N1-C6-N6	11.27	125.36	118.60
27	B8	574	A	N1-C6-N6	11.27	125.36	118.60
1	AA	1176	A	N1-C6-N6	11.26	125.36	118.60
27	B8	1287	A	N1-C6-N6	11.26	125.36	118.60
27	B8	2543	G	N1-C6-O6	11.26	126.66	119.90
26	B7	15	A	N1-C6-N6	11.26	125.35	118.60
27	B8	94	A	N1-C6-N6	11.26	125.35	118.60
1	AA	60	A	N1-C6-N6	11.25	125.35	118.60
27	B8	2856	A	N1-C6-N6	11.24	125.34	118.60
1	AA	908	A	N1-C6-N6	11.23	125.34	118.60
1	AA	1157	A	N1-C6-N6	11.23	125.34	118.60
1	AA	129	A	N1-C6-N6	11.22	125.33	118.60
1	AA	1150	A	N1-C6-N6	11.22	125.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	324	A	N1-C6-N6	11.22	125.33	118.60
27	B8	1679	A	N1-C6-N6	11.21	125.33	118.60
27	B8	1315	C	P-O3'-C3'	11.21	133.15	119.70
27	B8	1070	A	N1-C6-N6	11.21	125.32	118.60
1	AA	608	A	N1-C6-N6	11.20	125.32	118.60
27	B8	675	A	N1-C6-N6	11.20	125.32	118.60
27	B8	2750	A	N1-C6-N6	11.20	125.32	118.60
1	AA	1055	A	N1-C6-N6	11.19	125.32	118.60
1	AA	274	A	N1-C6-N6	11.18	125.31	118.60
27	B8	2829	A	N1-C6-N6	11.18	125.31	118.60
27	B8	118	A	N1-C6-N6	11.17	125.30	118.60
27	B8	1630	A	N1-C6-N6	11.16	125.30	118.60
1	AA	246	A	N1-C6-N6	11.16	125.30	118.60
27	B8	2564	A	N1-C6-N6	11.16	125.30	118.60
27	B8	1301	A	N1-C6-N6	11.15	125.29	118.60
27	B8	1307	A	N1-C6-N6	11.15	125.29	118.60
27	B8	1028	A	N1-C6-N6	11.15	125.29	118.60
27	B8	1690	A	N1-C6-N6	11.15	125.29	118.60
27	B8	727	A	N1-C6-N6	11.14	125.29	118.60
27	B8	1453	A	N1-C6-N6	11.14	125.29	118.60
1	AA	1206	G	N1-C6-O6	11.14	126.58	119.90
27	B8	2297	A	N1-C6-N6	11.13	125.28	118.60
27	B8	1021	A	N1-C6-N6	11.13	125.28	118.60
1	AA	1329	A	N1-C6-N6	11.13	125.28	118.60
1	AA	179	A	N1-C6-N6	11.12	125.27	118.60
27	B8	2764	A	N1-C6-N6	11.12	125.27	118.60
27	B8	2868	A	N1-C6-N6	11.12	125.27	118.60
27	B8	1853	A	N1-C6-N6	11.11	125.27	118.60
27	B8	2748	A	N1-C6-N6	11.11	125.27	118.60
27	B8	1854	A	N1-C6-N6	11.11	125.26	118.60
1	AA	554	A	N1-C6-N6	11.10	125.26	118.60
27	B8	279	A	N1-C6-N6	11.10	125.26	118.60
27	B8	1780	A	N1-C6-N6	11.10	125.26	118.60
27	B8	2015	A	N1-C6-N6	11.10	125.26	118.60
1	AA	1285	A	N1-C6-N6	11.10	125.26	118.60
27	B8	2119	A	N1-C6-N6	11.09	125.25	118.60
27	B8	1032	A	N1-C6-N6	11.08	125.25	118.60
1	AA	55	A	N1-C6-N6	11.07	125.24	118.60
27	B8	829	A	N1-C6-N6	11.07	125.24	118.60
1	AA	151	A	N1-C6-N6	11.05	125.23	118.60
3	AV	70	G	N1-C6-O6	11.05	126.53	119.90
27	B8	1126	A	N1-C6-N6	11.05	125.23	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1439	A	N1-C6-N6	11.05	125.23	118.60
1	AA	148	G	N1-C6-O6	11.04	126.52	119.90
27	B8	1393	A	N1-C6-N6	11.04	125.22	118.60
1	AA	428	G	N1-C6-O6	11.04	126.52	119.90
1	AA	860	A	N1-C6-N6	11.04	125.22	118.60
1	AA	195	A	N1-C6-N6	11.03	125.22	118.60
27	B8	181	A	N1-C6-N6	11.02	125.21	118.60
27	B8	528	A	N1-C6-N6	11.01	125.21	118.60
1	AA	753	A	N1-C6-N6	11.01	125.21	118.60
27	B8	1872	A	N1-C6-N6	11.01	125.20	118.60
1	AA	171	A	N1-C6-N6	11.01	125.20	118.60
27	B8	1668	A	N1-C6-N6	11.01	125.20	118.60
27	B8	1641	A	N1-C6-N6	11.00	125.20	118.60
27	B8	1652	A	N1-C6-N6	11.00	125.20	118.60
27	B8	2225	A	N1-C6-N6	11.00	125.20	118.60
27	B8	825	A	N1-C6-N6	10.99	125.19	118.60
1	AA	696	A	N1-C6-N6	10.99	125.19	118.60
27	B8	900	A	N1-C6-N6	10.99	125.19	118.60
1	AA	26	A	N1-C6-N6	10.98	125.19	118.60
27	B8	2335	A	N1-C6-N6	10.97	125.18	118.60
1	AA	766	A	N1-C6-N6	10.95	125.17	118.60
1	AA	65	A	N1-C6-N6	10.94	125.16	118.60
27	B8	768	G	N1-C6-O6	10.94	126.46	119.90
27	B8	256	A	N1-C6-N6	10.94	125.16	118.60
27	B8	1803	A	N1-C6-N6	10.94	125.16	118.60
1	AA	533	A	N1-C6-N6	10.93	125.16	118.60
27	B8	1381	G	N1-C6-O6	10.93	126.46	119.90
27	B8	2273	A	N1-C6-N6	10.93	125.16	118.60
26	B7	57	A	N1-C6-N6	10.93	125.16	118.60
1	AA	520	A	N1-C6-N6	10.92	125.15	118.60
27	B8	2366	A	N1-C6-N6	10.92	125.15	118.60
1	AA	22	G	N1-C6-O6	10.90	126.44	119.90
1	AA	109	A	N1-C6-N6	10.90	125.14	118.60
1	AA	116	A	N1-C6-N6	10.90	125.14	118.60
1	AA	1333	A	N1-C6-N6	10.90	125.14	118.60
1	AA	914	A	N1-C6-N6	10.90	125.14	118.60
27	B8	1205	A	N1-C6-N6	10.90	125.14	118.60
27	B8	654	A	N1-C6-N6	10.89	125.14	118.60
27	B8	2435	A	N1-C6-N6	10.89	125.13	118.60
1	AA	76	G	N1-C6-O6	10.88	126.43	119.90
27	B8	1701	A	N1-C6-N6	10.87	125.12	118.60
1	AA	329	A	N1-C6-N6	10.86	125.11	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	933	A	N1-C6-N6	10.86	125.11	118.60
1	AA	301	G	N1-C6-O6	10.85	126.41	119.90
1	AA	509	A	N1-C6-N6	10.85	125.11	118.60
1	AA	1101	A	N1-C6-N6	10.85	125.11	118.60
26	B7	34	A	N1-C6-N6	10.83	125.10	118.60
27	B8	2747	G	N1-C6-O6	10.83	126.40	119.90
27	B8	556	A	N1-C6-N6	10.82	125.09	118.60
1	AA	1005	A	N1-C6-N6	10.81	125.08	118.60
27	B8	2135	A	N1-C6-N6	10.81	125.08	118.60
26	B7	78	A	N1-C6-N6	10.80	125.08	118.60
27	B8	1552	A	N1-C6-N6	10.80	125.08	118.60
27	B8	266	G	N1-C6-O6	10.80	126.38	119.90
27	B8	2014	A	N1-C6-N6	10.79	125.08	118.60
27	B8	559	G	N1-C6-O6	10.79	126.38	119.90
27	B8	990	A	N1-C6-N6	10.79	125.07	118.60
27	B8	670	A	N1-C6-N6	10.79	125.07	118.60
1	AA	487	A	N1-C6-N6	10.78	125.07	118.60
1	AA	1392	G	N1-C6-O6	10.76	126.36	119.90
1	AA	431	A	N1-C6-N6	10.75	125.05	118.60
1	AA	674	G	N1-C6-O6	10.75	126.35	119.90
1	AA	1486	G	N1-C6-O6	10.75	126.35	119.90
1	AA	1034	G	N1-C6-O6	10.74	126.34	119.90
27	B8	2169	A	N1-C6-N6	10.74	125.04	118.60
1	AA	414	A	N1-C6-N6	10.74	125.04	118.60
27	B8	663	G	N1-C6-O6	10.74	126.34	119.90
27	B8	2033	A	N1-C6-N6	10.73	125.04	118.60
27	B8	916	G	N1-C6-O6	10.73	126.34	119.90
27	B8	1445	G	N1-C6-O6	10.72	126.33	119.90
27	B8	161	A	N1-C6-N6	10.71	125.03	118.60
27	B8	374	A	N1-C6-N6	10.71	125.03	118.60
1	AA	184	G	N1-C6-O6	10.71	126.32	119.90
1	AA	718	A	N1-C6-N6	10.71	125.02	118.60
27	B8	1783	A	N1-C6-N6	10.70	125.02	118.60
27	B8	2124	G	N1-C6-O6	10.70	126.32	119.90
1	AA	366	A	P-O3'-C3'	10.69	132.53	119.70
27	B8	505	A	N1-C6-N6	10.69	125.02	118.60
27	B8	2201	G	N1-C6-O6	10.69	126.31	119.90
27	B8	194	G	N1-C6-O6	10.69	126.31	119.90
27	B8	2778	A	N1-C6-N6	10.67	125.00	118.60
1	AA	584	G	N1-C6-O6	10.66	126.30	119.90
1	AA	1319	A	N1-C6-N6	10.66	125.00	118.60
27	B8	1885	A	N1-C6-N6	10.66	125.00	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	353	A	N1-C6-N6	10.63	124.98	118.60
27	B8	1717	A	N1-C6-N6	10.63	124.98	118.60
27	B8	2469	A	N1-C6-N6	10.63	124.98	118.60
27	B8	2298	A	N1-C6-N6	10.62	124.97	118.60
27	B8	1378	A	N1-C6-N6	10.62	124.97	118.60
27	B8	1975	G	N1-C6-O6	10.62	126.27	119.90
27	B8	2903	U	O4'-C1'-N1	10.61	116.69	108.20
27	B8	248	G	N1-C6-O6	10.61	126.26	119.90
27	B8	616	A	N1-C6-N6	10.59	124.96	118.60
1	AA	258	G	N1-C6-O6	10.59	126.25	119.90
1	AA	1275	A	N1-C6-N6	10.58	124.95	118.60
27	B8	1907	G	N1-C6-O6	10.58	126.25	119.90
27	B8	2234	G	N1-C6-O6	10.58	126.25	119.90
1	AA	168	G	N1-C6-O6	10.57	126.24	119.90
1	AA	484	G	N1-C6-O6	10.56	126.23	119.90
27	B8	820	A	N1-C6-N6	10.56	124.93	118.60
27	B8	2212	A	N1-C6-N6	10.55	124.93	118.60
1	AA	1289	A	N1-C6-N6	10.55	124.93	118.60
1	AA	1290	G	N1-C6-O6	10.55	126.23	119.90
27	B8	2052	A	N1-C6-N6	10.55	124.93	118.60
1	AA	973	G	N1-C6-O6	10.55	126.23	119.90
27	B8	2268	A	N1-C6-N6	10.54	124.92	118.60
27	B8	1522	A	N1-C6-N6	10.53	124.92	118.60
1	AA	687	A	N1-C6-N6	10.53	124.92	118.60
27	B8	1001	A	N1-C6-N6	10.52	124.91	118.60
27	B8	2054	A	N1-C6-N6	10.52	124.91	118.60
27	B8	2535	G	N1-C6-O6	10.52	126.21	119.90
27	B8	2485	G	N1-C6-O6	10.51	126.21	119.90
1	AA	1435	G	N1-C6-O6	10.49	126.19	119.90
27	B8	2392	A	N1-C6-N6	10.49	124.89	118.60
1	AA	782	A	N1-C6-N6	10.48	124.89	118.60
27	B8	103	A	N1-C6-N6	10.48	124.89	118.60
27	B8	2447	G	N1-C6-O6	10.48	126.19	119.90
1	AA	99	C	O4'-C1'-N1	10.48	116.58	108.20
1	AA	570	G	N1-C6-O6	10.48	126.19	119.90
27	B8	350	G	N1-C6-O6	10.48	126.19	119.90
27	B8	2024	G	N1-C6-O6	10.48	126.19	119.90
1	AA	417	G	N1-C6-O6	10.47	126.19	119.90
27	B8	2587	A	N1-C6-N6	10.47	124.88	118.60
27	B8	2673	G	N1-C6-O6	10.47	126.18	119.90
27	B8	1342	A	N1-C6-N6	10.47	124.88	118.60
27	B8	514	A	N1-C6-N6	10.46	124.88	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2741	A	N1-C6-N6	10.46	124.88	118.60
27	B8	1553	A	N1-C6-N6	10.46	124.88	118.60
27	B8	2027	G	N1-C6-O6	10.46	126.17	119.90
1	AA	275	G	N1-C6-O6	10.45	126.17	119.90
27	B8	1106	G	N1-C6-O6	10.45	126.17	119.90
27	B8	954	G	N1-C6-O6	10.45	126.17	119.90
27	B8	2624	G	N1-C6-O6	10.45	126.17	119.90
27	B8	346	A	N1-C6-N6	10.44	124.86	118.60
27	B8	2895	G	N1-C6-O6	10.43	126.16	119.90
1	AA	1033	G	N1-C6-O6	10.43	126.16	119.90
1	AA	1441	A	N1-C6-N6	10.43	124.86	118.60
1	AA	541	G	N1-C6-O6	10.42	126.15	119.90
27	B8	2227	A	N1-C6-N6	10.41	124.84	118.60
1	AA	1184	G	N1-C6-O6	10.40	126.14	119.90
27	B8	409	G	N1-C6-O6	10.40	126.14	119.90
27	B8	609	A	N1-C6-N6	10.40	124.84	118.60
1	AA	669	G	N1-C6-O6	10.39	126.13	119.90
27	B8	2279	G	N1-C6-O6	10.39	126.13	119.90
27	B8	424	G	N1-C6-O6	10.38	126.13	119.90
27	B8	538	A	N1-C6-N6	10.38	124.83	118.60
1	AA	454	G	N1-C6-O6	10.38	126.13	119.90
1	AA	259	G	N1-C6-O6	10.37	126.12	119.90
27	B8	2421	G	N1-C6-O6	10.37	126.12	119.90
26	B7	112	G	N1-C6-O6	10.36	126.12	119.90
27	B8	428	A	N1-C6-N6	10.36	124.82	118.60
1	AA	1191	A	N1-C6-N6	10.35	124.81	118.60
27	B8	1268	A	N1-C6-N6	10.35	124.81	118.60
1	AA	145	G	N1-C6-O6	10.34	126.11	119.90
27	B8	2304	G	N1-C6-O6	10.33	126.10	119.90
1	AA	457	G	N1-C6-O6	10.31	126.09	119.90
27	B8	757	G	N1-C6-O6	10.31	126.09	119.90
1	AA	616	G	N1-C6-O6	10.30	126.08	119.90
1	AA	1020	G	N1-C6-O6	10.30	126.08	119.90
27	B8	1743	G	N1-C6-O6	10.29	126.07	119.90
1	AA	1523	G	N1-C6-O6	10.28	126.07	119.90
27	B8	1422	G	N1-C6-O6	10.26	126.06	119.90
1	AA	778	G	N1-C6-O6	10.24	126.05	119.90
1	AA	1058	G	N1-C6-O6	10.24	126.05	119.90
1	AA	359	G	N1-C6-O6	10.24	126.04	119.90
27	B8	442	G	N1-C6-O6	10.24	126.04	119.90
1	AA	104	G	N1-C6-O6	10.23	126.04	119.90
27	B8	460	A	N1-C6-N6	10.23	124.74	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	628	G	N1-C6-O6	10.23	126.04	119.90
27	B8	1937	A	N1-C6-N6	10.23	124.74	118.60
1	AA	122	G	N1-C6-O6	10.22	126.03	119.90
27	B8	676	A	N1-C6-N6	10.22	124.73	118.60
26	B7	81	G	N1-C6-O6	10.21	126.03	119.90
27	B8	978	G	N1-C6-O6	10.21	126.03	119.90
1	AA	15	G	N1-C6-O6	10.21	126.03	119.90
1	AA	626	G	N1-C6-O6	10.21	126.03	119.90
27	B8	1492	G	N1-C6-O6	10.21	126.03	119.90
1	AA	1433	A	N1-C6-N6	10.19	124.72	118.60
27	B8	2363	G	N1-C6-O6	10.19	126.02	119.90
27	B8	1689	A	N1-C6-N6	10.19	124.71	118.60
1	AA	372	C	P-O3'-C3'	10.18	131.92	119.70
1	AA	1201	A	P-O3'-C3'	10.18	131.92	119.70
27	B8	735	A	N1-C6-N6	10.18	124.71	118.60
27	B8	1098	A	N1-C6-N6	10.18	124.70	118.60
27	B8	2601	C	P-O3'-C3'	10.18	131.91	119.70
27	B8	1785	A	N1-C6-N6	10.16	124.70	118.60
27	B8	1076	C	O4'-C1'-N1	10.15	116.32	108.20
27	B8	1627	G	N1-C6-O6	10.15	125.99	119.90
27	B8	2046	G	N1-C6-O6	10.15	125.99	119.90
27	B8	401	A	N1-C6-N6	10.15	124.69	118.60
27	B8	1655	A	N1-C6-N6	10.15	124.69	118.60
27	B8	2057	G	N1-C6-O6	10.15	125.99	119.90
27	B8	2714	G	N1-C6-O6	10.14	125.98	119.90
27	B8	244	A	N1-C6-N6	10.14	124.68	118.60
1	AA	164	G	N1-C6-O6	10.12	125.97	119.90
1	AA	1405	G	N1-C6-O6	10.12	125.97	119.90
27	B8	1157	G	N1-C6-O6	10.12	125.97	119.90
27	B8	2639	A	N1-C6-N6	10.12	124.67	118.60
1	AA	147	G	N1-C6-O6	10.12	125.97	119.90
27	B8	1649	G	N1-C6-O6	10.12	125.97	119.90
1	AA	933	G	N1-C6-O6	10.12	125.97	119.90
27	B8	501	A	N1-C6-N6	10.11	124.67	118.60
1	AA	601	G	N1-C6-O6	10.11	125.96	119.90
27	B8	784	G	N1-C6-O6	10.11	125.96	119.90
1	AA	1284	C	P-O3'-C3'	10.11	131.83	119.70
27	B8	1826	G	N1-C6-O6	10.11	125.96	119.90
1	AA	1048	G	N1-C6-O6	10.10	125.96	119.90
1	AA	424	G	N1-C6-O6	10.09	125.95	119.90
27	B8	2648	G	N1-C6-O6	10.09	125.95	119.90
1	AA	1338	G	O4'-C1'-N9	10.09	116.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2544	G	N1-C6-O6	10.08	125.95	119.90
27	B8	2692	G	N1-C6-O6	10.08	125.95	119.90
1	AA	627	G	N1-C6-O6	10.08	125.95	119.90
1	AA	1455	G	N1-C6-O6	10.07	125.94	119.90
27	B8	1059	G	N1-C6-O6	10.07	125.94	119.90
27	B8	524	G	N1-C6-O6	10.07	125.94	119.90
1	AA	1006	G	N1-C6-O6	10.07	125.94	119.90
1	AA	279	A	P-O3'-C3'	10.06	131.78	119.70
27	B8	1038	G	N1-C6-O6	10.06	125.94	119.90
1	AA	1072	G	N1-C6-O6	10.05	125.93	119.90
27	B8	108	G	N1-C6-O6	10.05	125.93	119.90
27	B8	2409	G	N1-C6-O6	10.05	125.93	119.90
1	AA	413	G	N1-C6-O6	10.04	125.92	119.90
27	B8	701	G	N1-C6-O6	10.04	125.92	119.90
27	B8	1479	G	N1-C6-O6	10.04	125.92	119.90
27	B8	2839	G	N1-C6-O6	10.04	125.92	119.90
27	B8	496	G	N1-C6-O6	10.03	125.92	119.90
27	B8	1338	G	N1-C6-O6	10.03	125.92	119.90
27	B8	141	G	N1-C6-O6	10.03	125.92	119.90
27	B8	533	G	N1-C6-O6	10.03	125.92	119.90
1	AA	786	G	N1-C6-O6	10.03	125.92	119.90
1	AA	724	G	N1-C6-O6	10.03	125.92	119.90
27	B8	864	G	N1-C6-O6	10.03	125.92	119.90
27	B8	1421	G	N1-C6-O6	10.03	125.92	119.90
27	B8	2400	G	N1-C6-O6	10.03	125.92	119.90
1	AA	667	G	N1-C6-O6	10.02	125.91	119.90
27	B8	471	A	N1-C6-N6	10.02	124.61	118.60
27	B8	777	G	N1-C6-O6	10.02	125.91	119.90
27	B8	2819	G	N1-C6-O6	10.02	125.91	119.90
27	B8	953	G	N1-C6-O6	10.02	125.91	119.90
27	B8	2478	A	N1-C6-N6	10.02	124.61	118.60
1	AA	1497	G	N1-C6-O6	10.01	125.91	119.90
27	B8	699	A	N1-C6-N6	10.01	124.61	118.60
1	AA	450	G	N1-C6-O6	10.01	125.90	119.90
27	B8	2472	G	N1-C6-O6	10.01	125.90	119.90
26	B7	45	A	N1-C6-N6	10.00	124.60	118.60
27	B8	371	A	N1-C6-N6	10.00	124.60	118.60
27	B8	2056	G	N1-C6-O6	10.00	125.90	119.90
1	AA	302	G	N1-C6-O6	9.99	125.89	119.90
27	B8	412	A	N1-C6-N6	9.98	124.59	118.60
27	B8	2894	G	N1-C6-O6	9.98	125.89	119.90
27	B8	1901	A	N1-C6-N6	9.98	124.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B7	54	G	N1-C6-O6	9.97	125.89	119.90
1	AA	75	G	N1-C6-O6	9.97	125.88	119.90
27	B8	662	G	N1-C6-O6	9.97	125.88	119.90
1	AA	849	G	N1-C6-O6	9.96	125.88	119.90
1	AA	889	A	N1-C6-N6	9.96	124.58	118.60
27	B8	81	G	N1-C6-O6	9.96	125.88	119.90
27	B8	2694	G	N1-C6-O6	9.96	125.88	119.90
27	B8	2147	A	P-O3'-C3'	9.96	131.65	119.70
27	B8	273	G	N1-C6-O6	9.96	125.87	119.90
1	AA	642	A	N1-C6-N6	9.96	124.57	118.60
1	AA	1323	G	N1-C6-O6	9.96	125.87	119.90
1	AA	951	G	N1-C6-O6	9.95	125.87	119.90
27	B8	1389	G	N1-C6-O6	9.95	125.87	119.90
1	AA	521	G	N1-C6-O6	9.95	125.87	119.90
27	B8	1465	G	N1-C6-O6	9.95	125.87	119.90
27	B8	1154	G	N1-C6-O6	9.95	125.87	119.90
27	B8	2414	G	N1-C6-O6	9.95	125.87	119.90
1	AA	138	G	N1-C6-O6	9.94	125.87	119.90
27	B8	1232	G	N1-C6-O6	9.94	125.87	119.90
27	B8	1515	A	O4'-C1'-N9	9.94	116.16	108.20
27	B8	1215	G	N1-C6-O6	9.94	125.87	119.90
1	AA	200	G	N1-C6-O6	9.94	125.86	119.90
26	B7	33	G	N1-C6-O6	9.94	125.86	119.90
26	B7	15	A	O4'-C1'-N9	9.94	116.15	108.20
1	AA	105	G	N1-C6-O6	9.94	125.86	119.90
1	AA	685	G	N1-C6-O6	9.92	125.86	119.90
27	B8	1815	A	N1-C6-N6	9.92	124.55	118.60
27	B8	2012	G	N1-C6-O6	9.92	125.85	119.90
27	B8	9	G	N1-C6-O6	9.92	125.85	119.90
27	B8	1896	G	N1-C6-O6	9.92	125.85	119.90
1	AA	279	A	N1-C6-N6	9.91	124.55	118.60
27	B8	1540	G	N1-C6-O6	9.91	125.85	119.90
27	B8	86	G	N1-C6-O6	9.91	125.84	119.90
1	AA	1133	G	N1-C6-O6	9.91	125.84	119.90
27	B8	2623	G	N1-C6-O6	9.91	125.84	119.90
27	B8	2583	G	N1-C6-O6	9.90	125.84	119.90
27	B8	2621	G	N1-C6-O6	9.90	125.84	119.90
27	B8	2383	G	N1-C6-O6	9.90	125.84	119.90
27	B8	520	G	N1-C6-O6	9.90	125.84	119.90
1	AA	39	G	N1-C6-O6	9.90	125.84	119.90
1	AA	1061	G	N1-C6-O6	9.90	125.84	119.90
27	B8	2803	G	N1-C6-O6	9.90	125.84	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	949	G	N1-C6-O6	9.89	125.84	119.90
27	B8	454	A	N1-C6-N6	9.89	124.54	118.60
27	B8	1182	G	N1-C6-O6	9.89	125.83	119.90
27	B8	2757	A	N1-C6-N6	9.89	124.53	118.60
1	AA	1164	G	N1-C6-O6	9.89	125.83	119.90
27	B8	875	G	N1-C6-O6	9.89	125.83	119.90
1	AA	57	G	N1-C6-O6	9.88	125.83	119.90
27	B8	659	G	N1-C6-O6	9.88	125.83	119.90
27	B8	2445	G	N1-C6-O6	9.88	125.83	119.90
26	B7	9	G	N1-C6-O6	9.88	125.83	119.90
27	B8	1435	G	N1-C6-O6	9.88	125.83	119.90
1	AA	838	G	N1-C6-O6	9.87	125.82	119.90
1	AA	711	G	N1-C6-O6	9.87	125.82	119.90
27	B8	2053	G	N1-C6-O6	9.87	125.82	119.90
27	B8	2574	G	N1-C6-O6	9.87	125.82	119.90
27	B8	2437	G	N1-C6-O6	9.87	125.82	119.90
27	B8	2140	G	N1-C6-O6	9.86	125.82	119.90
1	AA	812	G	N1-C6-O6	9.86	125.82	119.90
27	B8	291	G	N1-C6-O6	9.86	125.82	119.90
27	B8	1517	G	N1-C6-O6	9.86	125.82	119.90
27	B8	617	G	N1-C6-O6	9.86	125.82	119.90
1	AA	373	A	N1-C6-N6	9.86	124.51	118.60
27	B8	2709	G	N1-C6-O6	9.85	125.81	119.90
1	AA	617	G	N1-C6-O6	9.85	125.81	119.90
1	AA	1233	G	N1-C6-O6	9.85	125.81	119.90
1	AA	27	G	N1-C6-O6	9.85	125.81	119.90
1	AA	785	G	N1-C6-O6	9.85	125.81	119.90
27	B8	1034	G	N1-C6-O6	9.84	125.81	119.90
27	B8	1973	G	N1-C6-O6	9.84	125.81	119.90
1	AA	240	G	N1-C6-O6	9.84	125.81	119.90
1	AA	645	G	N1-C6-O6	9.84	125.80	119.90
1	AA	917	G	N1-C6-O6	9.84	125.80	119.90
27	B8	230	G	N1-C6-O6	9.83	125.80	119.90
27	B8	312	G	N1-C6-O6	9.83	125.80	119.90
27	B8	649	G	N1-C6-O6	9.83	125.80	119.90
1	AA	1419	G	N1-C6-O6	9.83	125.80	119.90
27	B8	2217	G	N1-C6-O6	9.83	125.80	119.90
27	B8	2702	G	N1-C6-O6	9.83	125.80	119.90
27	B8	1424	G	N1-C6-O6	9.82	125.80	119.90
27	B8	2631	G	N1-C6-O6	9.82	125.79	119.90
27	B8	483	A	N1-C6-N6	9.82	124.49	118.60
1	AA	117	G	N1-C6-O6	9.82	125.79	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	448	A	N1-C6-N6	9.82	124.49	118.60
27	B8	729	G	N1-C6-O6	9.82	125.79	119.90
1	AA	61	G	N1-C6-O6	9.81	125.79	119.90
27	B8	682	G	N1-C6-O6	9.81	125.79	119.90
27	B8	1193	G	N1-C6-O6	9.81	125.79	119.90
1	AA	115	G	N1-C6-O6	9.81	125.78	119.90
1	AA	1300	G	N1-C6-O6	9.81	125.78	119.90
27	B8	1809	A	N1-C6-N6	9.81	124.48	118.60
1	AA	1457	G	N1-C6-O6	9.81	125.78	119.90
27	B8	1538	G	N1-C6-O6	9.81	125.78	119.90
27	B8	1418	G	N1-C6-O6	9.80	125.78	119.90
27	B8	1797	G	N1-C6-O6	9.80	125.78	119.90
27	B8	2657	A	N1-C6-N6	9.80	124.48	118.60
27	B8	2221	G	N1-C6-O6	9.79	125.78	119.90
27	B8	1643	G	N1-C6-O6	9.79	125.78	119.90
1	AA	954	G	N1-C6-O6	9.79	125.77	119.90
26	B7	21	G	N1-C6-O6	9.78	125.77	119.90
27	B8	2722	G	N1-C6-O6	9.78	125.77	119.90
1	AA	45	G	N1-C6-O6	9.78	125.77	119.90
1	AA	1334	G	N1-C6-O6	9.78	125.77	119.90
27	B8	2093	G	N1-C6-O6	9.78	125.77	119.90
1	AA	1261	A	N1-C6-N6	9.77	124.46	118.60
27	B8	977	G	N1-C6-O6	9.77	125.76	119.90
27	B8	809	G	N1-C6-O6	9.77	125.76	119.90
27	B8	2654	A	N1-C6-N6	9.77	124.46	118.60
1	AA	1034	G	C5-C6-O6	-9.77	122.74	128.60
27	B8	2136	G	N1-C6-O6	9.77	125.76	119.90
1	AA	1511	G	N1-C6-O6	9.76	125.76	119.90
27	B8	123	G	N1-C6-O6	9.76	125.76	119.90
27	B8	2141	G	N1-C6-O6	9.76	125.76	119.90
27	B8	1239	G	N1-C6-O6	9.76	125.76	119.90
1	AA	1385	G	N1-C6-O6	9.76	125.75	119.90
27	B8	407	G	N1-C6-O6	9.76	125.75	119.90
1	AA	1193	G	N1-C6-O6	9.76	125.75	119.90
27	B8	400	G	N1-C6-O6	9.75	125.75	119.90
27	B8	2069	G	N1-C6-O6	9.75	125.75	119.90
27	B8	2123	G	N1-C6-O6	9.75	125.75	119.90
26	B7	10	G	N1-C6-O6	9.75	125.75	119.90
27	B8	1734	G	N1-C6-O6	9.75	125.75	119.90
27	B8	1218	G	N1-C6-O6	9.75	125.75	119.90
26	B7	86	G	N1-C6-O6	9.74	125.75	119.90
27	B8	1478	G	N1-C6-O6	9.74	125.75	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2812	G	N1-C6-O6	9.74	125.75	119.90
27	B8	1099	G	N1-C6-O6	9.74	125.74	119.90
27	B8	1191	G	N1-C6-O6	9.74	125.74	119.90
1	AA	455	G	N1-C6-O6	9.74	125.74	119.90
27	B8	326	G	N1-C6-O6	9.74	125.74	119.90
1	AA	1220	G	N1-C6-O6	9.73	125.74	119.90
27	B8	2315	G	N1-C6-O6	9.73	125.74	119.90
1	AA	1423	G	N1-C6-O6	9.73	125.74	119.90
1	AA	402	G	N1-C6-O6	9.73	125.74	119.90
27	B8	260	G	N1-C6-O6	9.73	125.74	119.90
27	B8	1055	G	N1-C6-O6	9.73	125.74	119.90
1	AA	497	G	N1-C6-O6	9.73	125.74	119.90
26	B7	106	G	N1-C6-O6	9.73	125.74	119.90
27	B8	1107	G	N1-C6-O6	9.73	125.74	119.90
1	AA	668	G	N1-C6-O6	9.72	125.73	119.90
27	B8	1308	A	N1-C6-N6	9.72	124.43	118.60
1	AA	1353	G	N1-C6-O6	9.72	125.73	119.90
27	B8	1016	G	N1-C6-O6	9.72	125.73	119.90
27	B8	1682	G	N1-C6-O6	9.72	125.73	119.90
1	AA	142	G	N1-C6-O6	9.71	125.73	119.90
27	B8	285	G	N1-C6-O6	9.71	125.73	119.90
1	AA	734	G	N1-C6-O6	9.71	125.73	119.90
27	B8	1546	G	N1-C6-O6	9.71	125.73	119.90
27	B8	1964	G	N1-C6-O6	9.71	125.73	119.90
1	AA	318	G	N1-C6-O6	9.71	125.73	119.90
27	B8	2718	G	N1-C6-O6	9.71	125.73	119.90
27	B8	2557	G	N1-C6-O6	9.71	125.72	119.90
27	B8	2801	G	N1-C6-O6	9.71	125.72	119.90
27	B8	410	G	N1-C6-O6	9.71	125.72	119.90
1	AA	449	G	C5-C6-O6	-9.70	122.78	128.60
27	B8	2556	C	O4'-C1'-N1	9.70	115.96	108.20
1	AA	1349	A	N1-C6-N6	9.70	124.42	118.60
1	AA	755	G	N1-C6-O6	9.69	125.72	119.90
1	AA	1288	A	N1-C6-N6	9.70	124.42	118.60
27	B8	287	G	N1-C6-O6	9.70	125.72	119.90
27	B8	2630	G	N1-C6-O6	9.69	125.71	119.90
1	AA	293	G	N1-C6-O6	9.69	125.71	119.90
1	AA	416	G	N1-C6-O6	9.69	125.71	119.90
27	B8	1560	G	N1-C6-O6	9.69	125.71	119.90
27	B8	2640	G	N1-C6-O6	9.69	125.71	119.90
27	B8	2685	G	N1-C6-O6	9.69	125.71	119.90
27	B8	2592	G	N1-C6-O6	9.68	125.71	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1422	G	N1-C6-O6	9.68	125.71	119.90
27	B8	760	G	N1-C6-O6	9.68	125.71	119.90
27	B8	425	G	N1-C6-O6	9.68	125.70	119.90
1	AA	1030	U	O4'-C1'-N1	9.67	115.94	108.20
1	AA	9	G	N1-C6-O6	9.66	125.70	119.90
27	B8	185	G	N1-C6-O6	9.66	125.70	119.90
27	B8	1932	A	N1-C6-N6	9.66	124.40	118.60
27	B8	939	G	N1-C6-O6	9.66	125.70	119.90
27	B8	2508	G	N1-C6-O6	9.66	125.70	119.90
27	B8	1190	G	N1-C6-O6	9.66	125.69	119.90
27	B8	1206	G	N1-C6-O6	9.66	125.69	119.90
27	B8	2115	G	N1-C6-O6	9.66	125.69	119.90
27	B8	2484	G	N1-C6-O6	9.66	125.69	119.90
27	B8	2498	C	O4'-C1'-N1	9.66	115.92	108.20
1	AA	1343	G	N1-C6-O6	9.65	125.69	119.90
27	B8	2040	G	N1-C6-O6	9.65	125.69	119.90
1	AA	1050	G	N1-C6-O6	9.65	125.69	119.90
1	AA	1373	G	N1-C6-O6	9.65	125.69	119.90
1	AA	639	G	N1-C6-O6	9.65	125.69	119.90
27	B8	220	G	N1-C6-O6	9.65	125.69	119.90
27	B8	2208	C	O4'-C1'-N1	9.64	115.92	108.20
27	B8	579	G	N1-C6-O6	9.64	125.68	119.90
27	B8	1792	G	N1-C6-O6	9.64	125.68	119.90
26	B7	66	A	P-O3'-C3'	9.63	131.26	119.70
27	B8	1948	G	N1-C6-O6	9.63	125.68	119.90
1	AA	319	G	N1-C6-O6	9.63	125.68	119.90
1	AA	1154	G	N1-C6-O6	9.63	125.68	119.90
27	B8	759	G	N1-C6-O6	9.63	125.68	119.90
1	AA	1087	G	N1-C6-O6	9.63	125.68	119.90
27	B8	377	G	N1-C6-O6	9.63	125.68	119.90
27	B8	836	G	N1-C6-O6	9.63	125.68	119.90
1	AA	802	A	N1-C6-N6	9.63	124.38	118.60
1	AA	851	G	C5-C6-O6	-9.63	122.83	128.60
27	B8	2323	G	N1-C6-O6	9.62	125.67	119.90
27	B8	2419	U	O4'-C1'-N1	9.62	115.90	108.20
1	AA	1515	G	N1-C6-O6	9.61	125.67	119.90
1	AA	714	G	N1-C6-O6	9.61	125.67	119.90
1	AA	945	G	N1-C6-O6	9.61	125.67	119.90
27	B8	1138	G	N1-C6-O6	9.61	125.67	119.90
1	AA	861	G	N1-C6-O6	9.61	125.66	119.90
1	AA	894	G	N1-C6-O6	9.61	125.66	119.90
1	AA	1041	G	N1-C6-O6	9.61	125.66	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	107	G	N1-C6-O6	9.61	125.66	119.90
27	B8	1482	G	N1-C6-O6	9.61	125.66	119.90
27	B8	2209	G	N1-C6-O6	9.61	125.66	119.90
27	B8	2235	G	N1-C6-O6	9.61	125.66	119.90
27	B8	2570	G	N1-C6-O6	9.61	125.66	119.90
27	B8	1037	G	N1-C6-O6	9.60	125.66	119.90
27	B8	402	A	N1-C6-N6	9.60	124.36	118.60
27	B8	1163	G	N1-C6-O6	9.60	125.66	119.90
27	B8	1214	A	N1-C6-N6	9.60	124.36	118.60
1	AA	1143	G	N1-C6-O6	9.60	125.66	119.90
27	B8	2128	G	N1-C6-O6	9.60	125.66	119.90
1	AA	227	G	N1-C6-O6	9.60	125.66	119.90
27	B8	186	G	N1-C6-O6	9.59	125.66	119.90
27	B8	797	G	N1-C6-O6	9.59	125.66	119.90
27	B8	1698	A	N1-C6-N6	9.59	124.36	118.60
27	B8	2330	G	N1-C6-O6	9.59	125.66	119.90
1	AA	428	G	C5-C6-O6	-9.59	122.85	128.60
26	B7	23	G	N1-C6-O6	9.59	125.65	119.90
27	B8	363	G	N1-C6-O6	9.59	125.65	119.90
1	AA	939	G	N1-C6-O6	9.59	125.65	119.90
27	B8	1296	G	N1-C6-O6	9.59	125.65	119.90
27	B8	1511	G	N1-C6-O6	9.59	125.65	119.90
1	AA	148	G	C5-C6-O6	-9.58	122.85	128.60
1	AA	877	G	N1-C6-O6	9.58	125.65	119.90
27	B8	798	G	N1-C6-O6	9.58	125.65	119.90
27	B8	1306	C	O4'-C1'-N1	9.58	115.86	108.20
27	B8	2599	G	N1-C6-O6	9.58	125.65	119.90
27	B8	2603	G	N1-C6-O6	9.58	125.65	119.90
1	AA	763	G	N1-C6-O6	9.57	125.64	119.90
3	AV	3	G	N1-C6-O6	9.57	125.64	119.90
27	B8	924	G	N1-C6-O6	9.57	125.64	119.90
27	B8	1660	G	N1-C6-O6	9.57	125.64	119.90
27	B8	1162	G	N1-C6-O6	9.57	125.64	119.90
27	B8	1124	G	N1-C6-O6	9.57	125.64	119.90
27	B8	2487	G	N1-C6-O6	9.57	125.64	119.90
27	B8	1845	G	N1-C6-O6	9.57	125.64	119.90
27	B8	1238	G	N1-C6-O6	9.56	125.64	119.90
1	AA	1221	G	N1-C6-O6	9.56	125.64	119.90
27	B8	1309	G	N1-C6-O6	9.56	125.64	119.90
27	B8	2399	G	N1-C6-O6	9.56	125.64	119.90
27	B8	70	G	N1-C6-O6	9.56	125.64	119.90
27	B8	396	G	N1-C6-O6	9.56	125.63	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1949	G	N1-C6-O6	9.56	125.64	119.90
1	AA	377	G	N1-C6-O6	9.55	125.63	119.90
27	B8	207	A	N1-C6-N6	9.55	124.33	118.60
27	B8	605	G	N1-C6-O6	9.55	125.63	119.90
27	B8	1545	A	N1-C6-N6	9.55	124.33	118.60
27	B8	1642	G	N1-C6-O6	9.55	125.63	119.90
27	B8	2664	G	C5-C6-O6	-9.55	122.87	128.60
27	B8	938	G	N1-C6-O6	9.55	125.63	119.90
27	B8	2588	G	N1-C6-O6	9.55	125.63	119.90
1	AA	1454	G	N1-C6-O6	9.54	125.63	119.90
1	AA	1494	G	N1-C6-O6	9.55	125.63	119.90
27	B8	122	G	N1-C6-O6	9.55	125.63	119.90
27	B8	1799	G	N1-C6-O6	9.55	125.63	119.90
27	B8	252	G	N1-C6-O6	9.54	125.63	119.90
27	B8	536	G	N1-C6-O6	9.54	125.63	119.90
1	AA	867	G	N1-C6-O6	9.54	125.62	119.90
27	B8	1510	G	C5-C6-O6	-9.54	122.88	128.60
1	AA	113	G	N1-C6-O6	9.54	125.62	119.90
27	B8	799	G	N1-C6-O6	9.54	125.62	119.90
27	B8	1179	G	N1-C6-O6	9.54	125.62	119.90
27	B8	1992	G	N1-C6-O6	9.54	125.62	119.90
27	B8	2641	G	N1-C6-O6	9.54	125.62	119.90
27	B8	550	C	O4'-C1'-N1	9.53	115.83	108.20
27	B8	976	G	N1-C6-O6	9.53	125.62	119.90
27	B8	1455	G	N1-C6-O6	9.53	125.62	119.90
27	B8	1651	G	N1-C6-O6	9.53	125.62	119.90
27	B8	2102	G	N1-C6-O6	9.53	125.62	119.90
27	B8	1093	G	N1-C6-O6	9.53	125.62	119.90
27	B8	1840	G	N1-C6-O6	9.53	125.62	119.90
27	B8	2464	G	N1-C6-O6	9.53	125.62	119.90
27	B8	2486	C	O4'-C1'-N1	9.53	115.82	108.20
27	B8	989	G	N1-C6-O6	9.52	125.61	119.90
27	B8	1137	G	N1-C6-O6	9.52	125.61	119.90
27	B8	2545	G	N1-C6-O6	9.52	125.61	119.90
1	AA	874	G	N1-C6-O6	9.52	125.61	119.90
27	B8	2677	G	N1-C6-O6	9.52	125.61	119.90
27	B8	1245	G	N1-C6-O6	9.51	125.61	119.90
1	AA	592	G	N1-C6-O6	9.51	125.61	119.90
27	B8	543	G	N1-C6-O6	9.51	125.61	119.90
27	B8	2643	G	N1-C6-O6	9.51	125.61	119.90
1	AA	892	A	N1-C6-N6	9.51	124.31	118.60
27	B8	1259	G	N1-C6-O6	9.51	125.61	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1292	G	N1-C6-O6	9.51	125.60	119.90
27	B8	2204	G	N1-C6-O6	9.51	125.60	119.90
27	B8	1954	G	N1-C6-O6	9.50	125.60	119.90
27	B8	212	G	N1-C6-O6	9.50	125.60	119.90
27	B8	1891	G	N1-C6-O6	9.50	125.60	119.90
1	AA	401	C	O4'-C1'-N1	9.50	115.80	108.20
1	AA	577	G	N1-C6-O6	9.50	125.60	119.90
27	B8	778	G	N1-C6-O6	9.50	125.60	119.90
27	B8	1659	G	N1-C6-O6	9.50	125.60	119.90
1	AA	725	G	N1-C6-O6	9.49	125.59	119.90
27	B8	1351	C	O4'-C1'-N1	9.49	115.79	108.20
1	AA	824	G	N1-C6-O6	9.49	125.59	119.90
1	AA	1174	G	N1-C6-O6	9.49	125.59	119.90
27	B8	2410	G	N1-C6-O6	9.49	125.59	119.90
27	B8	2674	G	N1-C6-O6	9.49	125.59	119.90
1	AA	779	C	O4'-C1'-N1	9.49	115.79	108.20
1	AA	846	G	N1-C6-O6	9.49	125.59	119.90
27	B8	121	G	N1-C6-O6	9.49	125.59	119.90
27	B8	2029	G	C5-C6-O6	-9.49	122.91	128.60
27	B8	1310	G	N1-C6-O6	9.49	125.59	119.90
1	AA	1310	G	N1-C6-O6	9.48	125.59	119.90
27	B8	408	G	N1-C6-O6	9.48	125.59	119.90
27	B8	1155	A	N1-C6-N6	9.48	124.29	118.60
27	B8	1707	G	N1-C6-O6	9.48	125.59	119.90
27	B8	245	G	N1-C6-O6	9.47	125.58	119.90
27	B8	1661	G	N1-C6-O6	9.47	125.58	119.90
1	AA	500	G	N1-C6-O6	9.47	125.58	119.90
27	B8	821	A	N1-C6-N6	9.47	124.28	118.60
27	B8	962	G	N1-C6-O6	9.47	125.58	119.90
27	B8	1906	G	N1-C6-O6	9.47	125.58	119.90
27	B8	2341	G	N1-C6-O6	9.47	125.58	119.90
1	AA	1127	G	N1-C6-O6	9.47	125.58	119.90
1	AA	198	G	N1-C6-O6	9.46	125.58	119.90
27	B8	77	G	N1-C6-O6	9.46	125.58	119.90
27	B8	2509	G	N1-C6-O6	9.46	125.58	119.90
27	B8	2716	C	O4'-C1'-N1	9.46	115.77	108.20
1	AA	615	G	N1-C6-O6	9.46	125.58	119.90
27	B8	1041	G	N1-C6-O6	9.46	125.58	119.90
27	B8	2078	C	O4'-C1'-N1	9.46	115.77	108.20
26	B7	83	G	N1-C6-O6	9.46	125.57	119.90
27	B8	2413	G	N1-C6-O6	9.46	125.57	119.90
1	AA	1386	G	N1-C6-O6	9.45	125.57	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	187	G	N1-C6-O6	9.45	125.57	119.90
27	B8	1256	G	N1-C6-O6	9.45	125.57	119.90
1	AA	791	G	N1-C6-O6	9.45	125.57	119.90
27	B8	2669	G	N1-C6-O6	9.45	125.57	119.90
27	B8	2731	G	N1-C6-O6	9.45	125.57	119.90
1	AA	347	G	N1-C6-O6	9.45	125.57	119.90
27	B8	717	C	O4'-C1'-N1	9.45	115.76	108.20
27	B8	1430	G	N1-C6-O6	9.45	125.57	119.90
27	B8	2355	G	N1-C6-O6	9.45	125.57	119.90
27	B8	2550	G	N1-C6-O6	9.45	125.57	119.90
27	B8	2732	G	N1-C6-O6	9.45	125.57	119.90
27	B8	998	C	O4'-C1'-N1	9.44	115.75	108.20
27	B8	1414	C	O4'-C1'-N1	9.44	115.75	108.20
1	AA	241	G	N1-C6-O6	9.44	125.56	119.90
27	B8	132	G	N1-C6-O6	9.44	125.56	119.90
27	B8	1601	G	N1-C6-O6	9.44	125.56	119.90
27	B8	1988	G	N1-C6-O6	9.44	125.56	119.90
27	B8	2782	G	N1-C6-O6	9.44	125.56	119.90
3	AV	23	G	N1-C6-O6	9.44	125.56	119.90
27	B8	585	G	N1-C6-O6	9.44	125.56	119.90
1	AA	213	G	N1-C6-O6	9.43	125.56	119.90
27	B8	258	G	N1-C6-O6	9.43	125.56	119.90
27	B8	319	G	N1-C6-O6	9.43	125.56	119.90
27	B8	966	G	N1-C6-O6	9.43	125.56	119.90
27	B8	2523	G	N1-C6-O6	9.43	125.56	119.90
1	AA	163	C	O4'-C1'-N1	9.43	115.74	108.20
27	B8	2110	G	N1-C6-O6	9.43	125.56	119.90
27	B8	1500	G	N1-C6-O6	9.43	125.56	119.90
27	B8	1904	G	N1-C6-O6	9.43	125.56	119.90
27	B8	914	G	N1-C6-O6	9.42	125.55	119.90
27	B8	1216	G	N1-C6-O6	9.42	125.55	119.90
27	B8	1429	G	N1-C6-O6	9.42	125.55	119.90
27	B8	1519	G	N1-C6-O6	9.42	125.56	119.90
27	B8	2276	G	N1-C6-O6	9.42	125.55	119.90
27	B8	1120	G	N1-C6-O6	9.42	125.55	119.90
27	B8	1731	G	N1-C6-O6	9.42	125.55	119.90
1	AA	666	G	N1-C6-O6	9.42	125.55	119.90
27	B8	1171	G	N1-C6-O6	9.41	125.55	119.90
27	B8	1448	G	N1-C6-O6	9.41	125.55	119.90
27	B8	1250	G	N1-C6-O6	9.41	125.55	119.90
27	B8	2838	G	N1-C6-O6	9.41	125.55	119.90
27	B8	792	A	P-O3'-C3'	9.41	130.99	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1011	G	N1-C6-O6	9.41	125.55	119.90
27	B8	1862	G	N1-C6-O6	9.41	125.55	119.90
27	B8	2242	G	N1-C6-O6	9.41	125.55	119.90
1	AA	1026	G	N1-C6-O6	9.41	125.54	119.90
27	B8	259	G	N1-C6-O6	9.41	125.54	119.90
1	AA	141	G	N1-C6-O6	9.40	125.54	119.90
27	B8	1530	G	N1-C6-O6	9.40	125.54	119.90
1	AA	903	G	N1-C6-O6	9.40	125.54	119.90
27	B8	700	G	N1-C6-O6	9.40	125.54	119.90
27	B8	297	G	N1-C6-O6	9.40	125.54	119.90
27	B8	261	G	N1-C6-O6	9.40	125.54	119.90
27	B8	535	G	N1-C6-O6	9.40	125.54	119.90
27	B8	723	C	O4'-C1'-N1	9.39	115.72	108.20
1	AA	731	G	N1-C6-O6	9.39	125.53	119.90
27	B8	1984	G	N1-C6-O6	9.39	125.53	119.90
1	AA	111	G	N1-C6-O6	9.39	125.53	119.90
26	B7	18	G	N1-C6-O6	9.39	125.53	119.90
1	AA	1238	A	N1-C6-N6	9.39	124.23	118.60
27	B8	214	G	N1-C6-O6	9.39	125.53	119.90
27	B8	1031	G	N1-C6-O6	9.39	125.53	119.90
27	B8	1	G	N1-C6-O6	9.39	125.53	119.90
1	AA	1002	G	N1-C6-O6	9.38	125.53	119.90
26	B7	6	G	N1-C6-O6	9.38	125.53	119.90
27	B8	952	G	N1-C6-O6	9.38	125.53	119.90
1	AA	491	G	N1-C6-O6	9.38	125.53	119.90
27	B8	1192	G	N1-C6-O6	9.38	125.53	119.90
1	AA	1032	G	N1-C6-O6	9.38	125.53	119.90
27	B8	189	G	N1-C6-O6	9.38	125.53	119.90
27	B8	1850	G	N1-C6-O6	9.38	125.53	119.90
1	AA	1198	G	N1-C6-O6	9.38	125.53	119.90
1	AA	1234	C	O4'-C1'-N1	9.38	115.70	108.20
1	AA	585	G	N1-C6-O6	9.38	125.53	119.90
1	AA	774	G	N1-C6-O6	9.37	125.52	119.90
27	B8	956	G	N1-C6-O6	9.37	125.52	119.90
1	AA	242	G	N1-C6-O6	9.37	125.52	119.90
27	B8	1168	G	N1-C6-O6	9.37	125.52	119.90
27	B8	2502	G	N1-C6-O6	9.37	125.52	119.90
27	B8	2744	G	N1-C6-O6	9.37	125.52	119.90
1	AA	1206	G	C5-C6-O6	-9.37	122.98	128.60
27	B8	468	G	N1-C6-O6	9.37	125.52	119.90
27	B8	2828	G	N1-C6-O6	9.36	125.52	119.90
3	AV	54	G	N1-C6-O6	9.36	125.52	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1388	G	N1-C6-O6	9.36	125.52	119.90
27	B8	1922	G	N1-C6-O6	9.36	125.52	119.90
27	B8	2846	G	N1-C6-O6	9.36	125.52	119.90
1	AA	314	C	O4'-C1'-N1	9.36	115.69	108.20
1	AA	929	G	N1-C6-O6	9.36	125.51	119.90
1	AA	604	G	N1-C6-O6	9.35	125.51	119.90
1	AA	671	G	N1-C6-O6	9.35	125.51	119.90
1	AA	1039	G	N1-C6-O6	9.35	125.51	119.90
27	B8	636	G	N1-C6-O6	9.35	125.51	119.90
27	B8	993	G	N1-C6-O6	9.35	125.51	119.90
27	B8	2107	G	N1-C6-O6	9.35	125.51	119.90
27	B8	2729	G	N1-C6-O6	9.35	125.51	119.90
1	AA	165	G	N1-C6-O6	9.35	125.51	119.90
27	B8	2895	G	C5-C6-O6	-9.35	122.99	128.60
27	B8	2759	G	N1-C6-O6	9.35	125.51	119.90
27	B8	424	G	C5-C6-O6	-9.35	122.99	128.60
27	B8	1358	G	N1-C6-O6	9.35	125.51	119.90
3	AV	47	G	N1-C6-O6	9.34	125.51	119.90
26	B7	7	G	N1-C6-O6	9.34	125.51	119.90
27	B8	2173	A	N1-C6-N6	9.34	124.20	118.60
27	B8	2325	G	N1-C6-O6	9.34	125.51	119.90
27	B8	2876	G	N1-C6-O6	9.34	125.50	119.90
1	AA	881	G	N1-C6-O6	9.34	125.50	119.90
26	B7	20	G	N1-C6-O6	9.34	125.50	119.90
3	AV	32	C	O4'-C1'-N1	9.34	115.67	108.20
27	B8	438	G	N1-C6-O6	9.34	125.50	119.90
1	AA	425	G	N1-C6-O6	9.33	125.50	119.90
27	B8	738	G	N1-C6-O6	9.33	125.50	119.90
27	B8	1724	G	N1-C6-O6	9.33	125.50	119.90
1	AA	836	G	N1-C6-O6	9.33	125.50	119.90
1	AA	902	G	N1-C6-O6	9.33	125.50	119.90
1	AA	1215	G	N1-C6-O6	9.33	125.50	119.90
27	B8	2490	G	N1-C6-O6	9.33	125.50	119.90
1	AA	548	G	N1-C6-O6	9.33	125.50	119.90
1	AA	1106	G	N1-C6-O6	9.32	125.49	119.90
26	B7	85	G	N1-C6-O6	9.32	125.49	119.90
27	B8	2582	G	N1-C6-O6	9.32	125.49	119.90
27	B8	215	G	N1-C6-O6	9.32	125.49	119.90
27	B8	1071	G	N1-C6-O6	9.32	125.49	119.90
27	B8	1281	G	N1-C6-O6	9.32	125.49	119.90
1	AA	203	G	N1-C6-O6	9.32	125.49	119.90
27	B8	2339	C	O4'-C1'-N1	9.32	115.66	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2443	C	O4'-C1'-N1	9.32	115.66	108.20
27	B8	2671	G	N1-C6-O6	9.32	125.49	119.90
27	B8	638	G	N1-C6-O6	9.32	125.49	119.90
27	B8	827	U	P-O3'-C3'	9.32	130.88	119.70
27	B8	1813	G	N1-C6-O6	9.32	125.49	119.90
27	B8	2686	G	N1-C6-O6	9.31	125.49	119.90
26	B7	35	C	O4'-C1'-N1	9.31	115.65	108.20
27	B8	276	U	O4'-C1'-N1	9.31	115.65	108.20
27	B8	1921	G	N1-C6-O6	9.31	125.49	119.90
1	AA	184	G	C5-C6-O6	-9.31	123.01	128.60
26	B7	44	G	N1-C6-O6	9.31	125.49	119.90
27	B8	1221	C	O4'-C1'-N1	9.31	115.65	108.20
27	B8	75	G	N1-C6-O6	9.31	125.48	119.90
1	AA	925	G	N1-C6-O6	9.31	125.48	119.90
1	AA	1469	C	O4'-C1'-N1	9.30	115.64	108.20
27	B8	1610	A	N1-C6-N6	9.30	124.18	118.60
1	AA	610	U	O4'-C1'-N1	9.30	115.64	108.20
1	AA	821	G	N1-C6-O6	9.30	125.48	119.90
27	B8	266	G	C5-C6-O6	-9.30	123.02	128.60
27	B8	893	C	O4'-C1'-N1	9.30	115.64	108.20
27	B8	1444	G	N1-C6-O6	9.30	125.48	119.90
27	B8	1910	G	C5-C6-O6	-9.30	123.02	128.60
27	B8	2889	C	O4'-C1'-N1	9.30	115.64	108.20
27	B8	2316	G	N1-C6-O6	9.30	125.48	119.90
1	AA	885	G	N1-C6-O6	9.30	125.48	119.90
27	B8	856	G	N1-C6-O6	9.30	125.48	119.90
27	B8	2228	G	N1-C6-O6	9.30	125.48	119.90
27	B8	2567	G	N1-C6-O6	9.30	125.48	119.90
27	B8	2633	G	N1-C6-O6	9.30	125.48	119.90
27	B8	241	A	N1-C6-N6	9.29	124.18	118.60
27	B8	578	G	N1-C6-O6	9.29	125.48	119.90
27	B8	1625	C	O4'-C1'-N1	9.30	115.64	108.20
27	B8	1202	G	N1-C6-O6	9.29	125.48	119.90
27	B8	1357	C	O4'-C1'-N1	9.29	115.63	108.20
27	B8	1860	G	N1-C6-O6	9.29	125.47	119.90
27	B8	1766	G	N1-C6-O6	9.29	125.47	119.90
1	AA	953	G	N1-C6-O6	9.28	125.47	119.90
1	AA	1138	G	N1-C6-O6	9.29	125.47	119.90
1	AA	1242	G	N1-C6-O6	9.29	125.47	119.90
27	B8	674	G	N1-C6-O6	9.29	125.47	119.90
26	B7	75	G	N1-C6-O6	9.28	125.47	119.90
1	AA	1514	G	N1-C6-O6	9.28	125.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	301	G	C5-C6-O6	-9.28	123.03	128.60
1	AA	1435	G	C5-C6-O6	-9.28	123.03	128.60
27	B8	843	G	N1-C6-O6	9.28	125.47	119.90
27	B8	2495	G	N1-C6-O6	9.28	125.47	119.90
27	B8	2543	G	C5-C6-O6	-9.28	123.03	128.60
27	B8	2725	A	N1-C6-N6	9.28	124.17	118.60
27	B8	2802	G	N1-C6-O6	9.28	125.47	119.90
1	AA	230	G	N1-C6-O6	9.28	125.47	119.90
27	B8	629	G	N1-C6-O6	9.28	125.47	119.90
27	B8	1645	G	N1-C6-O6	9.28	125.47	119.90
27	B8	2087	G	N1-C6-O6	9.28	125.47	119.90
27	B8	2403	C	O4'-C1'-N1	9.28	115.62	108.20
1	AA	1458	G	N1-C6-O6	9.28	125.47	119.90
27	B8	313	G	N1-C6-O6	9.28	125.47	119.90
27	B8	1653	G	N1-C6-O6	9.28	125.47	119.90
27	B8	1666	G	N1-C6-O6	9.28	125.47	119.90
27	B8	1925	C	O4'-C1'-N1	9.28	115.62	108.20
27	B8	2454	G	N1-C6-O6	9.28	125.47	119.90
1	AA	102	G	N1-C6-O6	9.27	125.46	119.90
1	AA	1438	G	N1-C6-O6	9.27	125.47	119.90
27	B8	1723	G	N1-C6-O6	9.27	125.47	119.90
1	AA	1144	G	N1-C6-O6	9.27	125.46	119.90
27	B8	1185	G	N1-C6-O6	9.27	125.46	119.90
1	AA	1462	C	O4'-C1'-N1	9.27	115.61	108.20
1	AA	1529	G	N1-C6-O6	9.27	125.46	119.90
26	B7	16	G	N1-C6-O6	9.27	125.46	119.90
27	B8	681	G	N1-C6-O6	9.27	125.46	119.90
27	B8	697	G	N1-C6-O6	9.27	125.46	119.90
27	B8	1835	G	N1-C6-O6	9.27	125.46	119.90
27	B8	974	G	N1-C6-O6	9.27	125.46	119.90
1	AA	462	G	N1-C6-O6	9.26	125.46	119.90
27	B8	2666	C	O4'-C1'-N1	9.26	115.61	108.20
1	AA	332	G	N1-C6-O6	9.26	125.46	119.90
27	B8	380	G	N1-C6-O6	9.26	125.46	119.90
27	B8	2290	G	N1-C6-O6	9.26	125.46	119.90
27	B8	1441	G	N1-C6-O6	9.26	125.46	119.90
27	B8	2251	G	N1-C6-O6	9.26	125.45	119.90
1	AA	337	G	N1-C6-O6	9.26	125.45	119.90
1	AA	1043	G	N1-C6-O6	9.26	125.45	119.90
27	B8	604	G	N1-C6-O6	9.25	125.45	119.90
27	B8	1136	G	N1-C6-O6	9.25	125.45	119.90
27	B8	1628	G	N1-C6-O6	9.25	125.45	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	46	G	N1-C6-O6	9.25	125.45	119.90
27	B8	695	G	N1-C6-O6	9.25	125.45	119.90
27	B8	770	G	N1-C6-O6	9.25	125.45	119.90
1	AA	978	A	N1-C6-N6	9.24	124.14	118.60
27	B8	1416	G	N1-C6-O6	9.24	125.44	119.90
27	B8	1622	G	N1-C6-O6	9.24	125.44	119.90
27	B8	289	G	N1-C6-O6	9.24	125.44	119.90
27	B8	1343	G	N1-C6-O6	9.24	125.44	119.90
27	B8	2852	G	N1-C6-O6	9.24	125.44	119.90
1	AA	1356	G	N1-C6-O6	9.23	125.44	119.90
27	B8	796	C	O4'-C1'-N1	9.23	115.59	108.20
27	B8	2428	G	N1-C6-O6	9.23	125.44	119.90
1	AA	299	G	N1-C6-O6	9.23	125.44	119.90
26	B7	61	G	N1-C6-O6	9.23	125.44	119.90
27	B8	151	C	O4'-C1'-N1	9.23	115.59	108.20
1	AA	1294	G	N1-C6-O6	9.23	125.44	119.90
1	AA	1526	G	N1-C6-O6	9.23	125.44	119.90
27	B8	1878	G	N1-C6-O6	9.23	125.44	119.90
27	B8	774	G	N1-C6-O6	9.23	125.44	119.90
27	B8	2642	G	N1-C6-O6	9.23	125.44	119.90
27	B8	35	G	N1-C6-O6	9.23	125.44	119.90
1	AA	988	G	N1-C6-O6	9.22	125.44	119.90
1	AA	404	G	N1-C6-O6	9.22	125.43	119.90
27	B8	647	G	N1-C6-O6	9.22	125.43	119.90
1	AA	1088	G	N1-C6-O6	9.22	125.43	119.90
27	B8	134	G	N1-C6-O6	9.22	125.43	119.90
27	B8	907	G	N1-C6-O6	9.22	125.43	119.90
27	B8	1116	G	N1-C6-O6	9.22	125.43	119.90
1	AA	670	G	N1-C6-O6	9.21	125.43	119.90
27	B8	271	G	N1-C6-O6	9.21	125.43	119.90
27	B8	656	G	N1-C6-O6	9.21	125.43	119.90
27	B8	1106	G	C5-C6-O6	-9.21	123.07	128.60
1	AA	962	C	O4'-C1'-N1	9.21	115.57	108.20
27	B8	469	G	N1-C6-O6	9.21	125.43	119.90
27	B8	2752	C	O4'-C1'-N1	9.21	115.57	108.20
27	B8	1491	G	N1-C6-O6	9.21	125.43	119.90
27	B8	2256	G	N1-C6-O6	9.21	125.43	119.90
27	B8	2415	G	N1-C6-O6	9.21	125.43	119.90
26	B7	84	G	N1-C6-O6	9.20	125.42	119.90
27	B8	2002	G	N1-C6-O6	9.20	125.42	119.90
27	B8	2693	G	N1-C6-O6	9.20	125.42	119.90
27	B8	2854	G	N1-C6-O6	9.20	125.42	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1087	G	N1-C6-O6	9.20	125.42	119.90
1	AA	1389	C	O4'-C1'-N1	9.20	115.56	108.20
27	B8	99	U	O4'-C1'-N1	9.20	115.56	108.20
27	B8	1361	G	N1-C6-O6	9.20	125.42	119.90
27	B8	1674	G	N1-C6-O6	9.19	125.42	119.90
1	AA	1415	G	N1-C6-O6	9.19	125.42	119.90
27	B8	2625	G	N1-C6-O6	9.19	125.41	119.90
1	AA	191	G	N1-C6-O6	9.19	125.41	119.90
27	B8	2777	G	N1-C6-O6	9.19	125.41	119.90
1	AA	538	G	N1-C6-O6	9.19	125.41	119.90
27	B8	1377	G	N1-C6-O6	9.19	125.41	119.90
27	B8	1450	G	N1-C6-O6	9.19	125.41	119.90
1	AA	529	G	N1-C6-O6	9.18	125.41	119.90
1	AA	1312	G	N1-C6-O6	9.18	125.41	119.90
27	B8	356	G	N1-C6-O6	9.18	125.41	119.90
27	B8	1842	G	N1-C6-O6	9.18	125.41	119.90
27	B8	1861	G	N1-C6-O6	9.18	125.41	119.90
1	AA	1124	G	N1-C6-O6	9.18	125.41	119.90
1	AA	1337	G	N1-C6-O6	9.18	125.41	119.90
27	B8	1261	C	O4'-C1'-N1	9.18	115.54	108.20
27	B8	2337	G	N1-C6-O6	9.18	125.41	119.90
27	B8	2763	G	N1-C6-O6	9.18	125.41	119.90
27	B8	325	G	N1-C6-O6	9.17	125.40	119.90
27	B8	733	G	N1-C6-O6	9.17	125.40	119.90
1	AA	31	G	N1-C6-O6	9.17	125.40	119.90
27	B8	1062	G	N1-C6-O6	9.17	125.40	119.90
27	B8	1730	C	P-O3'-C3'	9.17	130.70	119.70
27	B8	2246	G	N1-C6-O6	9.17	125.40	119.90
27	B8	2318	G	N1-C6-O6	9.17	125.40	119.90
26	B7	98	G	N1-C6-O6	9.16	125.40	119.90
27	B8	361	G	N1-C6-O6	9.16	125.40	119.90
27	B8	1410	G	N1-C6-O6	9.16	125.40	119.90
1	AA	688	G	N1-C6-O6	9.16	125.40	119.90
27	B8	1280	G	N1-C6-O6	9.16	125.40	119.90
1	AA	550	G	N1-C6-O6	9.16	125.39	119.90
1	AA	1255	G	N1-C6-O6	9.16	125.39	119.90
27	B8	768	G	C5-C6-O6	-9.16	123.11	128.60
27	B8	2405	G	N1-C6-O6	9.16	125.39	119.90
27	B8	205	G	N1-C6-O6	9.15	125.39	119.90
27	B8	1210	G	N1-C6-O6	9.15	125.39	119.90
27	B8	178	G	N1-C6-O6	9.15	125.39	119.90
27	B8	204	A	N1-C6-N6	9.15	124.09	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2230	G	N1-C6-O6	9.15	125.39	119.90
27	B8	2367	G	N1-C6-O6	9.15	125.39	119.90
3	AV	10	G	N1-C6-O6	9.15	125.39	119.90
26	B7	64	G	N1-C6-O6	9.15	125.39	119.90
27	B8	175	G	N1-C6-O6	9.15	125.39	119.90
27	B8	179	C	O4'-C1'-N1	9.15	115.52	108.20
27	B8	874	G	N1-C6-O6	9.15	125.39	119.90
27	B8	1371	G	N1-C6-O6	9.15	125.39	119.90
27	B8	2373	G	N1-C6-O6	9.15	125.39	119.90
1	AA	348	G	N1-C6-O6	9.14	125.39	119.90
27	B8	909	A	N1-C6-N6	9.14	124.09	118.60
27	B8	2389	G	N1-C6-O6	9.14	125.39	119.90
27	B8	940	G	N1-C6-O6	9.14	125.39	119.90
1	AA	1272	G	N1-C6-O6	9.14	125.38	119.90
1	AA	1459	G	N1-C6-O6	9.14	125.38	119.90
27	B8	375	G	N1-C6-O6	9.14	125.38	119.90
1	AA	42	G	N1-C6-O6	9.13	125.38	119.90
1	AA	289	G	N1-C6-O6	9.13	125.38	119.90
3	AV	70	G	C5-C6-O6	-9.14	123.12	128.60
1	AA	11	G	N1-C6-O6	9.13	125.38	119.90
27	B8	2132	U	O4'-C1'-N1	9.13	115.51	108.20
27	B8	2526	G	N1-C6-O6	9.13	125.38	119.90
27	B8	2869	G	N1-C6-O6	9.13	125.38	119.90
27	B8	847	U	O4'-C1'-N1	9.13	115.50	108.20
1	AA	400	C	O4'-C1'-N1	9.13	115.50	108.20
27	B8	17	G	N1-C6-O6	9.13	125.38	119.90
27	B8	971	G	N1-C6-O6	9.13	125.38	119.90
27	B8	1997	C	O4'-C1'-N1	9.13	115.50	108.20
1	AA	126	G	N1-C6-O6	9.13	125.38	119.90
1	AA	567	G	N1-C6-O6	9.12	125.38	119.90
3	AV	51	G	N1-C6-O6	9.13	125.38	119.90
1	AA	927	G	N1-C6-O6	9.12	125.37	119.90
27	B8	1846	G	N1-C6-O6	9.12	125.37	119.90
1	AA	1187	G	N1-C6-O6	9.12	125.37	119.90
1	AA	588	G	N1-C6-O6	9.12	125.37	119.90
1	AA	1047	G	N1-C6-O6	9.12	125.37	119.90
1	AA	276	G	N1-C6-O6	9.12	125.37	119.90
1	AA	158	G	N1-C6-O6	9.11	125.37	119.90
1	AA	388	G	N1-C6-O6	9.11	125.37	119.90
1	AA	444	G	N1-C6-O6	9.12	125.37	119.90
1	AA	730	G	N1-C6-O6	9.11	125.37	119.90
27	B8	1036	G	N1-C6-O6	9.11	125.37	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1220	G	N1-C6-O6	9.11	125.37	119.90
27	B8	1337	G	N1-C6-O6	9.11	125.37	119.90
1	AA	1033	G	C5-C6-O6	-9.11	123.14	128.60
1	AA	1153	G	N1-C6-O6	9.11	125.36	119.90
27	B8	785	G	N1-C6-O6	9.11	125.36	119.90
1	AA	542	G	N1-C6-O6	9.11	125.36	119.90
1	AA	1177	G	N1-C6-O6	9.11	125.36	119.90
26	B7	26	C	O4'-C1'-N1	9.11	115.48	108.20
27	B8	2396	G	N1-C6-O6	9.11	125.36	119.90
1	AA	196	A	N1-C6-N6	9.10	124.06	118.60
27	B8	930	G	N1-C6-O6	9.10	125.36	119.90
27	B8	2277	G	N1-C6-O6	9.10	125.36	119.90
1	AA	146	G	N1-C6-O6	9.10	125.36	119.90
1	AA	570	G	C5-C6-O6	-9.10	123.14	128.60
27	B8	283	G	N1-C6-O6	9.10	125.36	119.90
1	AA	1054	C	O4'-C1'-N1	9.10	115.48	108.20
27	B8	1177	G	N1-C6-O6	9.10	125.36	119.90
27	B8	1303	G	N1-C6-O6	9.10	125.36	119.90
27	B8	1751	U	O4'-C1'-N1	9.10	115.48	108.20
1	AA	887	G	N1-C6-O6	9.09	125.36	119.90
1	AA	1186	G	N1-C6-O6	9.09	125.36	119.90
1	AA	1309	G	N1-C6-O6	9.09	125.36	119.90
27	B8	584	C	O4'-C1'-N1	9.09	115.47	108.20
27	B8	841	G	N1-C6-O6	9.09	125.35	119.90
27	B8	2480	C	O4'-C1'-N1	9.09	115.47	108.20
27	B8	2862	G	N1-C6-O6	9.09	125.35	119.90
1	AA	361	G	N1-C6-O6	9.09	125.35	119.90
1	AA	872	A	N1-C6-N6	9.08	124.05	118.60
27	B8	712	G	N1-C6-O6	9.08	125.35	119.90
1	AA	776	G	N1-C6-O6	9.08	125.35	119.90
27	B8	1623	G	N1-C6-O6	9.08	125.35	119.90
27	B8	2488	G	N1-C6-O6	9.08	125.35	119.90
27	B8	1620	G	N1-C6-O6	9.07	125.34	119.90
1	AA	104	G	C5-C6-O6	-9.07	123.16	128.60
27	B8	1968	G	N1-C6-O6	9.07	125.34	119.90
1	AA	76	G	C5-C6-O6	-9.07	123.16	128.60
27	B8	406	G	N1-C6-O6	9.07	125.34	119.90
27	B8	1139	G	N1-C6-O6	9.07	125.34	119.90
27	B8	1369	G	N1-C6-O6	9.07	125.34	119.90
27	B8	1382	G	O4'-C1'-N9	9.07	115.45	108.20
27	B8	1719	G	N1-C6-O6	9.07	125.34	119.90
27	B8	992	C	O4'-C1'-N1	9.07	115.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2569	G	N1-C6-O6	9.07	125.34	119.90
27	B8	2708	G	N1-C6-O6	9.07	125.34	119.90
1	AA	544	G	N1-C6-O6	9.07	125.34	119.90
27	B8	85	G	N1-C6-O6	9.07	125.34	119.90
27	B8	1480	C	O4'-C1'-N1	9.07	115.45	108.20
1	AA	597	G	N1-C6-O6	9.06	125.34	119.90
1	AA	1299	A	N1-C6-N6	9.06	124.04	118.60
27	B8	2100	G	N1-C6-O6	9.06	125.34	119.90
1	AA	442	G	N1-C6-O6	9.06	125.34	119.90
1	AA	540	G	N1-C6-O6	9.06	125.34	119.90
1	AA	987	G	N1-C6-O6	9.06	125.34	119.90
27	B8	2190	G	N1-C6-O6	9.06	125.34	119.90
27	B8	2691	C	O4'-C1'-N1	9.06	115.45	108.20
27	B8	771	G	N1-C6-O6	9.06	125.34	119.90
27	B8	1696	G	N1-C6-O6	9.06	125.34	119.90
1	AA	100	G	N1-C6-O6	9.06	125.34	119.90
27	B8	2474	U	O4'-C1'-N1	9.06	115.45	108.20
27	B8	2864	G	N1-C6-O6	9.06	125.34	119.90
1	AA	1185	G	N1-C6-O6	9.06	125.33	119.90
1	AA	1401	G	N1-C6-O6	9.06	125.33	119.90
1	AA	1486	G	C5-C6-O6	-9.06	123.17	128.60
27	B8	110	G	N1-C6-O6	9.06	125.33	119.90
27	B8	2004	G	N1-C6-O6	9.06	125.33	119.90
1	AA	1258	G	N1-C6-O6	9.06	125.33	119.90
1	AA	830	G	N1-C6-O6	9.05	125.33	119.90
27	B8	327	G	N1-C6-O6	9.05	125.33	119.90
27	B8	1128	G	N1-C6-O6	9.05	125.33	119.90
27	B8	1407	G	N1-C6-O6	9.05	125.33	119.90
27	B8	1740	G	N1-C6-O6	9.05	125.33	119.90
1	AA	46	G	N1-C6-O6	9.05	125.33	119.90
1	AA	1104	G	N1-C6-O6	9.05	125.33	119.90
27	B8	1849	G	N1-C6-O6	9.05	125.33	119.90
27	B8	692	C	O4'-C1'-N1	9.05	115.44	108.20
27	B8	1449	G	N1-C6-O6	9.05	125.33	119.90
1	AA	848	C	O4'-C1'-N1	9.05	115.44	108.20
1	AA	1270	G	N1-C6-O6	9.05	125.33	119.90
27	B8	2382	G	N1-C6-O6	9.05	125.33	119.90
27	B8	124	G	N1-C6-O6	9.04	125.33	119.90
27	B8	763	G	N1-C6-O6	9.04	125.33	119.90
27	B8	1149	G	N1-C6-O6	9.04	125.33	119.90
1	AA	41	G	N1-C6-O6	9.04	125.33	119.90
27	B8	1663	G	N1-C6-O6	9.04	125.33	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	474	G	N1-C6-O6	9.04	125.32	119.90
1	AA	799	G	N1-C6-O6	9.04	125.32	119.90
27	B8	301	G	N1-C6-O6	9.04	125.32	119.90
27	B8	728	G	N1-C6-O6	9.04	125.32	119.90
27	B8	1633	G	N1-C6-O6	9.04	125.32	119.90
1	AA	721	G	N1-C6-O6	9.04	125.32	119.90
27	B8	776	G	N1-C6-O6	9.04	125.32	119.90
27	B8	1266	G	N1-C6-O6	9.04	125.32	119.90
27	B8	1863	G	N1-C6-O6	9.04	125.32	119.90
27	B8	1972	G	N1-C6-O6	9.04	125.32	119.90
27	B8	708	G	N1-C6-O6	9.03	125.32	119.90
27	B8	1380	G	N1-C6-O6	9.03	125.32	119.90
27	B8	1125	G	N1-C6-O6	9.03	125.32	119.90
27	B8	1225	G	N1-C6-O6	9.03	125.32	119.90
27	B8	27	G	N1-C6-O6	9.03	125.32	119.90
27	B8	1750	G	N1-C6-O6	9.03	125.32	119.90
1	AA	1370	G	N1-C6-O6	9.03	125.32	119.90
27	B8	2216	G	N1-C6-O6	9.03	125.32	119.90
1	AA	1241	G	N1-C6-O6	9.03	125.32	119.90
27	B8	119	A	N1-C6-N6	9.03	124.02	118.60
1	AA	251	G	N1-C6-O6	9.02	125.31	119.90
1	AA	1244	G	N1-C6-O6	9.02	125.31	119.90
1	AA	391	G	N1-C6-O6	9.02	125.31	119.90
1	AA	748	G	N1-C6-O6	9.02	125.31	119.90
1	AA	1141	C	O4'-C1'-N1	9.02	115.42	108.20
27	B8	302	C	O4'-C1'-N1	9.02	115.42	108.20
27	B8	498	G	N1-C6-O6	9.02	125.31	119.90
27	B8	2770	G	N1-C6-O6	9.02	125.31	119.90
27	B8	1592	C	O4'-C1'-N1	9.02	115.42	108.20
27	B8	780	G	N1-C6-O6	9.02	125.31	119.90
1	AA	64	G	N1-C6-O6	9.02	125.31	119.90
27	B8	1332	G	N1-C6-O6	9.02	125.31	119.90
27	B8	1516	G	N1-C6-O6	9.01	125.31	119.90
27	B8	2223	G	N1-C6-O6	9.01	125.31	119.90
27	B8	2280	G	N1-C6-O6	9.01	125.31	119.90
27	B8	612	G	N1-C6-O6	9.01	125.31	119.90
27	B8	1291	C	O4'-C1'-N1	9.01	115.41	108.20
27	B8	1684	G	N1-C6-O6	9.01	125.31	119.90
27	B8	2525	G	N1-C6-O6	9.01	125.31	119.90
27	B8	92	U	O4'-C1'-N1	9.01	115.41	108.20
27	B8	822	G	N1-C6-O6	9.01	125.31	119.90
27	B8	1164	C	O4'-C1'-N1	9.01	115.41	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	247	G	N1-C6-O6	9.01	125.31	119.90
27	B8	834	G	N1-C6-O6	9.01	125.31	119.90
1	AA	292	G	N1-C6-O6	9.01	125.31	119.90
1	AA	144	G	N1-C6-O6	9.01	125.30	119.90
1	AA	362	G	N1-C6-O6	9.00	125.30	119.90
1	AA	212	G	N1-C6-O6	9.00	125.30	119.90
1	AA	421	U	O4'-C1'-N1	9.00	115.40	108.20
1	AA	445	G	N1-C6-O6	9.00	125.30	119.90
1	AA	993	G	N1-C6-O6	9.00	125.30	119.90
27	B8	1404	C	O4'-C1'-N1	9.00	115.40	108.20
27	B8	2458	G	N1-C6-O6	9.00	125.30	119.90
27	B8	2890	G	N1-C6-O6	9.00	125.30	119.90
27	B8	1606	C	O4'-C1'-N1	9.00	115.40	108.20
27	B8	2485	G	C5-C6-O6	-9.00	123.20	128.60
27	B8	2061	G	N1-C6-O6	9.00	125.30	119.90
27	B8	2747	G	C5-C6-O6	-9.00	123.20	128.60
27	B8	23	G	N1-C6-O6	9.00	125.30	119.90
1	AA	859	G	N1-C6-O6	8.99	125.30	119.90
1	AA	1253	G	N1-C6-O6	8.99	125.30	119.90
1	AA	1460	C	O4'-C1'-N1	8.99	115.39	108.20
27	B8	298	G	N1-C6-O6	8.99	125.30	119.90
27	B8	551	G	N1-C6-O6	8.99	125.30	119.90
27	B8	775	G	N1-C6-O6	8.99	125.30	119.90
27	B8	1588	G	N1-C6-O6	8.99	125.30	119.90
27	B8	2218	G	N1-C6-O6	8.99	125.30	119.90
27	B8	307	G	N1-C6-O6	8.99	125.30	119.90
1	AA	324	G	N1-C6-O6	8.99	125.29	119.90
27	B8	411	G	N1-C6-O6	8.99	125.29	119.90
27	B8	1452	G	N1-C6-O6	8.99	125.30	119.90
27	B8	2831	G	N1-C6-O6	8.99	125.29	119.90
27	B8	1828	G	N1-C6-O6	8.99	125.29	119.90
27	B8	2293	G	N1-C6-O6	8.99	125.29	119.90
1	AA	1146	A	N1-C6-N6	8.99	123.99	118.60
1	AA	82	G	N1-C6-O6	8.99	125.29	119.90
1	AA	1296	C	O4'-C1'-N1	8.99	115.39	108.20
27	B8	303	G	N1-C6-O6	8.99	125.29	119.90
27	B8	630	G	N1-C6-O6	8.99	125.29	119.90
27	B8	1195	G	N1-C6-O6	8.99	125.29	119.90
27	B8	2038	G	N1-C6-O6	8.99	125.29	119.90
27	B8	1212	G	N1-C6-O6	8.98	125.29	119.90
1	AA	928	G	N1-C6-O6	8.98	125.29	119.90
1	AA	226	G	N1-C6-O6	8.98	125.29	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	682	G	N1-C6-O6	8.98	125.29	119.90
1	AA	971	G	N1-C6-O6	8.98	125.29	119.90
1	AA	1084	G	N1-C6-O6	8.98	125.29	119.90
27	B8	277	G	N1-C6-O6	8.98	125.29	119.90
27	B8	2303	G	N1-C6-O6	8.98	125.29	119.90
1	AA	220	G	N1-C6-O6	8.98	125.29	119.90
1	AA	527	G	N1-C6-O6	8.98	125.29	119.90
27	B8	188	G	N1-C6-O6	8.98	125.29	119.90
3	AV	15	G	N1-C6-O6	8.98	125.29	119.90
1	AA	1304	G	N1-C6-O6	8.97	125.28	119.90
27	B8	537	G	N1-C6-O6	8.97	125.28	119.90
27	B8	2661	G	N1-C6-O6	8.97	125.28	119.90
27	B8	862	G	N1-C6-O6	8.97	125.28	119.90
27	B8	1150	C	O4'-C1'-N1	8.97	115.38	108.20
1	AA	1530	G	N1-C6-O6	8.97	125.28	119.90
27	B8	1897	G	N1-C6-O6	8.97	125.28	119.90
27	B8	359	G	N1-C6-O6	8.97	125.28	119.90
27	B8	2121	G	N1-C6-O6	8.97	125.28	119.90
27	B8	2732	G	C5-C6-O6	-8.97	123.22	128.60
27	B8	7	G	N1-C6-O6	8.97	125.28	119.90
27	B8	942	G	N1-C6-O6	8.96	125.28	119.90
27	B8	1324	G	N1-C6-O6	8.96	125.28	119.90
27	B8	1436	G	N1-C6-O6	8.96	125.28	119.90
27	B8	2578	G	N1-C6-O6	8.96	125.28	119.90
1	AA	1276	G	N1-C6-O6	8.96	125.28	119.90
1	AA	803	G	N1-C6-O6	8.96	125.27	119.90
27	B8	57	C	O4'-C1'-N1	8.96	115.37	108.20
27	B8	923	G	N1-C6-O6	8.96	125.28	119.90
27	B8	463	G	N1-C6-O6	8.96	125.27	119.90
27	B8	997	G	N1-C6-O6	8.96	125.27	119.90
27	B8	1333	G	P-O3'-C3'	8.96	130.45	119.70
27	B8	1381	G	C5-C6-O6	-8.96	123.22	128.60
1	AA	505	G	N1-C6-O6	8.96	125.27	119.90
27	B8	1537	G	N1-C6-O6	8.96	125.27	119.90
27	B8	31	C	O4'-C1'-N1	8.95	115.36	108.20
27	B8	1475	G	N1-C6-O6	8.95	125.27	119.90
27	B8	1514	G	N1-C6-O6	8.95	125.27	119.90
27	B8	2844	G	N1-C6-O6	8.95	125.27	119.90
1	AA	147	G	C5-C6-O6	-8.95	123.23	128.60
1	AA	773	G	N1-C6-O6	8.95	125.27	119.90
27	B8	1445	G	C5-C6-O6	-8.95	123.23	128.60
27	B8	1767	G	N1-C6-O6	8.95	125.27	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1697	G	N1-C6-O6	8.95	125.27	119.90
27	B8	1063	G	N1-C6-O6	8.95	125.27	119.90
1	AA	1473	G	N1-C6-O6	8.95	125.27	119.90
27	B8	2857	G	N1-C6-O6	8.94	125.27	119.90
27	B8	2877	G	N1-C6-O6	8.95	125.27	119.90
1	AA	833	G	N1-C6-O6	8.94	125.27	119.90
27	B8	549	G	N1-C6-O6	8.94	125.27	119.90
1	AA	498	A	N1-C6-N6	8.94	123.96	118.60
27	B8	2697	G	N1-C6-O6	8.94	125.26	119.90
27	B8	916	G	C5-C6-O6	-8.94	123.24	128.60
27	B8	2867	G	N1-C6-O6	8.94	125.26	119.90
1	AA	1207	G	N1-C6-O6	8.94	125.26	119.90
27	B8	618	G	N1-C6-O6	8.94	125.26	119.90
27	B8	2717	C	O4'-C1'-N1	8.94	115.35	108.20
27	B8	736	C	O4'-C1'-N1	8.94	115.35	108.20
27	B8	1166	G	N1-C6-O6	8.94	125.26	119.90
1	AA	237	G	N1-C6-O6	8.93	125.26	119.90
1	AA	354	G	N1-C6-O6	8.93	125.26	119.90
1	AA	447	G	N1-C6-O6	8.93	125.26	119.90
27	B8	1811	G	N1-C6-O6	8.93	125.26	119.90
1	AA	944	G	N1-C6-O6	8.93	125.26	119.90
1	AA	1504	G	N1-C6-O6	8.93	125.26	119.90
3	AV	73	G	N1-C6-O6	8.93	125.26	119.90
27	B8	2645	G	N1-C6-O6	8.93	125.26	119.90
1	AA	710	G	N1-C6-O6	8.93	125.26	119.90
27	B8	518	G	N1-C6-O6	8.93	125.26	119.90
27	B8	1002	G	N1-C6-O6	8.93	125.26	119.90
27	B8	1160	G	N1-C6-O6	8.93	125.26	119.90
27	B8	2201	G	C5-C6-O6	-8.93	123.24	128.60
27	B8	24	G	N1-C6-O6	8.93	125.26	119.90
27	B8	1959	G	N1-C6-O6	8.93	125.26	119.90
27	B8	2773	C	O4'-C1'-N1	8.93	115.34	108.20
27	B8	2168	G	N1-C6-O6	8.92	125.25	119.90
27	B8	2730	C	O4'-C1'-N1	8.92	115.34	108.20
27	B8	2806	C	O4'-C1'-N1	8.92	115.34	108.20
1	AA	703	G	N1-C6-O6	8.92	125.25	119.90
27	B8	565	C	O4'-C1'-N1	8.92	115.34	108.20
27	B8	831	G	N1-C6-O6	8.92	125.25	119.90
27	B8	1442	U	O4'-C1'-N1	8.92	115.33	108.20
27	B8	2436	G	N1-C6-O6	8.92	125.25	119.90
27	B8	433	C	O4'-C1'-N1	8.92	115.33	108.20
27	B8	1334	G	N1-C6-O6	8.92	125.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1568	G	N1-C6-O6	8.92	125.25	119.90
27	B8	1733	G	N1-C6-O6	8.92	125.25	119.90
27	B8	2892	G	N1-C6-O6	8.92	125.25	119.90
27	B8	1157	G	C5-C6-O6	-8.91	123.25	128.60
27	B8	1248	G	N1-C6-O6	8.91	125.25	119.90
27	B8	1567	G	N1-C6-O6	8.91	125.25	119.90
27	B8	1604	C	O4'-C1'-N1	8.91	115.33	108.20
26	B7	51	G	N1-C6-O6	8.91	125.25	119.90
27	B8	969	G	N1-C6-O6	8.91	125.24	119.90
1	AA	490	C	O4'-C1'-N1	8.90	115.32	108.20
1	AA	1442	G	N1-C6-O6	8.90	125.24	119.90
3	AV	25	G	N1-C6-O6	8.90	125.24	119.90
1	AA	115	G	C5-C6-O6	-8.90	123.26	128.60
27	B8	295	G	N1-C6-O6	8.90	125.24	119.90
27	B8	2409	G	C5-C6-O6	-8.90	123.26	128.60
1	AA	558	G	N1-C6-O6	8.90	125.24	119.90
27	B8	136	G	N1-C6-O6	8.90	125.24	119.90
27	B8	1577	C	O4'-C1'-N1	8.90	115.32	108.20
1	AA	1392	G	C5-C6-O6	-8.90	123.26	128.60
27	B8	1555	G	N1-C6-O6	8.90	125.24	119.90
26	B7	79	G	N1-C6-O6	8.90	125.24	119.90
27	B8	1425	G	N1-C6-O6	8.90	125.24	119.90
1	AA	127	G	N1-C6-O6	8.89	125.24	119.90
3	AV	2	G	N1-C6-O6	8.89	125.24	119.90
27	B8	60	G	N1-C6-O6	8.89	125.24	119.90
27	B8	1299	G	N1-C6-O6	8.89	125.24	119.90
1	AA	331	G	N1-C6-O6	8.89	125.23	119.90
27	B8	232	G	N1-C6-O6	8.89	125.23	119.90
27	B8	864	G	C5-C6-O6	-8.89	123.27	128.60
27	B8	2494	G	N1-C6-O6	8.89	125.23	119.90
1	AA	1139	G	N1-C6-O6	8.89	125.23	119.90
1	AA	433	G	N1-C6-O6	8.89	125.23	119.90
27	B8	926	G	N1-C6-O6	8.89	125.23	119.90
1	AA	742	G	N1-C6-O6	8.88	125.23	119.90
26	B7	27	C	O4'-C1'-N1	8.88	115.31	108.20
27	B8	2894	G	C5-C6-O6	-8.89	123.27	128.60
1	AA	94	G	N1-C6-O6	8.88	125.23	119.90
27	B8	389	G	N1-C6-O6	8.88	125.23	119.90
27	B8	648	G	N1-C6-O6	8.88	125.23	119.90
27	B8	1047	G	N1-C6-O6	8.88	125.23	119.90
27	B8	2186	G	N1-C6-O6	8.88	125.23	119.90
27	B8	553	G	N1-C6-O6	8.88	125.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1368	G	N1-C6-O6	8.88	125.23	119.90
1	AA	1120	C	O4'-C1'-N1	8.88	115.30	108.20
27	B8	1814	G	N1-C6-O6	8.88	125.23	119.90
1	AA	69	G	N1-C6-O6	8.88	125.23	119.90
1	AA	399	G	N1-C6-O6	8.88	125.22	119.90
1	AA	1190	G	N1-C6-O6	8.88	125.22	119.90
26	B7	100	G	N1-C6-O6	8.87	125.22	119.90
27	B8	1223	G	N1-C6-O6	8.87	125.22	119.90
27	B8	2116	G	N1-C6-O6	8.88	125.22	119.90
1	AA	1290	G	C5-C6-O6	-8.87	123.28	128.60
26	B7	96	G	N1-C6-O6	8.87	125.22	119.90
27	B8	401	A	O4'-C1'-N9	8.87	115.30	108.20
27	B8	653	U	O4'-C1'-N1	8.87	115.30	108.20
27	B8	1681	G	N1-C6-O6	8.87	125.22	119.90
27	B8	1421	G	C5-C6-O6	-8.87	123.28	128.60
1	AA	973	G	C5-C6-O6	-8.87	123.28	128.60
1	AA	1439	G	N1-C6-O6	8.87	125.22	119.90
27	B8	1228	G	N1-C6-O6	8.87	125.22	119.90
27	B8	2724	U	O4'-C1'-N1	8.87	115.30	108.20
27	B8	1776	G	N1-C6-O6	8.87	125.22	119.90
27	B8	1824	G	N1-C6-O6	8.87	125.22	119.90
27	B8	2901	C	O4'-C1'-N1	8.87	115.29	108.20
1	AA	446	G	N1-C6-O6	8.86	125.22	119.90
1	AA	809	G	N1-C6-O6	8.87	125.22	119.90
1	AA	1426	G	N1-C6-O6	8.86	125.22	119.90
27	B8	254	G	N1-C6-O6	8.86	125.22	119.90
27	B8	885	C	O4'-C1'-N1	8.86	115.29	108.20
27	B8	1631	G	N1-C6-O6	8.86	125.22	119.90
27	B8	2028	U	O4'-C1'-N1	8.86	115.29	108.20
27	B8	2538	C	O4'-C1'-N1	8.87	115.29	108.20
1	AA	771	G	N1-C6-O6	8.86	125.22	119.90
1	AA	775	G	N1-C6-O6	8.86	125.22	119.90
1	AA	1305	G	N1-C6-O6	8.86	125.22	119.90
1	AA	1365	G	N1-C6-O6	8.86	125.22	119.90
27	B8	1945	G	N1-C6-O6	8.86	125.22	119.90
26	B7	107	G	N1-C6-O6	8.86	125.22	119.90
27	B8	15	G	N1-C6-O6	8.86	125.22	119.90
27	B8	2282	G	P-O3'-C3'	8.86	130.33	119.70
1	AA	369	G	N1-C6-O6	8.86	125.22	119.90
27	B8	458	G	N1-C6-O6	8.86	125.22	119.90
27	B8	467	G	N1-C6-O6	8.86	125.22	119.90
27	B8	622	G	N1-C6-O6	8.86	125.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	530	G	N1-C6-O6	8.86	125.21	119.90
1	AA	285	C	O4'-C1'-N1	8.86	115.28	108.20
1	AA	976	G	N1-C6-O6	8.86	125.21	119.90
3	AV	30	G	N1-C6-O6	8.86	125.21	119.90
27	B8	1524	G	N1-C6-O6	8.86	125.21	119.90
27	B8	1527	G	N1-C6-O6	8.86	125.21	119.90
1	AA	847	G	N1-C6-O6	8.85	125.21	119.90
27	B8	169	G	N1-C6-O6	8.85	125.21	119.90
27	B8	1152	C	O4'-C1'-N1	8.85	115.28	108.20
27	B8	1721	G	N1-C6-O6	8.85	125.21	119.90
1	AA	1064	G	N1-C6-O6	8.85	125.21	119.90
27	B8	859	G	N1-C6-O6	8.85	125.21	119.90
27	B8	1405	U	O4'-C1'-N1	8.85	115.28	108.20
27	B8	1581	G	N1-C6-O6	8.85	125.21	119.90
27	B8	1795	C	O4'-C1'-N1	8.85	115.28	108.20
27	B8	1933	G	N1-C6-O6	8.85	125.21	119.90
1	AA	79	G	N1-C6-O6	8.85	125.21	119.90
27	B8	45	G	N1-C6-O6	8.85	125.21	119.90
1	AA	880	C	O4'-C1'-N1	8.84	115.28	108.20
27	B8	2286	G	N1-C6-O6	8.84	125.21	119.90
27	B8	2371	G	N1-C6-O6	8.84	125.21	119.90
1	AA	424	G	C5-C6-O6	-8.84	123.30	128.60
1	AA	1108	G	N1-C6-O6	8.84	125.20	119.90
27	B8	263	G	N1-C6-O6	8.84	125.20	119.90
27	B8	524	G	C5-C6-O6	-8.84	123.30	128.60
27	B8	620	G	N1-C6-O6	8.84	125.20	119.90
27	B8	1994	C	O4'-C1'-N1	8.84	115.27	108.20
1	AA	423	G	N1-C6-O6	8.84	125.20	119.90
27	B8	1875	G	N1-C6-O6	8.84	125.20	119.90
27	B8	2529	G	N1-C6-O6	8.84	125.20	119.90
27	B8	2795	C	O4'-C1'-N1	8.84	115.27	108.20
1	AA	646	G	N1-C6-O6	8.83	125.20	119.90
1	AA	750	C	O4'-C1'-N1	8.83	115.27	108.20
27	B8	1753	G	N1-C6-O6	8.83	125.20	119.90
27	B8	2536	G	N1-C6-O6	8.83	125.20	119.90
27	B8	1283	G	N1-C6-O6	8.83	125.20	119.90
27	B8	2120	G	N1-C6-O6	8.83	125.20	119.90
27	B8	2843	G	N1-C6-O6	8.83	125.20	119.90
1	AA	674	G	C5-C6-O6	-8.83	123.30	128.60
27	B8	1903	G	N1-C6-O6	8.83	125.20	119.90
27	B8	2549	G	N1-C6-O6	8.83	125.20	119.90
27	B8	1374	G	N1-C6-O6	8.83	125.20	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1884	G	N1-C6-O6	8.83	125.19	119.90
1	AA	1057	G	N1-C6-O6	8.82	125.19	119.90
27	B8	86	G	C5-C6-O6	-8.82	123.31	128.60
27	B8	2853	C	O4'-C1'-N1	8.82	115.26	108.20
1	AA	963	G	N1-C6-O6	8.82	125.19	119.90
26	B7	113	C	O4'-C1'-N1	8.82	115.26	108.20
27	B8	48	G	N1-C6-O6	8.82	125.19	119.90
27	B8	51	G	N1-C6-O6	8.82	125.19	119.90
27	B8	473	G	N1-C6-O6	8.82	125.19	119.90
27	B8	2357	G	N1-C6-O6	8.82	125.19	119.90
27	B8	2360	G	N1-C6-O6	8.82	125.19	119.90
1	AA	378	G	N1-C6-O6	8.82	125.19	119.90
1	AA	869	G	N1-C6-O6	8.82	125.19	119.90
26	B7	116	G	N1-C6-O6	8.82	125.19	119.90
27	B8	1277	G	N1-C6-O6	8.82	125.19	119.90
27	B8	1873	G	N1-C6-O6	8.82	125.19	119.90
27	B8	664	G	N1-C6-O6	8.82	125.19	119.90
27	B8	2239	G	N1-C6-O6	8.82	125.19	119.90
27	B8	2870	C	O4'-C1'-N1	8.82	115.25	108.20
1	AA	406	G	N1-C6-O6	8.81	125.19	119.90
1	AA	1209	C	O4'-C1'-N1	8.81	115.25	108.20
27	B8	1186	G	N1-C6-O6	8.81	125.19	119.90
1	AA	255	G	N1-C6-O6	8.81	125.19	119.90
27	B8	1888	G	N1-C6-O6	8.81	125.19	119.90
1	AA	469	C	O4'-C1'-N1	8.81	115.25	108.20
27	B8	338	G	N1-C6-O6	8.81	125.19	119.90
27	B8	1649	G	C5-C6-O6	-8.81	123.31	128.60
27	B8	1763	G	N1-C6-O6	8.81	125.19	119.90
27	B8	1869	G	N1-C6-O6	8.81	125.19	119.90
27	B8	80	G	N1-C6-O6	8.81	125.19	119.90
1	AA	278	G	N1-C6-O6	8.81	125.18	119.90
1	AA	1488	G	N1-C6-O6	8.81	125.18	119.90
3	AV	72	C	O4'-C1'-N1	8.80	115.24	108.20
27	B8	58	G	N1-C6-O6	8.80	125.18	119.90
27	B8	372	G	N1-C6-O6	8.80	125.18	119.90
27	B8	855	G	N1-C6-O6	8.80	125.18	119.90
1	AA	1013	G	N1-C6-O6	8.80	125.18	119.90
27	B8	2465	C	O4'-C1'-N1	8.80	115.24	108.20
3	AV	43	G	N1-C6-O6	8.80	125.18	119.90
26	B7	17	C	O4'-C1'-N1	8.80	115.24	108.20
27	B8	950	G	N1-C6-O6	8.80	125.18	119.90
27	B8	818	G	N1-C6-O6	8.80	125.18	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1975	G	C5-C6-O6	-8.80	123.32	128.60
27	B8	2157	G	N1-C6-O6	8.80	125.18	119.90
27	B8	583	G	N1-C6-O6	8.79	125.18	119.90
27	B8	2455	G	N1-C6-O6	8.79	125.18	119.90
1	AA	584	G	C5-C6-O6	-8.79	123.32	128.60
26	B7	24	G	N1-C6-O6	8.79	125.18	119.90
27	B8	577	G	N1-C6-O6	8.79	125.18	119.90
1	AA	470	C	O4'-C1'-N1	8.79	115.23	108.20
27	B8	1243	C	O4'-C1'-N1	8.79	115.23	108.20
27	B8	2668	G	N1-C6-O6	8.79	125.17	119.90
3	AV	35	G	N1-C6-O6	8.79	125.17	119.90
26	B7	117	G	N1-C6-O6	8.79	125.17	119.90
27	B8	1288	G	N1-C6-O6	8.79	125.17	119.90
27	B8	1687	G	N1-C6-O6	8.79	125.17	119.90
27	B8	2049	G	N1-C6-O6	8.79	125.17	119.90
27	B8	418	C	O4'-C1'-N1	8.79	115.23	108.20
27	B8	2027	G	C5-C6-O6	-8.79	123.33	128.60
1	AA	1048	G	C5-C6-O6	-8.79	123.33	128.60
1	AA	581	G	N1-C6-O6	8.78	125.17	119.90
27	B8	157	C	O4'-C1'-N1	8.78	115.23	108.20
27	B8	2253	G	N1-C6-O6	8.78	125.17	119.90
27	B8	2446	G	N1-C6-O6	8.79	125.17	119.90
1	AA	350	G	N1-C6-O6	8.78	125.17	119.90
27	B8	248	G	C5-C6-O6	-8.78	123.33	128.60
27	B8	1074	G	N1-C6-O6	8.78	125.17	119.90
27	B8	1003	G	N1-C6-O6	8.78	125.17	119.90
27	B8	1110	G	N1-C6-O6	8.78	125.17	119.90
27	B8	1271	G	N1-C6-O6	8.78	125.17	119.90
27	B8	2524	G	N1-C6-O6	8.78	125.17	119.90
1	AA	481	G	N1-C6-O6	8.78	125.17	119.90
1	AA	966	G	N1-C6-O6	8.78	125.17	119.90
27	B8	1710	G	N1-C6-O6	8.78	125.17	119.90
27	B8	2592	G	C5-C6-O6	-8.78	123.33	128.60
1	AA	108	G	N1-C6-O6	8.78	125.17	119.90
1	AA	1387	G	N1-C6-O6	8.78	125.17	119.90
27	B8	2825	G	N1-C6-O6	8.78	125.17	119.90
27	B8	2834	G	N1-C6-O6	8.78	125.17	119.90
1	AA	394	G	N1-C6-O6	8.78	125.17	119.90
1	AA	1255	G	C5-C6-O6	-8.78	123.33	128.60
27	B8	2162	G	N1-C6-O6	8.78	125.17	119.90
1	AA	275	G	C5-C6-O6	-8.77	123.34	128.60
1	AA	656	G	N1-C6-O6	8.77	125.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1466	C	O4'-C1'-N1	8.77	115.22	108.20
27	B8	1839	G	N1-C6-O6	8.77	125.16	119.90
27	B8	2065	C	O4'-C1'-N1	8.77	115.22	108.20
27	B8	2623	G	C5-C6-O6	-8.77	123.34	128.60
1	AA	947	G	N1-C6-O6	8.77	125.16	119.90
27	B8	808	G	N1-C6-O6	8.77	125.16	119.90
27	B8	1619	G	N1-C6-O6	8.77	125.16	119.90
27	B8	1024	G	N1-C6-O6	8.77	125.16	119.90
27	B8	1356	G	N1-C6-O6	8.77	125.16	119.90
27	B8	1408	G	N1-C6-O6	8.77	125.16	119.90
27	B8	1986	C	O4'-C1'-N1	8.77	115.21	108.20
1	AA	713	G	N1-C6-O6	8.77	125.16	119.90
27	B8	69	C	O4'-C1'-N1	8.77	115.21	108.20
27	B8	257	C	O4'-C1'-N1	8.77	115.21	108.20
27	B8	857	G	N1-C6-O6	8.77	125.16	119.90
27	B8	1831	G	N1-C6-O6	8.77	125.16	119.90
1	AA	700	G	N1-C6-O6	8.76	125.16	119.90
1	AA	745	G	N1-C6-O6	8.76	125.16	119.90
27	B8	1051	G	N1-C6-O6	8.76	125.16	119.90
27	B8	2811	G	N1-C6-O6	8.76	125.16	119.90
27	B8	68	G	N1-C6-O6	8.76	125.16	119.90
27	B8	672	C	O4'-C1'-N1	8.76	115.21	108.20
27	B8	1049	C	O4'-C1'-N1	8.76	115.21	108.20
27	B8	2271	G	N1-C6-O6	8.76	125.16	119.90
27	B8	1823	G	N1-C6-O6	8.76	125.16	119.90
1	AA	281	G	N1-C6-O6	8.76	125.15	119.90
27	B8	117	G	N1-C6-O6	8.76	125.16	119.90
27	B8	1471	G	N1-C6-O6	8.76	125.15	119.90
1	AA	202	G	N1-C6-O6	8.75	125.15	119.90
1	AA	726	C	O4'-C1'-N1	8.75	115.20	108.20
27	B8	1346	G	N1-C6-O6	8.75	125.15	119.90
27	B8	1971	U	O4'-C1'-N1	8.75	115.20	108.20
27	B8	39	G	N1-C6-O6	8.75	125.15	119.90
27	B8	1702	G	N1-C6-O6	8.75	125.15	119.90
27	B8	555	G	N1-C6-O6	8.75	125.15	119.90
27	B8	663	G	C5-C6-O6	-8.75	123.35	128.60
27	B8	1292	G	N1-C6-O6	8.75	125.15	119.90
27	B8	2447	G	C5-C6-O6	-8.75	123.35	128.60
3	AV	45	G	N1-C6-O6	8.75	125.15	119.90
1	AA	661	G	N1-C6-O6	8.75	125.15	119.90
1	AA	852	G	N1-C6-O6	8.75	125.15	119.90
27	B8	130	C	O4'-C1'-N1	8.75	115.20	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	904	G	N1-C6-O6	8.75	125.15	119.90
27	B8	2780	G	N1-C6-O6	8.75	125.15	119.90
27	B8	334	C	O4'-C1'-N1	8.74	115.20	108.20
1	AA	858	G	N1-C6-O6	8.74	125.15	119.90
1	AA	1317	C	O4'-C1'-N1	8.74	115.19	108.20
26	B7	72	G	N1-C6-O6	8.74	125.15	119.90
27	B8	30	G	N1-C6-O6	8.74	125.15	119.90
27	B8	2237	G	N1-C6-O6	8.74	125.15	119.90
27	B8	2805	C	O4'-C1'-N1	8.74	115.20	108.20
27	B8	1025	G	N1-C6-O6	8.74	125.14	119.90
27	B8	1934	C	O4'-C1'-N1	8.74	115.19	108.20
27	B8	1699	G	N1-C6-O6	8.74	125.14	119.90
27	B8	1989	G	N1-C6-O6	8.74	125.14	119.90
27	B8	376	G	N1-C6-O6	8.74	125.14	119.90
1	AA	360	G	N1-C6-O6	8.73	125.14	119.90
1	AA	1024	G	N1-C6-O6	8.73	125.14	119.90
27	B8	379	G	N1-C6-O6	8.73	125.14	119.90
1	AA	844	G	N1-C6-O6	8.73	125.14	119.90
1	AA	1231	G	N1-C6-O6	8.73	125.14	119.90
27	B8	370	G	N1-C6-O6	8.73	125.14	119.90
27	B8	2553	G	N1-C6-O6	8.73	125.14	119.90
1	AA	575	G	N1-C6-O6	8.73	125.14	119.90
1	AA	1297	G	N1-C6-O6	8.73	125.14	119.90
1	AA	169	C	O4'-C1'-N1	8.73	115.18	108.20
27	B8	1627	G	C5-C6-O6	-8.73	123.36	128.60
27	B8	2368	C	O4'-C1'-N1	8.73	115.18	108.20
27	B8	2723	C	O4'-C1'-N1	8.73	115.18	108.20
1	AA	752	G	N1-C6-O6	8.72	125.14	119.90
1	AA	1003	G	N1-C6-O6	8.72	125.14	119.90
1	AA	193	C	O4'-C1'-N1	8.72	115.18	108.20
1	AA	616	G	C5-C6-O6	-8.72	123.37	128.60
1	AA	888	G	N1-C6-O6	8.72	125.13	119.90
27	B8	1311	G	N1-C6-O6	8.72	125.13	119.90
27	B8	489	G	N1-C6-O6	8.72	125.13	119.90
1	AA	346	G	N1-C6-O6	8.72	125.13	119.90
1	AA	606	G	N1-C6-O6	8.72	125.13	119.90
26	B7	102	G	N1-C6-O6	8.72	125.13	119.90
27	B8	517	C	O4'-C1'-N1	8.72	115.17	108.20
27	B8	891	G	O4'-C1'-N9	8.72	115.17	108.20
27	B8	98	G	N1-C6-O6	8.72	125.13	119.90
1	AA	769	G	N1-C6-O6	8.71	125.13	119.90
27	B8	1426	G	N1-C6-O6	8.71	125.13	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	517	G	N1-C6-O6	8.71	125.13	119.90
27	B8	2	G	N1-C6-O6	8.71	125.13	119.90
27	B8	1473	G	N1-C6-O6	8.71	125.13	119.90
27	B8	1756	G	N1-C6-O6	8.71	125.13	119.90
27	B8	2076	U	O4'-C1'-N1	8.71	115.17	108.20
27	B8	2532	G	N1-C6-O6	8.71	125.13	119.90
1	AA	112	G	N1-C6-O6	8.71	125.13	119.90
1	AA	398	U	O4'-C1'-N1	8.71	115.17	108.20
1	AA	419	C	O4'-C1'-N1	8.70	115.16	108.20
1	AA	1277	C	O4'-C1'-N1	8.71	115.16	108.20
27	B8	1827	U	O4'-C1'-N1	8.71	115.16	108.20
27	B8	2319	G	N1-C6-O6	8.71	125.12	119.90
27	B8	2379	G	N1-C6-O6	8.70	125.12	119.90
1	AA	357	G	N1-C6-O6	8.70	125.12	119.90
1	AA	524	G	N1-C6-O6	8.70	125.12	119.90
1	AA	1166	G	N1-C6-O6	8.70	125.12	119.90
27	B8	393	C	O4'-C1'-N1	8.70	115.16	108.20
27	B8	1703	G	N1-C6-O6	8.70	125.12	119.90
1	AA	1409	C	O4'-C1'-N1	8.70	115.16	108.20
27	B8	247	G	N1-C6-O6	8.70	125.12	119.90
27	B8	711	G	N1-C6-O6	8.70	125.12	119.90
1	AA	503	C	O4'-C1'-N1	8.69	115.16	108.20
1	AA	1316	G	N1-C6-O6	8.70	125.12	119.90
1	AA	1326	U	O4'-C1'-N1	8.69	115.16	108.20
27	B8	1432	G	N1-C6-O6	8.69	125.12	119.90
27	B8	2735	G	N1-C6-O6	8.69	125.12	119.90
1	AA	690	G	N1-C6-O6	8.69	125.11	119.90
1	AA	698	G	N1-C6-O6	8.69	125.11	119.90
1	AA	1099	G	N1-C6-O6	8.69	125.11	119.90
3	AV	44	G	N1-C6-O6	8.69	125.11	119.90
27	B8	725	G	N1-C6-O6	8.69	125.11	119.90
27	B8	1950	G	N1-C6-O6	8.69	125.11	119.90
27	B8	600	G	N1-C6-O6	8.69	125.11	119.90
27	B8	1542	U	O4'-C1'-N1	8.69	115.15	108.20
1	AA	172	A	N1-C6-N6	8.69	123.81	118.60
27	B8	704	G	N1-C6-O6	8.69	125.11	119.90
27	B8	805	G	N1-C6-O6	8.69	125.11	119.90
27	B8	2791	G	N1-C6-O6	8.69	125.11	119.90
1	AA	886	G	N1-C6-O6	8.69	125.11	119.90
1	AA	940	C	O4'-C1'-N1	8.69	115.15	108.20
27	B8	328	U	O4'-C1'-N1	8.69	115.15	108.20
27	B8	2144	G	N1-C6-O6	8.69	125.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2676	C	O4'-C1'-N1	8.69	115.15	108.20
27	B8	548	G	N1-C6-O6	8.69	125.11	119.90
27	B8	671	C	O4'-C1'-N1	8.69	115.15	108.20
27	B8	2462	C	O4'-C1'-N1	8.69	115.15	108.20
1	AA	1087	G	C5-C6-O6	-8.68	123.39	128.60
26	B7	112	G	C5-C6-O6	-8.68	123.39	128.60
27	B8	1279	G	N1-C6-O6	8.68	125.11	119.90
27	B8	1667	G	N1-C6-O6	8.68	125.11	119.90
1	AA	637	C	O4'-C1'-N1	8.68	115.14	108.20
1	AA	1182	G	N1-C6-O6	8.68	125.11	119.90
1	AA	506	G	N1-C6-O6	8.68	125.11	119.90
1	AA	1475	G	N1-C6-O6	8.68	125.11	119.90
27	B8	273	G	C5-C6-O6	-8.68	123.39	128.60
27	B8	1237	A	O4'-C1'-N9	8.68	115.14	108.20
2	AX	14	G	N1-C6-O6	8.68	125.11	119.90
26	B7	62	C	O4'-C1'-N1	8.68	115.14	108.20
27	B8	1930	G	N1-C6-O6	8.67	125.10	119.90
27	B8	2193	G	N1-C6-O6	8.67	125.10	119.90
27	B8	2638	G	N1-C6-O6	8.67	125.10	119.90
1	AA	761	G	N1-C6-O6	8.67	125.10	119.90
27	B8	159	G	N1-C6-O6	8.67	125.10	119.90
27	B8	1770	G	N1-C6-O6	8.67	125.10	119.90
1	AA	568	G	N1-C6-O6	8.67	125.10	119.90
1	AA	1432	G	N1-C6-O6	8.67	125.10	119.90
26	B7	71	C	O4'-C1'-N1	8.67	115.13	108.20
27	B8	1437	C	O4'-C1'-N1	8.67	115.13	108.20
27	B8	2138	G	N1-C6-O6	8.67	125.10	119.90
27	B8	43	G	N1-C6-O6	8.66	125.10	119.90
1	AA	1074	G	N1-C6-O6	8.66	125.10	119.90
27	B8	488	G	N1-C6-O6	8.66	125.10	119.90
1	AA	515	G	N1-C6-O6	8.66	125.10	119.90
27	B8	2737	G	N1-C6-O6	8.66	125.10	119.90
27	B8	533	G	C5-C6-O6	-8.66	123.41	128.60
27	B8	1099	G	C5-C6-O6	-8.66	123.41	128.60
27	B8	2353	G	N1-C6-O6	8.66	125.09	119.90
27	B8	2429	G	N1-C6-O6	8.66	125.09	119.90
1	AA	113	G	C5-C6-O6	-8.65	123.41	128.60
1	AA	628	G	N1-C6-O6	8.65	125.09	119.90
1	AA	856	C	O4'-C1'-N1	8.65	115.12	108.20
27	B8	495	G	N1-C6-O6	8.65	125.09	119.90
3	AV	37	G	N1-C6-O6	8.65	125.09	119.90
27	B8	579	G	C5-C6-O6	-8.65	123.41	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	336	C	O4'-C1'-N1	8.65	115.12	108.20
27	B8	506	G	N1-C6-O6	8.65	125.09	119.90
27	B8	707	G	N1-C6-O6	8.65	125.09	119.90
27	B8	651	G	N1-C6-O6	8.65	125.09	119.90
27	B8	2535	G	C5-C6-O6	-8.65	123.41	128.60
27	B8	2775	G	N1-C6-O6	8.65	125.09	119.90
27	B8	876	C	O4'-C1'-N1	8.65	115.12	108.20
27	B8	2659	G	N1-C6-O6	8.65	125.09	119.90
1	AA	1134	G	N1-C6-O6	8.65	125.09	119.90
27	B8	601	C	O4'-C1'-N1	8.65	115.12	108.20
1	AA	1222	G	N1-C6-O6	8.64	125.09	119.90
1	AA	1489	G	N1-C6-O6	8.64	125.09	119.90
27	B8	2364	C	O4'-C1'-N1	8.64	115.12	108.20
3	AV	20	G	N1-C6-O6	8.64	125.09	119.90
27	B8	2673	G	C5-C6-O6	-8.64	123.41	128.60
1	AA	1113	C	O4'-C1'-N1	8.64	115.11	108.20
27	B8	1115	G	N1-C6-O6	8.64	125.08	119.90
27	B8	2699	C	O4'-C1'-N1	8.64	115.11	108.20
27	B8	2751	G	N1-C6-O6	8.64	125.08	119.90
1	AA	1455	G	C5-C6-O6	-8.64	123.42	128.60
27	B8	625	G	N1-C6-O6	8.64	125.08	119.90
27	B8	2255	G	N1-C6-O6	8.64	125.08	119.90
27	B8	2544	G	C5-C6-O6	-8.64	123.42	128.60
1	AA	187	G	N1-C6-O6	8.64	125.08	119.90
27	B8	713	G	N1-C6-O6	8.64	125.08	119.90
27	B8	882	G	N1-C6-O6	8.63	125.08	119.90
27	B8	2365	G	N1-C6-O6	8.63	125.08	119.90
27	B8	2808	G	N1-C6-O6	8.63	125.08	119.90
27	B8	2822	G	N1-C6-O6	8.63	125.08	119.90
1	AA	75	G	C5-C6-O6	-8.63	123.42	128.60
27	B8	2885	G	N1-C6-O6	8.63	125.08	119.90
1	AA	733	G	N1-C6-O6	8.63	125.08	119.90
1	AA	1417	G	N1-C6-O6	8.63	125.08	119.90
27	B8	426	C	O4'-C1'-N1	8.63	115.11	108.20
27	B8	2045	C	O4'-C1'-N1	8.63	115.11	108.20
27	B8	2663	G	N1-C6-O6	8.63	125.08	119.90
1	AA	1172	C	O4'-C1'-N1	8.63	115.10	108.20
1	AA	1398	A	O4'-C1'-N9	8.63	115.10	108.20
26	B7	4	C	O4'-C1'-N1	8.63	115.10	108.20
27	B8	474	G	N1-C6-O6	8.63	125.08	119.90
27	B8	2338	C	O4'-C1'-N1	8.63	115.10	108.20
1	AA	1347	G	N1-C6-O6	8.62	125.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AV	12	G	N1-C6-O6	8.62	125.08	119.90
27	B8	493	G	N1-C6-O6	8.62	125.08	119.90
27	B8	1551	A	P-O3'-C3'	8.62	130.05	119.70
27	B8	2342	C	O4'-C1'-N1	8.63	115.10	108.20
27	B8	2289	G	N1-C6-O6	8.62	125.07	119.90
27	B8	2608	G	N1-C6-O6	8.62	125.08	119.90
1	AA	145	G	C5-C6-O6	-8.62	123.43	128.60
1	AA	310	G	N1-C6-O6	8.62	125.07	119.90
27	B8	757	G	C5-C6-O6	-8.62	123.43	128.60
1	AA	35	G	N1-C6-O6	8.62	125.07	119.90
1	AA	305	G	N1-C6-O6	8.62	125.07	119.90
1	AA	1331	G	N1-C6-O6	8.62	125.07	119.90
27	B8	1929	G	N1-C6-O6	8.62	125.07	119.90
27	B8	2127	G	N1-C6-O6	8.62	125.07	119.90
1	AA	297	G	N1-C6-O6	8.62	125.07	119.90
27	B8	1034	G	C5-C6-O6	-8.62	123.43	128.60
27	B8	143	C	O4'-C1'-N1	8.62	115.09	108.20
27	B8	1646	C	O4'-C1'-N1	8.62	115.09	108.20
27	B8	318	C	O4'-C1'-N1	8.62	115.09	108.20
27	B8	253	C	O4'-C1'-N1	8.62	115.09	108.20
27	B8	726	G	N1-C6-O6	8.62	125.07	119.90
27	B8	570	G	N1-C6-O6	8.61	125.07	119.90
27	B8	1092	C	O4'-C1'-N1	8.62	115.09	108.20
27	B8	1493	C	O4'-C1'-N1	8.62	115.09	108.20
27	B8	1538	G	C5-C6-O6	-8.62	123.43	128.60
1	AA	311	C	O4'-C1'-N1	8.61	115.09	108.20
1	AA	537	G	N1-C6-O6	8.61	125.07	119.90
27	B8	1333	G	N1-C6-O6	8.61	125.07	119.90
27	B8	1456	G	N1-C6-O6	8.61	125.07	119.90
1	AA	677	U	O4'-C1'-N1	8.61	115.09	108.20
1	AA	829	G	N1-C6-O6	8.61	125.07	119.90
1	AA	857	C	O4'-C1'-N1	8.61	115.09	108.20
1	AA	691	G	N1-C6-O6	8.61	125.06	119.90
27	B8	869	G	N1-C6-O6	8.61	125.07	119.90
27	B8	1364	G	N1-C6-O6	8.61	125.07	119.90
27	B8	2860	A	C4-C5-C6	8.61	121.31	117.00
27	B8	2863	C	O4'-C1'-N1	8.61	115.09	108.20
27	B8	623	C	O4'-C1'-N1	8.61	115.09	108.20
27	B8	891	G	N1-C6-O6	8.61	125.06	119.90
27	B8	1235	G	N1-C6-O6	8.61	125.06	119.90
27	B8	2331	G	N1-C6-O6	8.61	125.06	119.90
1	AA	370	C	O4'-C1'-N1	8.60	115.08	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1718	G	N1-C6-O6	8.60	125.06	119.90
27	B8	1857	G	N1-C6-O6	8.60	125.06	119.90
1	AA	626	G	C5-C6-O6	-8.60	123.44	128.60
1	AA	351	G	N1-C6-O6	8.60	125.06	119.90
3	AV	40	G	N1-C6-O6	8.60	125.06	119.90
27	B8	1907	G	C5-C6-O6	-8.60	123.44	128.60
1	AA	1521	C	O4'-C1'-N1	8.60	115.08	108.20
27	B8	2159	G	N1-C6-O6	8.60	125.06	119.90
1	AA	107	G	N1-C6-O6	8.60	125.06	119.90
1	AA	1094	G	N1-C6-O6	8.60	125.06	119.90
27	B8	2607	G	N1-C6-O6	8.59	125.06	119.90
27	B8	1459	G	N1-C6-O6	8.59	125.05	119.90
27	B8	1956	U	O4'-C1'-N1	8.59	115.07	108.20
1	AA	83	C	O4'-C1'-N1	8.59	115.07	108.20
1	AA	647	C	O4'-C1'-N1	8.59	115.07	108.20
1	AA	1278	G	N1-C6-O6	8.59	125.05	119.90
2	AX	20	G	N1-C6-O6	8.59	125.05	119.90
27	B8	481	G	N1-C6-O6	8.59	125.05	119.90
27	B8	1807	G	N1-C6-O6	8.59	125.05	119.90
27	B8	341	C	O4'-C1'-N1	8.58	115.07	108.20
27	B8	669	G	N1-C6-O6	8.58	125.05	119.90
27	B8	2470	G	N1-C6-O6	8.58	125.05	119.90
27	B8	446	G	N1-C6-O6	8.58	125.05	119.90
27	B8	634	C	O4'-C1'-N1	8.58	115.06	108.20
27	B8	1726	C	O4'-C1'-N1	8.58	115.06	108.20
27	B8	1068	G	N1-C6-O6	8.58	125.05	119.90
1	AA	134	G	N1-C6-O6	8.58	125.05	119.90
1	AA	1193	G	C5-C6-O6	-8.58	123.45	128.60
27	B8	22	C	O4'-C1'-N1	8.58	115.06	108.20
1	AA	159	G	N1-C6-O6	8.57	125.05	119.90
3	AV	7	G	N1-C6-O6	8.57	125.05	119.90
26	B7	105	G	N1-C6-O6	8.57	125.05	119.90
27	B8	500	G	N1-C6-O6	8.57	125.05	119.90
27	B8	561	G	N1-C6-O6	8.57	125.05	119.90
27	B8	1005	C	O4'-C1'-N1	8.57	115.06	108.20
27	B8	1501	G	N1-C6-O6	8.57	125.04	119.90
27	B8	1879	C	O4'-C1'-N1	8.57	115.06	108.20
27	B8	2658	C	O4'-C1'-N1	8.57	115.06	108.20
1	AA	708	C	O4'-C1'-N1	8.57	115.06	108.20
1	AA	1178	G	N1-C6-O6	8.57	125.04	119.90
27	B8	1006	C	O4'-C1'-N1	8.57	115.06	108.20
27	B8	2018	G	N1-C6-O6	8.57	125.04	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2206	C	O4'-C1'-N1	8.57	115.06	108.20
27	B8	2351	G	N1-C6-O6	8.57	125.04	119.90
27	B8	308	G	N1-C6-O6	8.57	125.04	119.90
27	B8	718	A	O4'-C1'-N9	8.57	115.06	108.20
27	B8	858	G	N1-C6-O6	8.57	125.04	119.90
27	B8	1339	G	N1-C6-O6	8.57	125.04	119.90
1	AA	290	C	O4'-C1'-N1	8.57	115.05	108.20
1	AA	501	C	O4'-C1'-N1	8.57	115.05	108.20
1	AA	1156	G	N1-C6-O6	8.57	125.04	119.90
3	AV	53	G	N1-C6-O6	8.57	125.04	119.90
27	B8	47	C	O4'-C1'-N1	8.57	115.05	108.20
27	B8	1844	C	O4'-C1'-N1	8.57	115.05	108.20
27	B8	2363	G	C5-C6-O6	-8.57	123.46	128.60
27	B8	1760	C	O4'-C1'-N1	8.57	115.05	108.20
27	B8	2787	C	O4'-C1'-N1	8.56	115.05	108.20
1	AA	359	G	C5-C6-O6	-8.56	123.46	128.60
3	AV	7	G	P-O3'-C3'	8.56	129.98	119.70
27	B8	381	G	N1-C6-O6	8.56	125.04	119.90
27	B8	417	C	O4'-C1'-N1	8.56	115.05	108.20
1	AA	1020	G	C5-C6-O6	-8.56	123.46	128.60
27	B8	367	G	N1-C6-O6	8.56	125.04	119.90
26	B7	114	C	O4'-C1'-N1	8.56	115.05	108.20
27	B8	1521	G	N1-C6-O6	8.56	125.04	119.90
27	B8	1550	C	O4'-C1'-N1	8.56	115.05	108.20
1	AA	128	G	N1-C6-O6	8.56	125.03	119.90
27	B8	2072	C	O4'-C1'-N1	8.56	115.05	108.20
27	B8	2156	G	N1-C6-O6	8.56	125.03	119.90
26	B7	91	C	O4'-C1'-N1	8.56	115.05	108.20
1	AA	667	G	C5-C6-O6	-8.55	123.47	128.60
26	B7	13	G	N1-C6-O6	8.55	125.03	119.90
27	B8	1715	G	N1-C6-O6	8.55	125.03	119.90
27	B8	2678	C	O4'-C1'-N1	8.55	115.04	108.20
27	B8	444	C	O4'-C1'-N1	8.55	115.04	108.20
27	B8	703	U	O4'-C1'-N1	8.55	115.04	108.20
27	B8	1812	U	O4'-C1'-N1	8.55	115.04	108.20
27	B8	2141	G	C5-C6-O6	-8.55	123.47	128.60
27	B8	2370	G	N1-C6-O6	8.55	125.03	119.90
27	B8	1	G	C5-C6-O6	-8.55	123.47	128.60
27	B8	2719	G	N1-C6-O6	8.55	125.03	119.90
1	AA	926	G	N1-C6-O6	8.54	125.03	119.90
27	B8	1483	G	N1-C6-O6	8.54	125.03	119.90
1	AA	272	C	O4'-C1'-N1	8.54	115.03	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	664	G	N1-C6-O6	8.54	125.03	119.90
27	B8	1298	C	O4'-C1'-N1	8.54	115.03	108.20
27	B8	2207	C	O4'-C1'-N1	8.54	115.03	108.20
27	B8	2688	G	N1-C6-O6	8.54	125.03	119.90
27	B8	1738	G	N1-C6-O6	8.54	125.02	119.90
1	AA	683	G	N1-C6-O6	8.54	125.02	119.90
26	B7	2	G	N1-C6-O6	8.54	125.02	119.90
27	B8	440	C	O4'-C1'-N1	8.54	115.03	108.20
27	B8	1227	G	N1-C6-O6	8.54	125.02	119.90
27	B8	2066	C	O4'-C1'-N1	8.54	115.03	108.20
27	B8	2749	A	N1-C6-N6	8.54	123.72	118.60
27	B8	2902	C	O4'-C1'-N1	8.54	115.03	108.20
1	AA	890	G	N1-C6-O6	8.54	125.02	119.90
1	AA	1079	G	N1-C6-O6	8.54	125.02	119.90
27	B8	619	G	N1-C6-O6	8.54	125.02	119.90
27	B8	817	C	O4'-C1'-N1	8.54	115.03	108.20
3	AV	46	G	N1-C6-O6	8.53	125.02	119.90
1	AA	417	G	C5-C6-O6	-8.53	123.48	128.60
1	AA	1089	G	N1-C6-O6	8.53	125.02	119.90
27	B8	1793	C	O4'-C1'-N1	8.53	115.03	108.20
27	B8	2252	G	N1-C6-O6	8.53	125.02	119.90
1	AA	1184	G	C5-C6-O6	-8.53	123.48	128.60
27	B8	1460	U	O4'-C1'-N1	8.53	115.03	108.20
1	AA	1068	G	N1-C6-O6	8.53	125.02	119.90
1	AA	1487	G	N1-C6-O6	8.53	125.02	119.90
1	AA	489	C	O4'-C1'-N1	8.53	115.02	108.20
27	B8	809	G	C5-C6-O6	-8.53	123.48	128.60
1	AA	972	C	O4'-C1'-N1	8.53	115.02	108.20
27	B8	168	G	N1-C6-O6	8.53	125.02	119.90
27	B8	512	G	N1-C6-O6	8.53	125.02	119.90
27	B8	180	G	N1-C6-O6	8.53	125.02	119.90
27	B8	559	G	C5-C6-O6	-8.53	123.48	128.60
27	B8	597	G	N1-C6-O6	8.53	125.02	119.90
27	B8	2848	G	N1-C6-O6	8.53	125.02	119.90
1	AA	124	C	O4'-C1'-N1	8.52	115.02	108.20
27	B8	557	C	O4'-C1'-N1	8.52	115.02	108.20
1	AA	639	G	C5-C6-O6	-8.52	123.49	128.60
1	AA	727	G	N1-C6-O6	8.52	125.01	119.90
27	B8	494	G	N1-C6-O6	8.52	125.01	119.90
27	B8	2816	G	N1-C6-O6	8.52	125.01	119.90
1	AA	122	G	C5-C6-O6	-8.52	123.49	128.60
1	AA	376	G	N1-C6-O6	8.52	125.01	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	657	U	O4'-C1'-N1	8.52	115.01	108.20
1	AA	1416	G	N1-C6-O6	8.52	125.01	119.90
27	B8	530	G	N1-C6-O6	8.52	125.01	119.90
26	B7	23	G	C5-C6-O6	-8.51	123.49	128.60
27	B8	881	G	N1-C6-O6	8.51	125.01	119.90
27	B8	1252	G	N1-C6-O6	8.51	125.01	119.90
1	AA	15	G	C5-C6-O6	-8.51	123.49	128.60
1	AA	741	G	N1-C6-O6	8.51	125.01	119.90
1	AA	1516	G	N1-C6-O6	8.51	125.01	119.90
26	B7	76	G	N1-C6-O6	8.51	125.01	119.90
27	B8	1741	C	O4'-C1'-N1	8.51	115.01	108.20
27	B8	1985	C	O4'-C1'-N1	8.51	115.01	108.20
27	B8	2324	U	O4'-C1'-N1	8.51	115.01	108.20
3	AV	1	C	O4'-C1'-N1	8.51	115.01	108.20
26	B7	41	G	N1-C6-O6	8.51	125.01	119.90
27	B8	2742	G	N1-C6-O6	8.51	125.01	119.90
27	B8	1146	C	O4'-C1'-N1	8.51	115.01	108.20
27	B8	2089	C	O4'-C1'-N1	8.51	115.00	108.20
27	B8	93	G	N1-C6-O6	8.51	125.00	119.90
1	AA	1279	G	N1-C6-O6	8.50	125.00	119.90
27	B8	242	G	N1-C6-O6	8.50	125.00	119.90
27	B8	366	C	O4'-C1'-N1	8.50	115.00	108.20
27	B8	1315	C	O4'-C1'-N1	8.50	115.00	108.20
1	AA	651	C	O4'-C1'-N1	8.50	115.00	108.20
27	B8	55	G	N1-C6-O6	8.50	125.00	119.90
27	B8	317	G	N1-C6-O6	8.50	125.00	119.90
27	B8	1038	G	C5-C6-O6	-8.50	123.50	128.60
1	AA	810	C	O4'-C1'-N1	8.50	115.00	108.20
27	B8	745	G	N1-C6-O6	8.50	125.00	119.90
1	AA	1260	G	N1-C6-O6	8.50	125.00	119.90
27	B8	413	C	O4'-C1'-N1	8.50	115.00	108.20
27	B8	1585	C	O4'-C1'-N1	8.50	115.00	108.20
27	B8	2032	G	N1-C6-O6	8.50	125.00	119.90
27	B8	2056	G	C5-C6-O6	-8.50	123.50	128.60
27	B8	2083	G	N1-C6-O6	8.50	125.00	119.90
27	B8	2466	C	O4'-C1'-N1	8.50	115.00	108.20
26	B7	54	G	C5-C6-O6	-8.49	123.50	128.60
27	B8	1892	C	O4'-C1'-N1	8.49	115.00	108.20
27	B8	2637	U	O4'-C1'-N1	8.49	115.00	108.20
27	B8	442	G	C5-C6-O6	-8.49	123.51	128.60
27	B8	1355	G	N1-C6-O6	8.49	124.99	119.90
1	AA	403	C	O4'-C1'-N1	8.49	114.99	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	388	G	N1-C6-O6	8.49	124.99	119.90
27	B8	737	C	O4'-C1'-N1	8.49	114.99	108.20
27	B8	2481	G	N1-C6-O6	8.49	124.99	119.90
1	AA	457	G	C5-C6-O6	-8.48	123.51	128.60
1	AA	879	C	O4'-C1'-N1	8.48	114.99	108.20
27	B8	1440	U	O4'-C1'-N1	8.48	114.99	108.20
1	AA	260	G	N1-C6-O6	8.48	124.99	119.90
27	B8	1197	G	N1-C6-O6	8.48	124.99	119.90
27	B8	1529	G	N1-C6-O6	8.48	124.99	119.90
1	AA	658	C	O4'-C1'-N1	8.48	114.98	108.20
1	AA	1524	C	O4'-C1'-N1	8.48	114.98	108.20
26	B7	33	G	C5-C6-O6	-8.48	123.51	128.60
1	AA	322	C	O4'-C1'-N1	8.48	114.98	108.20
1	AA	1405	G	C5-C6-O6	-8.48	123.51	128.60
27	B8	398	C	O4'-C1'-N1	8.48	114.98	108.20
1	AA	302	G	C5-C6-O6	-8.47	123.52	128.60
27	B8	1817	G	N1-C6-O6	8.47	124.98	119.90
1	AA	1421	G	N1-C6-O6	8.47	124.98	119.90
26	B7	56	G	N1-C6-O6	8.47	124.98	119.90
27	B8	2444	G	N1-C6-O6	8.47	124.98	119.90
1	AA	832	G	N1-C6-O6	8.47	124.98	119.90
1	AA	1077	G	N1-C6-O6	8.47	124.98	119.90
27	B8	1233	C	O4'-C1'-N1	8.47	114.98	108.20
27	B8	1867	G	N1-C6-O6	8.47	124.98	119.90
1	AA	22	G	C5-C6-O6	-8.47	123.52	128.60
27	B8	1447	C	O4'-C1'-N1	8.47	114.97	108.20
27	B8	333	G	N1-C6-O6	8.47	124.98	119.90
27	B8	1492	G	C5-C6-O6	-8.47	123.52	128.60
27	B8	1543	G	N1-C6-O6	8.47	124.98	119.90
27	B8	1686	C	O4'-C1'-N1	8.47	114.97	108.20
27	B8	2627	G	N1-C6-O6	8.47	124.98	119.90
1	AA	258	G	C5-C6-O6	-8.47	123.52	128.60
1	AA	942	G	N1-C6-O6	8.46	124.98	119.90
27	B8	2035	G	N1-C6-O6	8.46	124.98	119.90
1	AA	380	G	N1-C6-O6	8.46	124.98	119.90
27	B8	1515	A	N1-C6-N6	8.46	123.68	118.60
1	AA	1369	C	O4'-C1'-N1	8.46	114.97	108.20
27	B8	696	G	N1-C6-O6	8.46	124.97	119.90
27	B8	1236	G	N1-C6-O6	8.46	124.97	119.90
27	B8	1983	G	N1-C6-O6	8.46	124.97	119.90
1	AA	248	C	O4'-C1'-N1	8.46	114.96	108.20
27	B8	2694	G	C5-C6-O6	-8.46	123.53	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	450	G	N1-C6-O6	8.45	124.97	119.90
27	B8	777	G	C5-C6-O6	-8.46	123.53	128.60
1	AA	785	G	C5-C6-O6	-8.45	123.53	128.60
1	AA	1453	G	N1-C6-O6	8.45	124.97	119.90
27	B8	1973	G	C5-C6-O6	-8.45	123.53	128.60
27	B8	2133	G	N1-C6-O6	8.45	124.97	119.90
27	B8	2378	A	C4-C5-C6	8.45	121.23	117.00
1	AA	488	C	O4'-C1'-N1	8.45	114.96	108.20
27	B8	814	C	O4'-C1'-N1	8.45	114.96	108.20
27	B8	1896	G	C5-C6-O6	-8.45	123.53	128.60
27	B8	396	G	C5-C6-O6	-8.44	123.53	128.60
27	B8	1964	G	C5-C6-O6	-8.44	123.53	128.60
27	B8	1423	G	N1-C6-O6	8.44	124.97	119.90
27	B8	1401	G	N1-C6-O6	8.44	124.97	119.90
27	B8	1541	C	O4'-C1'-N1	8.44	114.95	108.20
27	B8	2624	G	C5-C6-O6	-8.44	123.53	128.60
1	AA	4	U	O4'-C1'-N1	8.44	114.95	108.20
27	B8	2269	G	N1-C6-O6	8.44	124.96	119.90
27	B8	2437	G	C5-C6-O6	-8.44	123.54	128.60
27	B8	2594	C	O4'-C1'-N1	8.44	114.95	108.20
27	B8	2597	G	N1-C6-O6	8.44	124.96	119.90
1	AA	235	C	O4'-C1'-N1	8.44	114.95	108.20
1	AA	486	U	O4'-C1'-N1	8.44	114.95	108.20
27	B8	1843	C	O4'-C1'-N1	8.44	114.95	108.20
27	B8	2512	C	O4'-C1'-N1	8.44	114.95	108.20
1	AA	1384	C	O4'-C1'-N1	8.44	114.95	108.20
3	AV	68	G	N1-C6-O6	8.44	124.96	119.90
27	B8	1682	G	C5-C6-O6	-8.44	123.54	128.60
27	B8	192	C	O4'-C1'-N1	8.43	114.94	108.20
27	B8	2214	C	O4'-C1'-N1	8.43	114.95	108.20
1	AA	168	G	C5-C6-O6	-8.43	123.54	128.60
1	AA	1505	G	N1-C6-O6	8.43	124.96	119.90
1	AA	1018	G	N1-C6-O6	8.43	124.96	119.90
1	AA	1265	C	O4'-C1'-N1	8.43	114.94	108.20
1	AA	259	G	C5-C6-O6	-8.43	123.55	128.60
1	AA	941	G	N1-C6-O6	8.43	124.95	119.90
1	AA	257	G	N1-C6-O6	8.42	124.95	119.90
1	AA	650	G	N1-C6-O6	8.42	124.95	119.90
1	AA	1175	G	N1-C6-O6	8.42	124.95	119.90
27	B8	16	C	O4'-C1'-N1	8.42	114.94	108.20
27	B8	679	C	O4'-C1'-N1	8.42	114.94	108.20
27	B8	1947	C	O4'-C1'-N1	8.42	114.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	38	G	N1-C6-O6	8.42	124.95	119.90
27	B8	2858	C	O4'-C1'-N1	8.42	114.94	108.20
1	AA	440	C	O4'-C1'-N1	8.42	114.94	108.20
1	AA	931	C	O4'-C1'-N1	8.42	114.94	108.20
1	AA	326	G	N1-C6-O6	8.41	124.95	119.90
1	AA	800	G	N1-C6-O6	8.41	124.95	119.90
27	B8	880	G	N1-C6-O6	8.41	124.95	119.90
27	B8	1180	U	O4'-C1'-N1	8.41	114.93	108.20
27	B8	935	C	O4'-C1'-N1	8.41	114.93	108.20
27	B8	2576	G	N1-C6-O6	8.41	124.95	119.90
1	AA	215	C	O4'-C1'-N1	8.41	114.93	108.20
1	AA	614	C	O4'-C1'-N1	8.41	114.93	108.20
26	B7	97	C	O4'-C1'-N1	8.41	114.93	108.20
27	B8	1239	G	C5-C6-O6	-8.41	123.55	128.60
27	B8	316	C	O4'-C1'-N1	8.41	114.93	108.20
27	B8	1017	G	N1-C6-O6	8.41	124.94	119.90
27	B8	1061	U	C2-N1-C1'	8.41	127.79	117.70
27	B8	1183	U	O4'-C1'-N1	8.41	114.93	108.20
1	AA	1058	G	C5-C6-O6	-8.41	123.56	128.60
27	B8	2361	G	N1-C6-O6	8.41	124.94	119.90
1	AA	86	G	N1-C6-O6	8.40	124.94	119.90
27	B8	1695	G	N1-C6-O6	8.40	124.94	119.90
27	B8	2874	C	O4'-C1'-N1	8.40	114.92	108.20
1	AA	812	G	C5-C6-O6	-8.40	123.56	128.60
1	AA	1338	G	N1-C6-O6	8.40	124.94	119.90
27	B8	315	G	N1-C6-O6	8.40	124.94	119.90
27	B8	486	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	2294	G	N1-C6-O6	8.40	124.94	119.90
27	B8	2414	G	C5-C6-O6	-8.40	123.56	128.60
27	B8	564	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	765	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	1957	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	491	G	N1-C6-O6	8.40	124.94	119.90
27	B8	948	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	2055	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	2332	C	O4'-C1'-N1	8.40	114.92	108.20
27	B8	2591	C	O4'-C1'-N1	8.39	114.92	108.20
27	B8	2644	G	N1-C6-O6	8.39	124.94	119.90
1	AA	201	G	N1-C6-O6	8.39	124.94	119.90
27	B8	2842	G	N1-C6-O6	8.39	124.94	119.90
1	AA	1154	G	C5-C6-O6	-8.39	123.56	128.60
27	B8	2421	G	C5-C6-O6	-8.39	123.56	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1217	C	O4'-C1'-N1	8.39	114.91	108.20
27	B8	2124	G	C5-C6-O6	-8.39	123.57	128.60
27	B8	2215	C	O4'-C1'-N1	8.39	114.91	108.20
26	B7	118	C	O4'-C1'-N1	8.39	114.91	108.20
27	B8	1587	G	N1-C6-O6	8.39	124.93	119.90
27	B8	1908	C	O4'-C1'-N1	8.39	114.91	108.20
27	B8	2177	C	O4'-C1'-N1	8.38	114.91	108.20
27	B8	2264	C	O4'-C1'-N1	8.38	114.91	108.20
1	AA	818	G	N1-C6-O6	8.38	124.93	119.90
3	AV	19	G	N1-C6-O6	8.38	124.93	119.90
27	B8	830	G	N1-C6-O6	8.38	124.93	119.90
27	B8	922	C	O4'-C1'-N1	8.38	114.91	108.20
27	B8	1187	G	N1-C6-O6	8.38	124.93	119.90
27	B8	1788	C	O4'-C1'-N1	8.38	114.91	108.20
27	B8	2618	G	N1-C6-O6	8.38	124.93	119.90
27	B8	2655	G	N1-C6-O6	8.38	124.93	119.90
1	AA	1273	C	O4'-C1'-N1	8.38	114.90	108.20
1	AA	693	G	N1-C6-O6	8.38	124.93	119.90
1	AA	90	C	O4'-C1'-N1	8.38	114.90	108.20
1	AA	1203	C	O4'-C1'-N1	8.38	114.90	108.20
27	B8	951	C	O4'-C1'-N1	8.37	114.90	108.20
27	B8	1743	G	C5-C6-O6	-8.37	123.58	128.60
27	B8	2774	C	O4'-C1'-N1	8.38	114.90	108.20
27	B8	836	G	C5-C6-O6	-8.37	123.58	128.60
27	B8	662	G	C5-C6-O6	-8.37	123.58	128.60
27	B8	1704	C	O4'-C1'-N1	8.37	114.90	108.20
27	B8	2048	G	N1-C6-O6	8.37	124.92	119.90
27	B8	2397	G	N1-C6-O6	8.37	124.92	119.90
1	AA	1382	C	O4'-C1'-N1	8.37	114.90	108.20
27	B8	1935	G	N1-C6-O6	8.37	124.92	119.90
27	B8	452	G	N1-C6-O6	8.37	124.92	119.90
27	B8	1685	C	O4'-C1'-N1	8.37	114.89	108.20
27	B8	1931	U	O4'-C1'-N1	8.36	114.89	108.20
1	AA	211	G	N1-C6-O6	8.36	124.92	119.90
27	B8	2683	C	O4'-C1'-N1	8.36	114.89	108.20
27	B8	329	G	N1-C6-O6	8.36	124.92	119.90
27	B8	1331	G	N1-C6-O6	8.36	124.92	119.90
27	B8	2507	C	O4'-C1'-N1	8.36	114.89	108.20
3	AV	36	G	N1-C6-O6	8.36	124.91	119.90
1	AA	895	G	N1-C6-O6	8.35	124.91	119.90
1	AA	1259	C	O4'-C1'-N1	8.35	114.88	108.20
26	B7	81	G	C5-C6-O6	-8.35	123.59	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1464	G	N1-C6-O6	8.35	124.91	119.90
1	AA	97	G	N1-C6-O6	8.35	124.91	119.90
1	AA	1361	G	N1-C6-O6	8.35	124.91	119.90
27	B8	1967	C	O4'-C1'-N1	8.35	114.88	108.20
1	AA	1049	U	P-O3'-C3'	8.35	129.72	119.70
1	AA	1325	C	O4'-C1'-N1	8.35	114.88	108.20
27	B8	20	C	O4'-C1'-N1	8.34	114.87	108.20
27	B8	194	G	C5-C6-O6	-8.34	123.59	128.60
27	B8	795	C	O4'-C1'-N1	8.34	114.87	108.20
27	B8	1465	G	C5-C6-O6	-8.34	123.59	128.60
27	B8	2257	U	O4'-C1'-N1	8.34	114.87	108.20
27	B8	929	U	O4'-C1'-N1	8.34	114.87	108.20
27	B8	903	C	O4'-C1'-N1	8.34	114.87	108.20
27	B8	1140	C	O4'-C1'-N1	8.34	114.87	108.20
27	B8	1739	A	N1-C6-N6	8.34	123.60	118.60
1	AA	582	C	O4'-C1'-N1	8.34	114.87	108.20
1	AA	613	C	O4'-C1'-N1	8.34	114.87	108.20
1	AA	1016	A	C4-C5-C6	8.34	121.17	117.00
27	B8	2282	G	N1-C6-O6	8.34	124.90	119.90
27	B8	1184	U	O4'-C1'-N1	8.34	114.87	108.20
27	B8	846	U	O4'-C1'-N1	8.33	114.87	108.20
27	B8	1122	G	N1-C6-O6	8.33	124.90	119.90
27	B8	1026	G	N1-C6-O6	8.33	124.90	119.90
3	AV	65	C	O4'-C1'-N1	8.33	114.86	108.20
27	B8	1370	C	O4'-C1'-N1	8.33	114.86	108.20
27	B8	690	G	N1-C6-O6	8.33	124.90	119.90
1	AA	1461	G	N1-C6-O6	8.33	124.90	119.90
27	B8	260	G	C5-C6-O6	-8.33	123.60	128.60
27	B8	897	C	O4'-C1'-N1	8.33	114.86	108.20
26	B7	38	C	O4'-C1'-N1	8.32	114.86	108.20
27	B8	700	G	C5-C6-O6	-8.32	123.61	128.60
27	B8	748	G	N1-C6-O6	8.32	124.89	119.90
27	B8	1114	C	O4'-C1'-N1	8.32	114.86	108.20
1	AA	1164	G	C5-C6-O6	-8.32	123.61	128.60
27	B8	558	U	O4'-C1'-N1	8.32	114.86	108.20
27	B8	2410	G	C5-C6-O6	-8.32	123.61	128.60
27	B8	684	G	N1-C6-O6	8.32	124.89	119.90
3	AV	50	G	N1-C6-O6	8.32	124.89	119.90
27	B8	2140	G	C5-C6-O6	-8.32	123.61	128.60
1	AA	304	U	O4'-C1'-N1	8.31	114.85	108.20
1	AA	1148	U	O4'-C1'-N1	8.31	114.85	108.20
1	AA	1344	C	O4'-C1'-N1	8.31	114.85	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1362	C	O4'-C1'-N1	8.31	114.85	108.20
1	AA	1268	G	N1-C6-O6	8.31	124.89	119.90
1	AA	842	U	O4'-C1'-N1	8.31	114.85	108.20
1	AA	1515	G	C5-C6-O6	-8.31	123.61	128.60
27	B8	2224	G	N1-C6-O6	8.31	124.89	119.90
27	B8	1769	U	O4'-C1'-N1	8.31	114.85	108.20
27	B8	2595	G	N1-C6-O6	8.31	124.89	119.90
1	AA	21	G	N1-C6-O6	8.30	124.88	119.90
1	AA	936	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	1153	C	O4'-C1'-N1	8.31	114.84	108.20
1	AA	1038	C	O4'-C1'-N1	8.30	114.84	108.20
1	AA	1355	G	N1-C6-O6	8.30	124.88	119.90
27	B8	97	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	112	U	O4'-C1'-N1	8.30	114.84	108.20
27	B8	210	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	350	G	C5-C6-O6	-8.30	123.62	128.60
27	B8	784	G	O4'-C1'-N9	8.30	114.84	108.20
27	B8	977	G	C5-C6-O6	-8.30	123.62	128.60
27	B8	1575	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	2010	G	N1-C6-O6	8.30	124.88	119.90
1	AA	6	G	N1-C6-O6	8.30	124.88	119.90
26	B7	10	G	C5-C6-O6	-8.30	123.62	128.60
27	B8	186	G	C5-C6-O6	-8.30	123.62	128.60
27	B8	1605	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	2839	G	C5-C6-O6	-8.30	123.62	128.60
27	B8	854	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	870	U	O4'-C1'-N1	8.30	114.84	108.20
27	B8	1874	C	O4'-C1'-N1	8.30	114.84	108.20
26	B7	60	C	O4'-C1'-N1	8.30	114.84	108.20
27	B8	1300	G	N1-C6-O6	8.30	124.88	119.90
27	B8	2067	G	N1-C6-O6	8.30	124.88	119.90
1	AA	268	U	O4'-C1'-N1	8.29	114.83	108.20
1	AA	45	G	C5-C6-O6	-8.29	123.62	128.60
1	AA	633	G	N1-C6-O6	8.29	124.88	119.90
1	AA	882	C	O4'-C1'-N1	8.29	114.83	108.20
1	AA	910	C	O4'-C1'-N1	8.29	114.83	108.20
1	AA	985	C	O4'-C1'-N1	8.29	114.83	108.20
27	B8	2350	C	O4'-C1'-N1	8.29	114.83	108.20
1	AA	379	C	O4'-C1'-N1	8.29	114.83	108.20
27	B8	1056	G	N1-C6-O6	8.29	124.87	119.90
27	B8	1737	G	N1-C6-O6	8.29	124.87	119.90
27	B8	2417	C	O4'-C1'-N1	8.29	114.83	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2803	G	C5-C6-O6	-8.29	123.63	128.60
1	AA	594	U	O4'-C1'-N1	8.28	114.83	108.20
1	AA	216	U	O4'-C1'-N1	8.28	114.83	108.20
1	AA	519	C	O4'-C1'-N1	8.28	114.83	108.20
27	B8	1613	G	N1-C6-O6	8.28	124.87	119.90
1	AA	57	G	C5-C6-O6	-8.28	123.63	128.60
1	AA	1026	G	C5-C6-O6	-8.28	123.63	128.60
27	B8	1391	U	O4'-C1'-N1	8.28	114.82	108.20
27	B8	2222	C	O4'-C1'-N1	8.28	114.82	108.20
1	AA	838	G	C5-C6-O6	-8.28	123.64	128.60
27	B8	312	G	C5-C6-O6	-8.28	123.64	128.60
27	B8	875	G	C5-C6-O6	-8.28	123.64	128.60
27	B8	2023	C	O4'-C1'-N1	8.28	114.82	108.20
27	B8	2304	G	C5-C6-O6	-8.28	123.63	128.60
27	B8	2640	G	C5-C6-O6	-8.28	123.64	128.60
27	B8	2855	C	O4'-C1'-N1	8.28	114.82	108.20
1	AA	627	G	C5-C6-O6	-8.27	123.64	128.60
27	B8	185	G	C5-C6-O6	-8.27	123.64	128.60
27	B8	326	G	C5-C6-O6	-8.27	123.64	128.60
27	B8	2391	G	N1-C6-O6	8.27	124.86	119.90
1	AA	254	G	N1-C6-O6	8.27	124.86	119.90
27	B8	2400	G	C5-C6-O6	-8.27	123.64	128.60
27	B8	2649	C	O4'-C1'-N1	8.27	114.82	108.20
1	AA	557	G	N1-C6-O6	8.27	124.86	119.90
1	AA	1239	A	N1-C6-N6	8.27	123.56	118.60
27	B8	853	C	O4'-C1'-N1	8.27	114.82	108.20
27	B8	985	C	O4'-C1'-N1	8.27	114.82	108.20
27	B8	1167	C	O4'-C1'-N1	8.27	114.82	108.20
1	AA	689	C	O4'-C1'-N1	8.27	114.81	108.20
27	B8	816	C	O4'-C1'-N1	8.27	114.82	108.20
1	AA	1517	G	N1-C6-O6	8.27	124.86	119.90
1	AA	1520	C	O4'-C1'-N1	8.27	114.81	108.20
3	AV	75	C	O4'-C1'-N1	8.27	114.82	108.20
27	B8	208	C	O4'-C1'-N1	8.27	114.81	108.20
27	B8	2285	C	O4'-C1'-N1	8.27	114.81	108.20
27	B8	26	G	N1-C6-O6	8.27	124.86	119.90
27	B8	2620	C	O4'-C1'-N1	8.27	114.81	108.20
27	B8	987	C	O4'-C1'-N1	8.26	114.81	108.20
27	B8	2574	G	C5-C6-O6	-8.26	123.64	128.60
27	B8	137	U	O4'-C1'-N1	8.26	114.81	108.20
1	AA	385	C	O4'-C1'-N1	8.26	114.81	108.20
1	AA	1495	U	O4'-C1'-N1	8.26	114.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	409	U	O4'-C1'-N1	8.26	114.81	108.20
1	AA	1071	C	O4'-C1'-N1	8.26	114.81	108.20
27	B8	36	G	N1-C6-O6	8.26	124.86	119.90
27	B8	1826	G	C5-C6-O6	-8.26	123.64	128.60
1	AA	755	G	C5-C6-O6	-8.26	123.64	128.60
1	AA	1371	G	N1-C6-O6	8.26	124.85	119.90
26	B7	92	C	O4'-C1'-N1	8.26	114.81	108.20
1	AA	823	C	O4'-C1'-N1	8.25	114.80	108.20
27	B8	129	C	O4'-C1'-N1	8.25	114.80	108.20
27	B8	1573	G	N1-C6-O6	8.25	124.85	119.90
1	AA	756	C	O4'-C1'-N1	8.25	114.80	108.20
1	AA	898	G	N1-C6-O6	8.25	124.85	119.90
26	B7	63	C	O4'-C1'-N1	8.25	114.80	108.20
27	B8	1980	G	N1-C6-O6	8.25	124.85	119.90
1	AA	319	G	C5-C6-O6	-8.24	123.65	128.60
1	AA	455	G	C5-C6-O6	-8.24	123.65	128.60
1	AA	580	C	O4'-C1'-N1	8.24	114.80	108.20
27	B8	201	C	O4'-C1'-N1	8.24	114.80	108.20
1	AA	732	C	O4'-C1'-N1	8.24	114.79	108.20
27	B8	687	C	O4'-C1'-N1	8.24	114.79	108.20
27	B8	1547	C	O4'-C1'-N1	8.24	114.79	108.20
1	AA	999	C	O4'-C1'-N1	8.24	114.79	108.20
27	B8	121	G	C5-C6-O6	-8.24	123.66	128.60
27	B8	409	G	C5-C6-O6	-8.24	123.66	128.60
27	B8	1270	C	O4'-C1'-N1	8.24	114.79	108.20
27	B8	2217	G	C5-C6-O6	-8.24	123.66	128.60
26	B7	9	G	C5-C6-O6	-8.24	123.66	128.60
27	B8	539	G	N1-C6-O6	8.24	124.84	119.90
27	B8	2362	C	O4'-C1'-N1	8.24	114.79	108.20
27	B8	2704	C	O4'-C1'-N1	8.24	114.79	108.20
1	AA	778	G	C5-C6-O6	-8.23	123.66	128.60
3	AV	67	C	O4'-C1'-N1	8.23	114.79	108.20
27	B8	2559	C	O4'-C1'-N1	8.23	114.79	108.20
1	AA	105	G	C5-C6-O6	-8.23	123.66	128.60
27	B8	1191	G	C5-C6-O6	-8.23	123.66	128.60
1	AA	764	C	O4'-C1'-N1	8.23	114.78	108.20
27	B8	1540	G	C5-C6-O6	-8.23	123.66	128.60
1	AA	1266	G	N1-C6-O6	8.23	124.84	119.90
27	B8	109	C	O4'-C1'-N1	8.23	114.78	108.20
27	B8	968	C	O4'-C1'-N1	8.23	114.78	108.20
1	AA	899	C	O4'-C1'-N1	8.23	114.78	108.20
27	B8	954	G	C5-C6-O6	-8.23	123.66	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2648	G	C5-C6-O6	-8.23	123.66	128.60
27	B8	2896	C	O4'-C1'-N1	8.23	114.78	108.20
27	B8	2715	C	O4'-C1'-N1	8.23	114.78	108.20
1	AA	269	C	O4'-C1'-N1	8.22	114.78	108.20
27	B8	355	U	O4'-C1'-N1	8.22	114.78	108.20
27	B8	1961	C	O4'-C1'-N1	8.22	114.78	108.20
1	AA	668	G	C5-C6-O6	-8.22	123.67	128.60
27	B8	2641	G	C5-C6-O6	-8.22	123.67	128.60
27	B8	465	G	N1-C6-O6	8.22	124.83	119.90
27	B8	673	C	O4'-C1'-N1	8.21	114.77	108.20
27	B8	2380	C	O4'-C1'-N1	8.21	114.77	108.20
1	AA	291	U	O4'-C1'-N1	8.21	114.77	108.20
1	AA	392	C	O4'-C1'-N1	8.21	114.77	108.20
27	B8	879	G	N1-C6-O6	8.21	124.83	119.90
26	B7	110	C	O4'-C1'-N1	8.21	114.77	108.20
1	AA	1002	G	C5-C6-O6	-8.21	123.67	128.60
26	B7	90	C	O4'-C1'-N1	8.21	114.77	108.20
27	B8	54	G	N1-C6-O6	8.21	124.83	119.90
27	B8	245	G	C5-C6-O6	-8.21	123.67	128.60
27	B8	1837	C	O4'-C1'-N1	8.21	114.77	108.20
1	AA	85	U	O4'-C1'-N1	8.20	114.76	108.20
1	AA	286	C	O4'-C1'-N1	8.20	114.76	108.20
1	AA	232	G	N1-C6-O6	8.20	124.82	119.90
1	AA	731	G	C5-C6-O6	-8.20	123.68	128.60
1	AA	1352	C	O4'-C1'-N1	8.20	114.76	108.20
27	B8	81	G	C5-C6-O6	-8.20	123.68	128.60
27	B8	2819	G	C5-C6-O6	-8.20	123.68	128.60
1	AA	138	G	C5-C6-O6	-8.20	123.68	128.60
1	AA	853	C	O4'-C1'-N1	8.20	114.76	108.20
27	B8	331	C	O4'-C1'-N1	8.20	114.76	108.20
27	B8	476	G	N1-C6-O6	8.20	124.82	119.90
27	B8	2057	G	C5-C6-O6	-8.19	123.68	128.60
27	B8	2185	U	O4'-C1'-N1	8.19	114.76	108.20
27	B8	2424	C	O4'-C1'-N1	8.19	114.75	108.20
27	B8	2801	G	C5-C6-O6	-8.20	123.68	128.60
27	B8	2588	G	C5-C6-O6	-8.19	123.68	128.60
1	AA	1328	C	O4'-C1'-N1	8.19	114.75	108.20
27	B8	1293	C	O4'-C1'-N1	8.19	114.75	108.20
27	B8	2557	G	C5-C6-O6	-8.19	123.69	128.60
27	B8	2722	G	C5-C6-O6	-8.19	123.69	128.60
1	AA	454	G	C5-C6-O6	-8.19	123.69	128.60
27	B8	611	C	O4'-C1'-N1	8.19	114.75	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1341	G	N1-C6-O6	8.19	124.81	119.90
27	B8	2283	C	O4'-C1'-N1	8.19	114.75	108.20
1	AA	1132	C	O4'-C1'-N1	8.19	114.75	108.20
27	B8	2375	G	N1-C6-O6	8.19	124.81	119.90
1	AA	998	C	O4'-C1'-N1	8.18	114.75	108.20
1	AA	1320	C	O4'-C1'-N1	8.18	114.75	108.20
1	AA	1414	U	O4'-C1'-N1	8.18	114.75	108.20
1	AA	242	G	C5-C6-O6	-8.18	123.69	128.60
1	AA	786	G	C5-C6-O6	-8.18	123.69	128.60
3	AV	6	C	O4'-C1'-N1	8.18	114.75	108.20
27	B8	1435	G	C5-C6-O6	-8.18	123.69	128.60
1	AA	1454	G	C5-C6-O6	-8.18	123.69	128.60
27	B8	425	G	C5-C6-O6	-8.18	123.69	128.60
27	B8	2581	G	N1-C6-O6	8.18	124.81	119.90
27	B8	2631	G	C5-C6-O6	-8.18	123.69	128.60
1	AA	264	C	O4'-C1'-N1	8.18	114.74	108.20
1	AA	1136	C	O4'-C1'-N1	8.18	114.74	108.20
27	B8	496	G	C5-C6-O6	-8.18	123.69	128.60
27	B8	1858	A	N1-C6-N6	8.18	123.51	118.60
27	B8	1463	C	O4'-C1'-N1	8.18	114.74	108.20
27	B8	1734	G	C5-C6-O6	-8.17	123.70	128.60
1	AA	587	G	N1-C6-O6	8.17	124.80	119.90
1	AA	654	G	N1-C6-O6	8.17	124.80	119.90
27	B8	617	G	C5-C6-O6	-8.17	123.70	128.60
27	B8	754	U	O4'-C1'-N1	8.17	114.73	108.20
1	AA	475	C	O4'-C1'-N1	8.17	114.73	108.20
1	AA	1323	G	C5-C6-O6	-8.17	123.70	128.60
27	B8	784	G	C5-C6-O6	-8.17	123.70	128.60
1	AA	384	G	N1-C6-O6	8.16	124.80	119.90
1	AA	484	G	C5-C6-O6	-8.16	123.70	128.60
1	AA	426	U	O4'-C1'-N1	8.16	114.73	108.20
1	AA	578	C	O4'-C1'-N1	8.16	114.73	108.20
1	AA	722	G	N1-C6-O6	8.16	124.80	119.90
1	AA	1263	C	O4'-C1'-N1	8.16	114.73	108.20
1	AA	1283	U	O4'-C1'-N1	8.16	114.73	108.20
27	B8	88	G	N1-C6-O6	8.16	124.80	119.90
27	B8	105	C	O4'-C1'-N1	8.16	114.73	108.20
27	B8	236	C	O4'-C1'-N1	8.16	114.73	108.20
27	B8	386	G	N1-C6-O6	8.16	124.80	119.90
27	B8	2515	C	O4'-C1'-N1	8.16	114.73	108.20
1	AA	1484	C	O4'-C1'-N1	8.16	114.73	108.20
27	B8	1917	U	O4'-C1'-N1	8.16	114.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1200	C	O4'-C1'-N1	8.15	114.72	108.20
1	AA	765	G	N1-C6-O6	8.15	124.79	119.90
1	AA	1343	G	C5-C6-O6	-8.15	123.71	128.60
27	B8	731	C	O4'-C1'-N1	8.15	114.72	108.20
27	B8	986	C	O4'-C1'-N1	8.15	114.72	108.20
27	B8	1561	C	O4'-C1'-N1	8.15	114.72	108.20
27	B8	2714	G	C5-C6-O6	-8.15	123.71	128.60
27	B8	2859	G	N1-C6-O6	8.15	124.79	119.90
1	AA	1525	G	N1-C6-O6	8.15	124.79	119.90
27	B8	2520	C	O4'-C1'-N1	8.15	114.72	108.20
1	AA	162	A	C4-C5-C6	8.15	121.07	117.00
27	B8	1949	G	C5-C6-O6	-8.15	123.71	128.60
27	B8	2483	C	O4'-C1'-N1	8.15	114.72	108.20
1	AA	948	C	O4'-C1'-N1	8.14	114.72	108.20
1	AA	1096	C	O4'-C1'-N1	8.14	114.71	108.20
27	B8	1488	C	O4'-C1'-N1	8.14	114.71	108.20
27	B8	2200	C	O4'-C1'-N1	8.14	114.71	108.20
1	AA	84	U	O4'-C1'-N1	8.13	114.71	108.20
27	B8	633	A	C4-C5-C6	8.13	121.07	117.00
27	B8	991	C	O4'-C1'-N1	8.13	114.71	108.20
27	B8	1171	G	C5-C6-O6	-8.13	123.72	128.60
27	B8	1424	G	C5-C6-O6	-8.13	123.72	128.60
27	B8	520	G	C5-C6-O6	-8.13	123.72	128.60
27	B8	724	U	O4'-C1'-N1	8.13	114.70	108.20
27	B8	1595	C	O4'-C1'-N1	8.13	114.71	108.20
27	B8	2248	C	O4'-C1'-N1	8.13	114.71	108.20
27	B8	628	G	C5-C6-O6	-8.13	123.72	128.60
1	AA	188	C	O4'-C1'-N1	8.13	114.70	108.20
27	B8	1213	A	C4-C5-C6	8.13	121.06	117.00
27	B8	2628	C	O4'-C1'-N1	8.13	114.70	108.20
27	B8	212	G	C5-C6-O6	-8.12	123.72	128.60
27	B8	1319	C	O4'-C1'-N1	8.12	114.70	108.20
27	B8	970	U	O4'-C1'-N1	8.12	114.70	108.20
1	AA	1037	C	O4'-C1'-N1	8.12	114.70	108.20
1	AA	1510	C	O4'-C1'-N1	8.12	114.70	108.20
27	B8	445	C	O4'-C1'-N1	8.12	114.70	108.20
1	AA	222	C	O4'-C1'-N1	8.12	114.69	108.20
1	AA	1109	C	O4'-C1'-N1	8.12	114.69	108.20
27	B8	801	G	N1-C6-O6	8.12	124.77	119.90
27	B8	1493	C	C2-N1-C1'	8.12	127.73	118.80
1	AA	1069	C	O4'-C1'-N1	8.12	114.69	108.20
27	B8	337	C	O4'-C1'-N1	8.12	114.69	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	556	C	O4'-C1'-N1	8.11	114.69	108.20
1	AA	883	C	O4'-C1'-N1	8.11	114.69	108.20
3	AV	26	C	O4'-C1'-N1	8.11	114.69	108.20
1	AA	51	A	P-O3'-C3'	8.11	129.43	119.70
1	AA	458	U	O4'-C1'-N1	8.11	114.69	108.20
1	AA	660	C	O4'-C1'-N1	8.11	114.69	108.20
26	B7	28	C	O4'-C1'-N1	8.11	114.69	108.20
27	B8	894	U	O4'-C1'-N1	8.11	114.69	108.20
27	B8	1102	C	O4'-C1'-N1	8.11	114.69	108.20
27	B8	1112	G	N1-C6-O6	8.11	124.77	119.90
27	B8	1990	C	O4'-C1'-N1	8.11	114.69	108.20
27	B8	2299	U	O4'-C1'-N1	8.11	114.69	108.20
1	AA	106	C	O4'-C1'-N1	8.11	114.69	108.20
1	AA	1143	G	C5-C6-O6	-8.11	123.74	128.60
27	B8	1108	U	O4'-C1'-N1	8.11	114.68	108.20
27	B8	1338	G	C5-C6-O6	-8.11	123.74	128.60
27	B8	1728	C	O4'-C1'-N1	8.11	114.69	108.20
1	AA	995	C	O4'-C1'-N1	8.10	114.68	108.20
1	AA	1449	C	O4'-C1'-N1	8.10	114.68	108.20
27	B8	163	C	O4'-C1'-N1	8.10	114.68	108.20
27	B8	2420	C	O4'-C1'-N1	8.10	114.68	108.20
1	AA	1523	G	C5-C6-O6	-8.10	123.74	128.60
27	B8	147	C	O4'-C1'-N1	8.10	114.68	108.20
27	B8	1075	C	O4'-C1'-N1	8.10	114.68	108.20
1	AA	27	G	C5-C6-O6	-8.10	123.74	128.60
27	B8	1100	C	O4'-C1'-N1	8.10	114.68	108.20
27	B8	1546	G	C5-C6-O6	-8.10	123.74	128.60
27	B8	2539	C	O4'-C1'-N1	8.10	114.68	108.20
1	AA	34	C	O4'-C1'-N1	8.10	114.68	108.20
1	AA	61	G	C5-C6-O6	-8.10	123.74	128.60
1	AA	190	A	C4-C5-C6	8.10	121.05	117.00
3	AV	21	U	O4'-C1'-N1	8.10	114.68	108.20
27	B8	598	U	O4'-C1'-N1	8.10	114.68	108.20
27	B8	2300	C	O4'-C1'-N1	8.10	114.68	108.20
27	B8	2794	C	O4'-C1'-N1	8.10	114.68	108.20
1	AA	1098	C	O4'-C1'-N1	8.09	114.67	108.20
27	B8	1835	G	C5-C6-O6	-8.09	123.75	128.60
1	AA	1051	C	O4'-C1'-N1	8.09	114.67	108.20
1	AA	1391	U	O4'-C1'-N1	8.09	114.67	108.20
27	B8	2046	G	C5-C6-O6	-8.09	123.75	128.60
27	B8	2226	C	O4'-C1'-N1	8.09	114.67	108.20
1	AA	1482	G	N1-C6-O6	8.09	124.75	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1042	G	N1-C6-O6	8.09	124.75	119.90
27	B8	1658	C	O4'-C1'-N1	8.09	114.67	108.20
27	B8	1893	C	O4'-C1'-N1	8.09	114.67	108.20
27	B8	2523	G	C5-C6-O6	-8.09	123.75	128.60
27	B8	237	C	O4'-C1'-N1	8.09	114.67	108.20
27	B8	949	G	C5-C6-O6	-8.09	123.75	128.60
27	B8	283	G	O4'-C1'-N9	8.08	114.67	108.20
27	B8	1022	G	N1-C6-O6	8.08	124.75	119.90
1	AA	507	C	O4'-C1'-N1	8.08	114.66	108.20
1	AA	1379	G	N1-C6-O6	8.08	124.75	119.90
26	B7	8	C	O4'-C1'-N1	8.08	114.67	108.20
27	B8	2772	C	O4'-C1'-N1	8.08	114.66	108.20
27	B8	2812	G	C5-C6-O6	-8.08	123.75	128.60
27	B8	1059	G	C5-C6-O6	-8.08	123.75	128.60
27	B8	116	C	O4'-C1'-N1	8.07	114.66	108.20
27	B8	953	G	C5-C6-O6	-8.07	123.75	128.60
27	B8	2383	G	C5-C6-O6	-8.07	123.75	128.60
27	B8	6	A	C5-C6-N6	-8.07	117.24	123.70
27	B8	2345	G	N1-C6-O6	8.07	124.74	119.90
27	B8	2540	C	O4'-C1'-N1	8.07	114.66	108.20
1	AA	178	C	O4'-C1'-N1	8.07	114.65	108.20
27	B8	1822	C	O4'-C1'-N1	8.07	114.65	108.20
1	AA	525	C	O4'-C1'-N1	8.07	114.65	108.20
1	AA	1027	C	N3-C4-N4	8.07	123.65	118.00
27	B8	1386	C	O4'-C1'-N1	8.07	114.65	108.20
1	AA	150	U	O4'-C1'-N1	8.06	114.65	108.20
1	AA	1491	G	N1-C6-O6	8.06	124.74	119.90
27	B8	198	C	O4'-C1'-N1	8.06	114.65	108.20
27	B8	523	C	O4'-C1'-N1	8.06	114.65	108.20
27	B8	2148	G	N1-C6-O6	8.06	124.74	119.90
27	B8	973	A	N1-C6-N6	8.06	123.44	118.60
27	B8	2039	U	O4'-C1'-N1	8.06	114.65	108.20
1	AA	724	G	C5-C6-O6	-8.06	123.76	128.60
1	AA	868	C	O4'-C1'-N1	8.06	114.65	108.20
27	B8	1107	G	C5-C6-O6	-8.06	123.76	128.60
27	B8	1121	C	O4'-C1'-N1	8.06	114.65	108.20
27	B8	1259	G	C5-C6-O6	-8.06	123.76	128.60
27	B8	1642	G	C5-C6-O6	-8.06	123.76	128.60
26	B7	6	G	C5-C6-O6	-8.06	123.77	128.60
26	B7	85	G	C5-C6-O6	-8.06	123.77	128.60
27	B8	407	G	C5-C6-O6	-8.06	123.76	128.60
27	B8	1723	G	C5-C6-O6	-8.06	123.77	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2301	C	O4'-C1'-N1	8.06	114.65	108.20
27	B8	9	G	C5-C6-O6	-8.06	123.77	128.60
1	AA	1388	C	O4'-C1'-N1	8.05	114.64	108.20
27	B8	719	C	O4'-C1'-N1	8.05	114.64	108.20
27	B8	1422	G	C5-C6-O6	-8.05	123.77	128.60
27	B8	2234	G	C5-C6-O6	-8.05	123.77	128.60
27	B8	2359	C	O4'-C1'-N1	8.05	114.64	108.20
1	AA	1385	G	C5-C6-O6	-8.05	123.77	128.60
27	B8	2450	A	N1-C6-N6	8.05	123.43	118.60
1	AA	504	C	O4'-C1'-N1	8.05	114.64	108.20
1	AA	1386	G	C5-C6-O6	-8.05	123.77	128.60
27	B8	183	C	O4'-C1'-N1	8.05	114.64	108.20
27	B8	540	C	O4'-C1'-N1	8.05	114.64	108.20
27	B8	1920	C	O4'-C1'-N1	8.05	114.64	108.20
1	AA	1090	U	O4'-C1'-N1	8.04	114.64	108.20
1	AA	1218	C	O4'-C1'-N1	8.04	114.64	108.20
1	AA	111	G	C5-C6-O6	-8.04	123.78	128.60
1	AA	522	C	O4'-C1'-N1	8.04	114.63	108.20
27	B8	729	G	C5-C6-O6	-8.04	123.77	128.60
27	B8	963	U	O4'-C1'-N1	8.04	114.63	108.20
27	B8	1123	C	O4'-C1'-N1	8.04	114.63	108.20
1	AA	1001	C	O4'-C1'-N1	8.04	114.63	108.20
27	B8	1345	C	O4'-C1'-N1	8.04	114.63	108.20
27	B8	1736	U	O4'-C1'-N1	8.04	114.63	108.20
27	B8	2666	C	C2-N1-C1'	8.04	127.64	118.80
27	B8	758	C	O4'-C1'-N1	8.04	114.63	108.20
27	B8	798	G	C5-C6-O6	-8.04	123.78	128.60
27	B8	2527	C	O4'-C1'-N1	8.04	114.63	108.20
27	B8	2667	C	O4'-C1'-N1	8.04	114.63	108.20
1	AA	861	G	C5-C6-O6	-8.04	123.78	128.60
27	B8	1415	U	O4'-C1'-N1	8.04	114.63	108.20
1	AA	468	A	O4'-C1'-N9	8.03	114.63	108.20
1	AA	808	C	O4'-C1'-N1	8.03	114.63	108.20
27	B8	1193	G	C5-C6-O6	-8.03	123.78	128.60
27	B8	2053	G	C5-C6-O6	-8.04	123.78	128.60
1	AA	601	G	C5-C6-O6	-8.03	123.78	128.60
1	AA	632	U	O4'-C1'-N1	8.03	114.63	108.20
1	AA	1337	G	C5-C6-O6	-8.03	123.78	128.60
27	B8	2295	C	O4'-C1'-N1	8.03	114.63	108.20
27	B8	66	C	O4'-C1'-N1	8.03	114.62	108.20
27	B8	2463	C	O4'-C1'-N1	8.03	114.62	108.20
1	AA	1509	C	O4'-C1'-N1	8.03	114.62	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2276	G	C5-C6-O6	-8.03	123.78	128.60
27	B8	77	G	C5-C6-O6	-8.03	123.78	128.60
27	B8	2175	C	O4'-C1'-N1	8.03	114.62	108.20
1	AA	1262	C	O4'-C1'-N1	8.03	114.62	108.20
27	B8	1072	C	O4'-C1'-N1	8.03	114.62	108.20
27	B8	2260	C	O4'-C1'-N1	8.03	114.62	108.20
27	B8	732	C	O4'-C1'-N1	8.03	114.62	108.20
27	B8	1594	U	O4'-C1'-N1	8.03	114.62	108.20
1	AA	1045	C	O4'-C1'-N1	8.02	114.62	108.20
27	B8	976	G	C5-C6-O6	-8.02	123.79	128.60
27	B8	2261	C	O4'-C1'-N1	8.02	114.62	108.20
27	B8	2521	C	O4'-C1'-N1	8.02	114.62	108.20
1	AA	922	G	N1-C6-O6	8.02	124.71	119.90
27	B8	2830	C	O4'-C1'-N1	8.02	114.62	108.20
27	B8	2432	A	O4'-C1'-N9	8.02	114.61	108.20
27	B8	2625	G	C5-C6-O6	-8.02	123.79	128.60
1	AA	585	G	C5-C6-O6	-8.02	123.79	128.60
1	AA	636	U	O4'-C1'-N1	8.02	114.61	108.20
1	AA	1485	U	O4'-C1'-N1	8.02	114.61	108.20
26	B7	68	C	O4'-C1'-N1	8.02	114.61	108.20
27	B8	832	U	O4'-C1'-N1	8.02	114.61	108.20
27	B8	2841	C	O4'-C1'-N1	8.02	114.61	108.20
1	AA	623	C	O4'-C1'-N1	8.01	114.61	108.20
27	B8	1182	G	C5-C6-O6	-8.01	123.79	128.60
27	B8	2128	G	C5-C6-O6	-8.01	123.79	128.60
27	B8	2254	C	O4'-C1'-N1	8.01	114.61	108.20
1	AA	39	G	C5-C6-O6	-8.01	123.80	128.60
27	B8	682	G	C5-C6-O6	-8.01	123.79	128.60
27	B8	1905	C	O4'-C1'-N1	8.01	114.61	108.20
27	B8	2505	G	N1-C6-O6	8.01	124.71	119.90
27	B8	2744	G	C5-C6-O6	-8.01	123.79	128.60
1	AA	43	C	O4'-C1'-N1	8.01	114.61	108.20
1	AA	402	G	C5-C6-O6	-8.01	123.80	128.60
1	AA	1293	C	O4'-C1'-N1	8.01	114.61	108.20
27	B8	1571	A	C4-C5-C6	8.01	121.00	117.00
27	B8	978	G	C5-C6-O6	-8.01	123.80	128.60
27	B8	2347	C	O4'-C1'-N1	8.01	114.60	108.20
27	B8	457	A	N1-C6-N6	8.00	123.40	118.60
27	B8	2279	G	C5-C6-O6	-8.00	123.80	128.60
27	B8	2603	G	C5-C6-O6	-8.00	123.80	128.60
27	B8	2238	G	N1-C6-O6	8.00	124.70	119.90
1	AA	1245	C	O4'-C1'-N1	8.00	114.60	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AV	31	U	O4'-C1'-N1	8.00	114.60	108.20
27	B8	1656	C	O4'-C1'-N1	8.00	114.60	108.20
1	AA	1300	G	P-O3'-C3'	8.00	129.30	119.70
1	AA	23	C	O4'-C1'-N1	8.00	114.60	108.20
1	AA	317	U	O4'-C1'-N1	8.00	114.60	108.20
1	AA	1086	U	O4'-C1'-N1	8.00	114.60	108.20
27	B8	1305	C	O4'-C1'-N1	8.00	114.60	108.20
27	B8	305	C	O4'-C1'-N1	8.00	114.60	108.20
1	AA	624	C	O4'-C1'-N1	7.99	114.59	108.20
1	AA	1411	C	O4'-C1'-N1	7.99	114.59	108.20
27	B8	153	U	O4'-C1'-N1	7.99	114.59	108.20
27	B8	238	C	O4'-C1'-N1	7.99	114.59	108.20
27	B8	566	U	O4'-C1'-N1	7.99	114.59	108.20
27	B8	1030	C	O4'-C1'-N1	7.99	114.59	108.20
27	B8	1651	G	C5-C6-O6	-7.99	123.80	128.60
27	B8	1924	C	O4'-C1'-N1	7.99	114.59	108.20
1	AA	551	U	O4'-C1'-N1	7.99	114.59	108.20
27	B8	1023	U	O4'-C1'-N1	7.99	114.59	108.20
27	B8	2081	U	O4'-C1'-N1	7.99	114.59	108.20
27	B8	106	C	O4'-C1'-N1	7.99	114.59	108.20
27	B8	1105	U	O4'-C1'-N1	7.99	114.59	108.20
27	B8	2508	G	C5-C6-O6	-7.99	123.81	128.60
1	AA	89	U	O4'-C1'-N1	7.99	114.59	108.20
3	AV	47	G	C5-C6-O6	-7.99	123.81	128.60
27	B8	1109	C	O4'-C1'-N1	7.99	114.59	108.20
27	B8	1124	G	C5-C6-O6	-7.99	123.81	128.60
1	AA	413	G	C5-C6-O6	-7.99	123.81	128.60
27	B8	938	G	C5-C6-O6	-7.99	123.81	128.60
27	B8	1135	C	O4'-C1'-N1	7.99	114.59	108.20
27	B8	1948	G	C5-C6-O6	-7.99	123.81	128.60
1	AA	876	C	O4'-C1'-N1	7.98	114.59	108.20
27	B8	1417	C	O4'-C1'-N1	7.98	114.59	108.20
27	B8	2024	G	C5-C6-O6	-7.98	123.81	128.60
3	AV	3	G	C5-C6-O6	-7.98	123.81	128.60
27	B8	351	C	O4'-C1'-N1	7.98	114.59	108.20
27	B8	1245	G	C5-C6-O6	-7.98	123.81	128.60
1	AA	300	A	O4'-C1'-N9	7.98	114.58	108.20
1	AA	1470	U	O4'-C1'-N1	7.98	114.58	108.20
27	B8	287	G	C5-C6-O6	-7.98	123.81	128.60
1	AA	740	U	O4'-C1'-N1	7.98	114.58	108.20
27	B8	170	U	O4'-C1'-N1	7.98	114.58	108.20
27	B8	1101	U	O4'-C1'-N1	7.98	114.58	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	701	G	C5-C6-O6	-7.98	123.81	128.60
27	B8	2596	U	O4'-C1'-N1	7.98	114.58	108.20
1	AA	867	G	C5-C6-O6	-7.97	123.81	128.60
1	AA	1050	G	C5-C6-O6	-7.97	123.81	128.60
1	AA	152	A	N1-C6-N6	7.97	123.38	118.60
27	B8	1232	G	C5-C6-O6	-7.97	123.82	128.60
27	B8	823	C	O4'-C1'-N1	7.97	114.58	108.20
1	AA	17	U	O4'-C1'-N1	7.97	114.58	108.20
27	B8	265	A	O4'-C1'-N9	7.97	114.58	108.20
27	B8	649	G	C5-C6-O6	-7.97	123.82	128.60
27	B8	1520	U	O4'-C1'-N1	7.97	114.58	108.20
27	B8	1562	U	O4'-C1'-N1	7.97	114.58	108.20
27	B8	2558	C	O4'-C1'-N1	7.97	114.58	108.20
1	AA	153	C	O4'-C1'-N1	7.97	114.57	108.20
1	AA	267	C	O4'-C1'-N1	7.97	114.57	108.20
27	B8	787	C	O4'-C1'-N1	7.97	114.57	108.20
27	B8	2157	G	O4'-C1'-N9	7.97	114.57	108.20
27	B8	2315	G	C5-C6-O6	-7.97	123.82	128.60
1	AA	1029	U	O4'-C1'-N1	7.96	114.57	108.20
26	B7	7	G	C5-C6-O6	-7.96	123.82	128.60
27	B8	177	G	N1-C6-O6	7.96	124.68	119.90
27	B8	919	U	O4'-C1'-N1	7.96	114.57	108.20
27	B8	2651	C	O4'-C1'-N1	7.96	114.57	108.20
27	B8	385	C	O4'-C1'-N1	7.96	114.57	108.20
1	AA	114	U	O4'-C1'-N1	7.96	114.56	108.20
1	AA	1133	G	C5-C6-O6	-7.96	123.83	128.60
27	B8	581	C	O4'-C1'-N1	7.96	114.57	108.20
27	B8	2195	U	O4'-C1'-N1	7.96	114.56	108.20
27	B8	1016	G	C5-C6-O6	-7.96	123.83	128.60
27	B8	1207	C	O4'-C1'-N1	7.96	114.56	108.20
27	B8	1661	G	C5-C6-O6	-7.96	123.83	128.60
27	B8	1162	G	C5-C6-O6	-7.95	123.83	128.60
27	B8	1278	C	O4'-C1'-N1	7.95	114.56	108.20
27	B8	2599	G	C5-C6-O6	-7.95	123.83	128.60
26	B7	22	U	O4'-C1'-N1	7.95	114.56	108.20
1	AA	142	G	C5-C6-O6	-7.95	123.83	128.60
27	B8	1518	C	O4'-C1'-N1	7.95	114.56	108.20
1	AA	1075	U	O4'-C1'-N1	7.95	114.56	108.20
27	B8	383	C	O4'-C1'-N1	7.95	114.56	108.20
27	B8	759	G	C5-C6-O6	-7.95	123.83	128.60
27	B8	1429	G	C5-C6-O6	-7.95	123.83	128.60
1	AA	52	C	O4'-C1'-N1	7.95	114.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1479	G	C5-C6-O6	-7.95	123.83	128.60
1	AA	214	C	O4'-C1'-N1	7.95	114.56	108.20
1	AA	739	C	O4'-C1'-N1	7.95	114.56	108.20
27	B8	1816	C	O4'-C1'-N1	7.95	114.56	108.20
27	B8	1890	A	N1-C6-N6	7.94	123.37	118.60
27	B8	2250	G	N1-C6-O6	7.94	124.67	119.90
1	AA	1401	G	C5-C6-O6	-7.94	123.83	128.60
27	B8	1258	U	O4'-C1'-N1	7.94	114.55	108.20
27	B8	2484	G	C5-C6-O6	-7.94	123.83	128.60
27	B8	2804	U	O4'-C1'-N1	7.94	114.55	108.20
1	AA	1041	G	C5-C6-O6	-7.94	123.84	128.60
27	B8	1181	U	O4'-C1'-N1	7.94	114.55	108.20
27	B8	2096	C	O4'-C1'-N1	7.94	114.55	108.20
1	AA	798	U	O4'-C1'-N1	7.94	114.55	108.20
27	B8	680	C	O4'-C1'-N1	7.94	114.55	108.20
27	B8	1031	G	C5-C6-O6	-7.94	123.84	128.60
27	B8	2021	C	O4'-C1'-N1	7.94	114.55	108.20
1	AA	1061	G	C5-C6-O6	-7.94	123.84	128.60
1	AA	951	G	C5-C6-O6	-7.93	123.84	128.60
3	AV	39	U	O4'-C1'-N1	7.93	114.55	108.20
27	B8	164	C	O4'-C1'-N1	7.93	114.55	108.20
27	B8	1145	C	O4'-C1'-N1	7.93	114.55	108.20
27	B8	1206	G	C5-C6-O6	-7.93	123.84	128.60
27	B8	1389	G	C5-C6-O6	-7.93	123.84	128.60
27	B8	46	G	C5-C6-O6	-7.93	123.84	128.60
27	B8	131	A	O4'-C1'-N9	7.93	114.55	108.20
1	AA	1210	C	O4'-C1'-N1	7.93	114.54	108.20
27	B8	2643	G	C5-C6-O6	-7.93	123.84	128.60
27	B8	1131	G	N1-C6-O6	7.93	124.66	119.90
27	B8	1154	G	C5-C6-O6	-7.93	123.84	128.60
27	B8	2329	U	O4'-C1'-N1	7.93	114.54	108.20
26	B7	3	C	O4'-C1'-N1	7.93	114.54	108.20
1	AA	1039	G	C5-C6-O6	-7.92	123.84	128.60
27	B8	898	C	O4'-C1'-N1	7.92	114.54	108.20
27	B8	2390	U	O4'-C1'-N1	7.92	114.54	108.20
27	B8	2579	C	O4'-C1'-N1	7.92	114.54	108.20
27	B8	815	C	O4'-C1'-N1	7.92	114.54	108.20
27	B8	230	G	C5-C6-O6	-7.92	123.85	128.60
27	B8	363	G	C5-C6-O6	-7.92	123.85	128.60
1	AA	186	C	O4'-C1'-N1	7.92	114.53	108.20
1	AA	271	C	O4'-C1'-N1	7.92	114.53	108.20
1	AA	617	G	C5-C6-O6	-7.92	123.85	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	824	G	C5-C6-O6	-7.92	123.85	128.60
27	B8	799	G	C5-C6-O6	-7.92	123.85	128.60
27	B8	2458	G	O4'-C1'-N9	7.92	114.53	108.20
1	AA	518	C	O4'-C1'-N1	7.92	114.53	108.20
27	B8	288	U	O4'-C1'-N1	7.92	114.53	108.20
1	AA	1497	G	C5-C6-O6	-7.91	123.85	128.60
27	B8	414	C	O4'-C1'-N1	7.91	114.53	108.20
27	B8	1643	G	C5-C6-O6	-7.91	123.85	128.60
27	B8	2069	G	C5-C6-O6	-7.91	123.85	128.60
1	AA	538	G	C5-C6-O6	-7.91	123.85	128.60
27	B8	202	U	O4'-C1'-N1	7.91	114.53	108.20
27	B8	487	C	O4'-C1'-N1	7.91	114.53	108.20
1	AA	1010	U	O4'-C1'-N1	7.91	114.53	108.20
27	B8	1418	G	C5-C6-O6	-7.91	123.85	128.60
27	B8	2802	G	C5-C6-O6	-7.91	123.86	128.60
27	B8	1768	C	O4'-C1'-N1	7.91	114.53	108.20
27	B8	2785	C	O4'-C1'-N1	7.91	114.53	108.20
26	B7	111	U	O4'-C1'-N1	7.91	114.52	108.20
27	B8	1531	C	O4'-C1'-N1	7.91	114.52	108.20
1	AA	1366	C	O4'-C1'-N1	7.90	114.52	108.20
26	B7	88	C	O4'-C1'-N1	7.90	114.52	108.20
1	AA	135	C	O4'-C1'-N1	7.90	114.52	108.20
1	AA	821	G	C5-C6-O6	-7.90	123.86	128.60
1	AA	1478	U	O4'-C1'-N1	7.90	114.52	108.20
27	B8	2441	U	O4'-C1'-N1	7.90	114.52	108.20
27	B8	2464	G	C5-C6-O6	-7.90	123.86	128.60
27	B8	1914	C	O4'-C1'-N1	7.90	114.52	108.20
27	B8	2396	G	C5-C6-O6	-7.90	123.86	128.60
1	AA	234	C	O4'-C1'-N1	7.90	114.52	108.20
27	B8	946	C	O4'-C1'-N1	7.90	114.52	108.20
1	AA	450	G	C5-C6-O6	-7.90	123.86	128.60
27	B8	1706	C	O4'-C1'-N1	7.90	114.52	108.20
1	AA	241	G	C5-C6-O6	-7.89	123.86	128.60
26	B7	36	C	O4'-C1'-N1	7.89	114.51	108.20
27	B8	224	U	O4'-C1'-N1	7.89	114.51	108.20
27	B8	867	C	O4'-C1'-N1	7.89	114.51	108.20
27	B8	1462	C	O4'-C1'-N1	7.89	114.51	108.20
27	B8	2416	C	O4'-C1'-N1	7.89	114.51	108.20
27	B8	914	G	C5-C6-O6	-7.89	123.86	128.60
27	B8	1170	C	O4'-C1'-N1	7.89	114.51	108.20
1	AA	634	C	O4'-C1'-N1	7.89	114.51	108.20
27	B8	807	U	O4'-C1'-N1	7.89	114.51	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1563	U	O4'-C1'-N1	7.89	114.51	108.20
1	AA	117	G	C5-C6-O6	-7.89	123.87	128.60
1	AA	146	G	C5-C6-O6	-7.89	123.87	128.60
1	AA	583	A	N1-C6-N6	7.89	123.33	118.60
1	AA	744	C	O4'-C1'-N1	7.89	114.51	108.20
1	AA	862	C	O4'-C1'-N1	7.89	114.51	108.20
1	AA	513	C	O4'-C1'-N1	7.88	114.51	108.20
27	B8	2063	C	O4'-C1'-N1	7.88	114.51	108.20
27	B8	797	G	C5-C6-O6	-7.88	123.87	128.60
27	B8	1093	G	C5-C6-O6	-7.88	123.87	128.60
27	B8	2867	G	O4'-C1'-N9	7.88	114.51	108.20
1	AA	849	G	C5-C6-O6	-7.88	123.87	128.60
3	AV	11	C	O4'-C1'-N1	7.88	114.50	108.20
27	B8	812	C	O4'-C1'-N1	7.88	114.50	108.20
27	B8	1343	G	C5-C6-O6	-7.88	123.87	128.60
27	B8	2146	C	O4'-C1'-N1	7.88	114.50	108.20
27	B8	2093	G	C5-C6-O6	-7.88	123.87	128.60
1	AA	986	U	O4'-C1'-N1	7.88	114.50	108.20
27	B8	924	G	C5-C6-O6	-7.88	123.87	128.60
27	B8	2630	G	C5-C6-O6	-7.88	123.87	128.60
1	AA	835	U	O4'-C1'-N1	7.87	114.50	108.20
1	AA	1006	G	C5-C6-O6	-7.87	123.88	128.60
27	B8	115	C	O4'-C1'-N1	7.87	114.50	108.20
27	B8	2824	C	O4'-C1'-N1	7.87	114.50	108.20
1	AA	500	G	C5-C6-O6	-7.87	123.88	128.60
1	AA	592	G	C5-C6-O6	-7.87	123.88	128.60
1	AA	1282	C	O4'-C1'-N1	7.87	114.50	108.20
27	B8	123	G	C5-C6-O6	-7.87	123.88	128.60
27	B8	1909	C	O4'-C1'-N1	7.87	114.50	108.20
27	B8	2880	C	O4'-C1'-N1	7.87	114.50	108.20
27	B8	1289	C	O4'-C1'-N1	7.87	114.50	108.20
27	B8	593	U	O4'-C1'-N1	7.87	114.50	108.20
27	B8	650	C	O4'-C1'-N1	7.87	114.49	108.20
27	B8	1530	G	C5-C6-O6	-7.87	123.88	128.60
27	B8	2189	U	O4'-C1'-N1	7.87	114.50	108.20
1	AA	334	C	O4'-C1'-N1	7.86	114.49	108.20
27	B8	509	C	O4'-C1'-N1	7.86	114.49	108.20
27	B8	534	U	O4'-C1'-N1	7.86	114.49	108.20
27	B8	1083	U	O4'-C1'-N1	7.86	114.49	108.20
27	B8	1238	G	C5-C6-O6	-7.86	123.88	128.60
27	B8	1691	C	O4'-C1'-N1	7.86	114.49	108.20
1	AA	9	G	C5-C6-O6	-7.86	123.88	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	599	C	O4'-C1'-N1	7.86	114.49	108.20
27	B8	234	U	O4'-C1'-N1	7.86	114.49	108.20
27	B8	252	G	C5-C6-O6	-7.86	123.88	128.60
27	B8	902	C	O4'-C1'-N1	7.86	114.49	108.20
27	B8	1297	C	O4'-C1'-N1	7.86	114.49	108.20
27	B8	2041	U	O4'-C1'-N1	7.86	114.49	108.20
1	AA	487	A	C4-C5-C6	7.86	120.93	117.00
27	B8	1752	C	O4'-C1'-N1	7.86	114.49	108.20
27	B8	2698	U	O4'-C1'-N1	7.86	114.49	108.20
27	B8	325	G	C5-C6-O6	-7.86	123.89	128.60
27	B8	2782	G	C5-C6-O6	-7.85	123.89	128.60
1	AA	1425	U	O4'-C1'-N1	7.85	114.48	108.20
3	AV	62	C	O4'-C1'-N1	7.85	114.48	108.20
27	B8	1888	G	O4'-C1'-N9	7.85	114.48	108.20
1	AA	191	G	C5-C6-O6	-7.85	123.89	128.60
1	AA	225	C	O4'-C1'-N1	7.85	114.48	108.20
1	AA	970	C	O4'-C1'-N1	7.85	114.48	108.20
3	AV	23	G	C5-C6-O6	-7.85	123.89	128.60
27	B8	209	C	O4'-C1'-N1	7.85	114.48	108.20
1	AA	308	C	O4'-C1'-N1	7.85	114.48	108.20
1	AA	1220	G	C5-C6-O6	-7.85	123.89	128.60
1	AA	176	C	O4'-C1'-N1	7.84	114.48	108.20
1	AA	207	C	O4'-C1'-N1	7.84	114.48	108.20
27	B8	2221	G	C5-C6-O6	-7.84	123.89	128.60
27	B8	2467	C	O4'-C1'-N1	7.84	114.48	108.20
1	AA	1540	U	O4'-C1'-N1	7.84	114.47	108.20
1	AA	25	C	O4'-C1'-N1	7.84	114.47	108.20
1	AA	917	G	C5-C6-O6	-7.84	123.90	128.60
26	B7	117	G	P-O3'-C3'	7.84	129.11	119.70
27	B8	605	G	C5-C6-O6	-7.84	123.89	128.60
27	B8	822	G	C5-C6-O6	-7.84	123.89	128.60
27	B8	2232	C	O4'-C1'-N1	7.84	114.47	108.20
26	B7	106	G	C5-C6-O6	-7.84	123.90	128.60
27	B8	141	G	C5-C6-O6	-7.84	123.90	128.60
27	B8	1455	G	C5-C6-O6	-7.84	123.90	128.60
27	B8	1727	C	O4'-C1'-N1	7.84	114.47	108.20
27	B8	1850	G	C5-C6-O6	-7.84	123.90	128.60
1	AA	1230	C	O4'-C1'-N1	7.84	114.47	108.20
27	B8	552	U	O4'-C1'-N1	7.84	114.47	108.20
27	B8	2104	C	O4'-C1'-N1	7.84	114.47	108.20
1	AA	543	U	O4'-C1'-N1	7.84	114.47	108.20
1	AA	748	G	C5-C6-O6	-7.84	123.90	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1149	C	O4'-C1'-N1	7.84	114.47	108.20
26	B7	86	G	C5-C6-O6	-7.84	123.90	128.60
27	B8	1673	G	N1-C6-O6	7.84	124.60	119.90
27	B8	2209	G	C5-C6-O6	-7.84	123.90	128.60
1	AA	266	G	N1-C6-O6	7.83	124.60	119.90
27	B8	485	C	O4'-C1'-N1	7.83	114.47	108.20
27	B8	2530	A	O4'-C1'-N9	7.83	114.47	108.20
1	AA	1072	G	C5-C6-O6	-7.83	123.90	128.60
1	AA	1147	C	O4'-C1'-N1	7.83	114.47	108.20
26	B7	84	G	C5-C6-O6	-7.83	123.90	128.60
27	B8	1427	A	N1-C6-N6	7.83	123.30	118.60
27	B8	1816	C	C2-N1-C1'	7.83	127.42	118.80
27	B8	2355	G	C5-C6-O6	-7.83	123.90	128.60
27	B8	1806	C	O4'-C1'-N1	7.83	114.47	108.20
27	B8	2323	G	C5-C6-O6	-7.83	123.90	128.60
27	B8	2325	G	C5-C6-O6	-7.83	123.90	128.60
1	AA	361	G	C5-C6-O6	-7.83	123.90	128.60
27	B8	767	U	O4'-C1'-N1	7.83	114.46	108.20
27	B8	834	G	C5-C6-O6	-7.83	123.90	128.60
27	B8	1448	G	C5-C6-O6	-7.83	123.90	128.60
27	B8	1196	C	O4'-C1'-N1	7.83	114.46	108.20
27	B8	1902	C	O4'-C1'-N1	7.83	114.46	108.20
1	AA	335	C	O4'-C1'-N1	7.83	114.46	108.20
27	B8	267	C	O4'-C1'-N1	7.83	114.46	108.20
27	B8	1517	G	C5-C6-O6	-7.83	123.91	128.60
27	B8	2548	U	O4'-C1'-N1	7.83	114.46	108.20
27	B8	1832	C	O4'-C1'-N1	7.82	114.46	108.20
27	B8	1188	U	O4'-C1'-N1	7.82	114.46	108.20
27	B8	1472	C	O4'-C1'-N1	7.82	114.46	108.20
27	B8	1612	C	O4'-C1'-N1	7.82	114.46	108.20
27	B8	1636	U	O4'-C1'-N1	7.82	114.46	108.20
27	B8	1766	G	C5-C6-O6	-7.82	123.91	128.60
27	B8	1999	C	O4'-C1'-N1	7.82	114.46	108.20
27	B8	2861	U	O4'-C1'-N1	7.82	114.46	108.20
27	B8	274	C	O4'-C1'-N1	7.82	114.45	108.20
27	B8	467	G	C5-C6-O6	-7.82	123.91	128.60
27	B8	995	C	O4'-C1'-N1	7.82	114.45	108.20
27	B8	1372	U	O4'-C1'-N1	7.82	114.45	108.20
27	B8	2677	G	C5-C6-O6	-7.82	123.91	128.60
1	AA	36	C	O4'-C1'-N1	7.82	114.45	108.20
27	B8	1256	G	C5-C6-O6	-7.82	123.91	128.60
27	B8	2382	G	C5-C6-O6	-7.81	123.91	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	140	C	O4'-C1'-N1	7.81	114.45	108.20
27	B8	778	G	C5-C6-O6	-7.81	123.91	128.60
27	B8	61	C	O4'-C1'-N1	7.81	114.45	108.20
27	B8	1323	C	O4'-C1'-N1	7.81	114.45	108.20
27	B8	2718	G	C5-C6-O6	-7.81	123.91	128.60
1	AA	492	C	O4'-C1'-N1	7.81	114.45	108.20
1	AA	645	G	C5-C6-O6	-7.81	123.92	128.60
1	AA	1531	A	O4'-C1'-N9	7.81	114.45	108.20
1	AA	428	G	P-O3'-C3'	7.81	129.07	119.70
27	B8	214	G	C5-C6-O6	-7.81	123.92	128.60
27	B8	850	U	O4'-C1'-N1	7.81	114.45	108.20
27	B8	1601	G	C5-C6-O6	-7.81	123.92	128.60
27	B8	2827	C	O4'-C1'-N1	7.81	114.45	108.20
1	AA	425	G	C5-C6-O6	-7.80	123.92	128.60
1	AA	1272	G	C5-C6-O6	-7.80	123.92	128.60
3	AV	71	C	O4'-C1'-N1	7.80	114.44	108.20
27	B8	246	C	O4'-C1'-N1	7.80	114.44	108.20
27	B8	1058	U	O4'-C1'-N1	7.80	114.44	108.20
27	B8	1904	G	C5-C6-O6	-7.80	123.92	128.60
1	AA	725	G	C5-C6-O6	-7.80	123.92	128.60
1	AA	738	C	O4'-C1'-N1	7.80	114.44	108.20
27	B8	108	G	C5-C6-O6	-7.80	123.92	128.60
1	AA	933	G	C5-C6-O6	-7.80	123.92	128.60
27	B8	851	C	O4'-C1'-N1	7.80	114.44	108.20
27	B8	1119	U	O4'-C1'-N1	7.80	114.44	108.20
1	AA	165	G	C5-C6-O6	-7.79	123.92	128.60
1	AA	439	U	O4'-C1'-N1	7.79	114.44	108.20
27	B8	1192	G	C5-C6-O6	-7.79	123.92	128.60
27	B8	239	C	O4'-C1'-N1	7.79	114.43	108.20
27	B8	1796	U	O4'-C1'-N1	7.79	114.44	108.20
1	AA	341	C	O4'-C1'-N1	7.79	114.43	108.20
1	AA	620	C	O4'-C1'-N1	7.79	114.43	108.20
27	B8	2228	G	C5-C6-O6	-7.79	123.92	128.60
27	B8	2703	C	O4'-C1'-N1	7.79	114.43	108.20
27	B8	1457	U	O4'-C1'-N1	7.79	114.43	108.20
1	AA	1494	G	C5-C6-O6	-7.79	123.93	128.60
27	B8	468	G	C5-C6-O6	-7.79	123.93	128.60
27	B8	2120	G	P-O3'-C3'	7.79	129.04	119.70
1	AA	1190	G	P-O3'-C3'	7.79	129.04	119.70
27	B8	2652	C	O4'-C1'-N1	7.79	114.43	108.20
1	AA	1276	G	C5-C6-O6	-7.79	123.93	128.60
27	B8	2509	G	C5-C6-O6	-7.79	123.93	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	894	G	C5-C6-O6	-7.78	123.93	128.60
1	AA	1310	G	C5-C6-O6	-7.78	123.93	128.60
27	B8	2153	C	O4'-C1'-N1	7.78	114.43	108.20
1	AA	164	G	C5-C6-O6	-7.78	123.93	128.60
1	AA	567	G	C5-C6-O6	-7.78	123.93	128.60
26	B7	73	A	C4-C5-C6	7.78	120.89	117.00
27	B8	1094	U	O4'-C1'-N1	7.78	114.42	108.20
27	B8	806	C	O4'-C1'-N1	7.78	114.42	108.20
27	B8	1954	G	C5-C6-O6	-7.78	123.93	128.60
1	AA	1334	G	C5-C6-O6	-7.78	123.93	128.60
1	AA	1471	U	O4'-C1'-N1	7.78	114.42	108.20
27	B8	1534	U	O4'-C1'-N1	7.78	114.42	108.20
27	B8	2731	G	C5-C6-O6	-7.78	123.93	128.60
1	AA	87	C	O4'-C1'-N1	7.78	114.42	108.20
1	AA	377	G	C5-C6-O6	-7.78	123.93	128.60
27	B8	678	C	O4'-C1'-N1	7.78	114.42	108.20
27	B8	2502	G	C5-C6-O6	-7.77	123.94	128.60
1	AA	289	G	C5-C6-O6	-7.77	123.94	128.60
1	AA	669	G	C5-C6-O6	-7.77	123.94	128.60
1	AA	763	G	C5-C6-O6	-7.77	123.94	128.60
27	B8	1784	A	C5-C6-N6	-7.77	117.48	123.70
1	AA	797	C	O4'-C1'-N1	7.77	114.42	108.20
1	AA	1018	G	O4'-C1'-N9	7.77	114.42	108.20
1	AA	1407	C	O4'-C1'-N1	7.77	114.41	108.20
27	B8	394	C	O4'-C1'-N1	7.77	114.42	108.20
27	B8	2134	A	O4'-C1'-N9	7.77	114.41	108.20
27	B8	2550	G	C5-C6-O6	-7.77	123.94	128.60
1	AA	1162	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	416	U	O4'-C1'-N1	7.76	114.41	108.20
27	B8	2854	G	C5-C6-O6	-7.76	123.94	128.60
1	AA	527	G	C5-C6-O6	-7.76	123.94	128.60
1	AA	586	C	O4'-C1'-N1	7.76	114.41	108.20
1	AA	685	G	C5-C6-O6	-7.76	123.94	128.60
1	AA	1336	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	1044	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	1348	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	2263	C	O4'-C1'-N1	7.76	114.41	108.20
1	AA	284	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	2838	G	C5-C6-O6	-7.76	123.94	128.60
27	B8	2011	U	O4'-C1'-N1	7.76	114.41	108.20
1	AA	477	C	O4'-C1'-N1	7.76	114.41	108.20
1	AA	1205	U	O4'-C1'-N1	7.76	114.41	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1443	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	2084	C	O4'-C1'-N1	7.76	114.41	108.20
27	B8	843	G	C5-C6-O6	-7.75	123.95	128.60
27	B8	1731	G	C5-C6-O6	-7.75	123.95	128.60
27	B8	1790	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	156	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	1181	G	N1-C6-O6	7.75	124.55	119.90
3	AV	54	G	C5-C6-O6	-7.75	123.95	128.60
27	B8	1804	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	312	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	347	G	C5-C6-O6	-7.75	123.95	128.60
27	B8	964	C	O4'-C1'-N1	7.75	114.40	108.20
27	B8	2040	G	C5-C6-O6	-7.75	123.95	128.60
1	AA	544	G	C5-C6-O6	-7.75	123.95	128.60
27	B8	883	G	N1-C6-O6	7.75	124.55	119.90
1	AA	707	U	O4'-C1'-N1	7.75	114.40	108.20
27	B8	32	C	O4'-C1'-N1	7.75	114.40	108.20
27	B8	128	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	897	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	924	C	O4'-C1'-N1	7.75	114.40	108.20
1	AA	1040	U	O4'-C1'-N1	7.75	114.40	108.20
1	AA	939	G	C5-C6-O6	-7.74	123.95	128.60
1	AA	541	G	C5-C6-O6	-7.74	123.95	128.60
1	AA	1121	U	O4'-C1'-N1	7.74	114.39	108.20
27	B8	2582	G	C5-C6-O6	-7.74	123.96	128.60
27	B8	2692	G	C5-C6-O6	-7.74	123.96	128.60
1	AA	1195	C	O4'-C1'-N1	7.74	114.39	108.20
27	B8	2472	G	C5-C6-O6	-7.74	123.96	128.60
27	B8	2510	C	O4'-C1'-N1	7.74	114.39	108.20
27	B8	1670	C	O4'-C1'-N1	7.73	114.39	108.20
27	B8	2136	G	C5-C6-O6	-7.73	123.96	128.60
27	B8	1375	U	O4'-C1'-N1	7.73	114.39	108.20
1	AA	404	G	C5-C6-O6	-7.73	123.96	128.60
1	AA	1031	C	O4'-C1'-N1	7.73	114.38	108.20
1	AA	1427	C	O4'-C1'-N1	7.73	114.38	108.20
27	B8	2155	U	O4'-C1'-N1	7.73	114.38	108.20
27	B8	811	U	O4'-C1'-N1	7.73	114.38	108.20
27	B8	2098	U	O4'-C1'-N1	7.73	114.38	108.20
1	AA	58	C	O4'-C1'-N1	7.72	114.38	108.20
27	B8	7	G	C5-C6-O6	-7.72	123.97	128.60
27	B8	921	C	O4'-C1'-N1	7.72	114.38	108.20
27	B8	2233	U	O4'-C1'-N1	7.72	114.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1519	G	C5-C6-O6	-7.72	123.97	128.60
27	B8	2851	A	N1-C6-N6	7.72	123.23	118.60
27	B8	1056	G	O4'-C1'-N9	7.72	114.38	108.20
27	B8	1792	G	C5-C6-O6	-7.72	123.97	128.60
27	B8	2125	G	N1-C6-O6	7.72	124.53	119.90
27	B8	2739	U	O4'-C1'-N1	7.72	114.38	108.20
1	AA	175	C	O4'-C1'-N1	7.72	114.37	108.20
1	AA	1059	C	O4'-C1'-N1	7.72	114.38	108.20
1	AA	1053	G	N1-C6-O6	7.72	124.53	119.90
27	B8	813	U	O4'-C1'-N1	7.72	114.37	108.20
27	B8	1478	G	C5-C6-O6	-7.72	123.97	128.60
27	B8	2404	U	O4'-C1'-N1	7.71	114.37	108.20
26	B7	1	U	O4'-C1'-N1	7.71	114.37	108.20
27	B8	2091	C	O4'-C1'-N1	7.71	114.37	108.20
1	AA	240	G	C5-C6-O6	-7.71	123.97	128.60
1	AA	806	C	O4'-C1'-N1	7.71	114.37	108.20
1	AA	1383	C	O4'-C1'-N1	7.71	114.37	108.20
27	B8	1296	G	C5-C6-O6	-7.71	123.97	128.60
27	B8	41	C	O4'-C1'-N1	7.71	114.37	108.20
27	B8	1988	G	C5-C6-O6	-7.71	123.97	128.60
1	AA	217	C	O4'-C1'-N1	7.71	114.37	108.20
1	AA	997	U	O4'-C1'-N1	7.71	114.37	108.20
3	AV	10	G	C5-C6-O6	-7.71	123.97	128.60
27	B8	1799	G	C5-C6-O6	-7.71	123.97	128.60
27	B8	2230	G	C5-C6-O6	-7.71	123.97	128.60
27	B8	2729	G	C5-C6-O6	-7.71	123.97	128.60
27	B8	1215	G	C5-C6-O6	-7.71	123.98	128.60
27	B8	2573	C	O4'-C1'-N1	7.71	114.36	108.20
27	B8	291	G	C5-C6-O6	-7.71	123.98	128.60
27	B8	2343	U	O4'-C1'-N1	7.71	114.36	108.20
27	B8	2240	U	O4'-C1'-N1	7.70	114.36	108.20
27	B8	2766	A	C5-C6-N6	-7.70	117.54	123.70
26	B7	49	C	O4'-C1'-N1	7.70	114.36	108.20
27	B8	211	C	O4'-C1'-N1	7.70	114.36	108.20
27	B8	240	C	O4'-C1'-N1	7.70	114.36	108.20
27	B8	2777	G	C5-C6-O6	-7.70	123.98	128.60
1	AA	497	G	C5-C6-O6	-7.70	123.98	128.60
1	AA	604	G	C5-C6-O6	-7.70	123.98	128.60
1	AA	788	U	O4'-C1'-N1	7.70	114.36	108.20
1	AA	1128	C	O4'-C1'-N1	7.70	114.36	108.20
27	B8	835	C	O4'-C1'-N1	7.70	114.36	108.20
27	B8	1281	G	C5-C6-O6	-7.70	123.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2789	C	O4'-C1'-N1	7.70	114.36	108.20
1	AA	1097	C	O4'-C1'-N1	7.70	114.36	108.20
1	AA	930	C	O4'-C1'-N1	7.70	114.36	108.20
27	B8	2554	U	O4'-C1'-N1	7.70	114.36	108.20
27	B8	1118	C	O4'-C1'-N1	7.69	114.36	108.20
27	B8	436	C	O4'-C1'-N1	7.69	114.36	108.20
27	B8	1218	G	C5-C6-O6	-7.69	123.98	128.60
1	AA	443	C	O4'-C1'-N1	7.69	114.35	108.20
27	B8	319	G	C5-C6-O6	-7.69	123.99	128.60
27	B8	659	G	C5-C6-O6	-7.69	123.99	128.60
27	B8	1906	G	C5-C6-O6	-7.69	123.98	128.60
27	B8	2161	C	P-O3'-C3'	7.69	128.93	119.70
27	B8	292	U	O4'-C1'-N1	7.69	114.35	108.20
27	B8	635	C	O4'-C1'-N1	7.69	114.35	108.20
1	AA	136	C	O4'-C1'-N1	7.69	114.35	108.20
1	AA	1253	G	C5-C6-O6	-7.69	123.99	128.60
26	B7	67	G	N1-C6-O6	7.69	124.51	119.90
1	AA	1174	G	C5-C6-O6	-7.69	123.99	128.60
27	B8	18	U	O4'-C1'-N1	7.69	114.35	108.20
1	AA	1292	G	C5-C6-O6	-7.68	123.99	128.60
27	B8	2202	U	O4'-C1'-N1	7.68	114.35	108.20
1	AA	18	C	O4'-C1'-N1	7.68	114.35	108.20
1	AA	680	C	O4'-C1'-N1	7.68	114.35	108.20
27	B8	85	G	C5-C6-O6	-7.68	123.99	128.60
27	B8	1830	C	O4'-C1'-N1	7.68	114.35	108.20
27	B8	2899	A	C5-C6-N6	-7.68	117.55	123.70
27	B8	1511	G	C5-C6-O6	-7.68	123.99	128.60
27	B8	1684	G	C5-C6-O6	-7.68	123.99	128.60
26	B7	93	C	O4'-C1'-N1	7.68	114.34	108.20
1	AA	552	U	O4'-C1'-N1	7.68	114.34	108.20
1	AA	1309	G	C5-C6-O6	-7.68	123.99	128.60
1	AA	1511	G	C5-C6-O6	-7.68	123.99	128.60
27	B8	1277	G	O4'-C1'-N9	7.68	114.34	108.20
27	B8	1657	U	O4'-C1'-N1	7.68	114.34	108.20
27	B8	2506	U	O4'-C1'-N1	7.68	114.34	108.20
1	AA	859	G	C5-C6-O6	-7.67	124.00	128.60
1	AA	1215	G	C5-C6-O6	-7.67	124.00	128.60
3	AV	42	C	O4'-C1'-N1	7.67	114.34	108.20
27	B8	17	G	C5-C6-O6	-7.67	124.00	128.60
27	B8	1979	U	O4'-C1'-N1	7.67	114.34	108.20
27	B8	2743	U	O4'-C1'-N1	7.67	114.34	108.20
1	AA	41	G	C5-C6-O6	-7.67	124.00	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	184	C	O4'-C1'-N1	7.67	114.34	108.20
1	AA	774	G	C5-C6-O6	-7.67	124.00	128.60
27	B8	1104	C	O4'-C1'-N1	7.67	114.33	108.20
27	B8	1113	U	O4'-C1'-N1	7.67	114.33	108.20
27	B8	2277	G	C5-C6-O6	-7.67	124.00	128.60
1	AA	1514	G	C5-C6-O6	-7.67	124.00	128.60
27	B8	285	G	C5-C6-O6	-7.67	124.00	128.60
27	B8	1432	G	O4'-C1'-N9	7.67	114.33	108.20
27	B8	1526	C	O4'-C1'-N1	7.67	114.33	108.20
1	AA	62	U	O4'-C1'-N1	7.66	114.33	108.20
1	AA	494	G	N1-C6-O6	7.66	124.50	119.90
1	AA	1364	U	O4'-C1'-N1	7.66	114.33	108.20
27	B8	2229	U	O4'-C1'-N1	7.66	114.33	108.20
27	B8	2308	G	N1-C6-O6	7.66	124.50	119.90
1	AA	418	C	O4'-C1'-N1	7.66	114.33	108.20
1	AA	203	G	O4'-C1'-N9	7.66	114.33	108.20
27	B8	2636	C	O4'-C1'-N1	7.66	114.33	108.20
2	AX	17	C	O4'-C1'-N1	7.66	114.33	108.20
3	AV	57	C	O4'-C1'-N1	7.66	114.33	108.20
27	B8	1317	G	N1-C6-O6	7.66	124.50	119.90
27	B8	2460	U	O4'-C1'-N1	7.66	114.33	108.20
27	B8	400	G	C5-C6-O6	-7.66	124.01	128.60
27	B8	937	C	O4'-C1'-N1	7.66	114.33	108.20
27	B8	2043	C	O4'-C1'-N1	7.66	114.33	108.20
27	B8	258	G	C5-C6-O6	-7.66	124.01	128.60
27	B8	1250	G	C5-C6-O6	-7.66	124.01	128.60
27	B8	838	C	O4'-C1'-N1	7.65	114.32	108.20
27	B8	1581	G	C5-C6-O6	-7.65	124.01	128.60
1	AA	734	G	C5-C6-O6	-7.65	124.01	128.60
1	AA	758	C	O4'-C1'-N1	7.65	114.32	108.20
1	AA	1107	C	O4'-C1'-N1	7.65	114.32	108.20
27	B8	40	U	O4'-C1'-N1	7.65	114.32	108.20
27	B8	966	G	C5-C6-O6	-7.65	124.01	128.60
27	B8	1921	G	C5-C6-O6	-7.65	124.01	128.60
27	B8	2671	G	C5-C6-O6	-7.65	124.01	128.60
1	AA	170	U	O4'-C1'-N1	7.65	114.32	108.20
1	AA	954	G	C5-C6-O6	-7.65	124.01	128.60
1	AA	1424	U	O4'-C1'-N1	7.65	114.32	108.20
27	B8	290	U	O4'-C1'-N1	7.65	114.32	108.20
1	AA	337	G	C5-C6-O6	-7.65	124.01	128.60
1	AA	1448	C	O4'-C1'-N1	7.65	114.32	108.20
26	B7	47	C	O4'-C1'-N1	7.65	114.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1930	G	O4'-C1'-N9	7.65	114.32	108.20
1	AA	1237	C	O4'-C1'-N1	7.65	114.32	108.20
1	AA	1161	C	O4'-C1'-N1	7.64	114.31	108.20
1	AA	476	U	O4'-C1'-N1	7.64	114.31	108.20
27	B8	2626	C	O4'-C1'-N1	7.64	114.31	108.20
1	AA	679	C	O4'-C1'-N1	7.64	114.31	108.20
27	B8	624	C	O4'-C1'-N1	7.64	114.31	108.20
27	B8	763	G	C5-C6-O6	-7.64	124.02	128.60
27	B8	901	C	O4'-C1'-N1	7.64	114.31	108.20
27	B8	940	G	C5-C6-O6	-7.64	124.02	128.60
1	AA	902	G	C5-C6-O6	-7.64	124.02	128.60
1	AA	1252	A	C5-C6-N6	-7.64	117.59	123.70
27	B8	779	U	O4'-C1'-N1	7.64	114.31	108.20
27	B8	2430	A	C4-C5-C6	7.64	120.82	117.00
1	AA	1247	U	O4'-C1'-N1	7.63	114.31	108.20
27	B8	27	G	O4'-C1'-N9	7.63	114.31	108.20
27	B8	250	G	N1-C6-O6	7.63	124.48	119.90
27	B8	2783	U	O4'-C1'-N1	7.63	114.31	108.20
1	AA	540	G	C5-C6-O6	-7.63	124.02	128.60
27	B8	2306	C	O4'-C1'-N1	7.63	114.31	108.20
3	AV	66	U	O4'-C1'-N1	7.63	114.30	108.20
27	B8	110	G	C5-C6-O6	-7.63	124.02	128.60
27	B8	1201	U	O4'-C1'-N1	7.63	114.30	108.20
1	AA	688	G	C5-C6-O6	-7.63	124.02	128.60
27	B8	2798	U	O4'-C1'-N1	7.63	114.30	108.20
27	B8	2876	G	C5-C6-O6	-7.63	124.02	128.60
27	B8	261	G	C5-C6-O6	-7.62	124.03	128.60
27	B8	1179	G	C5-C6-O6	-7.62	124.03	128.60
1	AA	854	U	O4'-C1'-N1	7.62	114.30	108.20
27	B8	1290	C	O4'-C1'-N1	7.62	114.30	108.20
1	AA	846	G	C5-C6-O6	-7.62	124.03	128.60
1	AA	1390	U	O4'-C1'-N1	7.62	114.30	108.20
27	B8	275	C	O4'-C1'-N1	7.62	114.30	108.20
27	B8	1399	C	O4'-C1'-N1	7.62	114.30	108.20
27	B8	1482	G	C5-C6-O6	-7.62	124.03	128.60
1	AA	206	C	O4'-C1'-N1	7.62	114.30	108.20
27	B8	1977	A	C5-C6-N6	-7.62	117.60	123.70
1	AA	141	G	C5-C6-O6	-7.62	124.03	128.60
1	AA	1140	C	O4'-C1'-N1	7.62	114.29	108.20
27	B8	677	A	C5-C6-N6	-7.62	117.61	123.70
27	B8	863	A	C5-C6-N6	-7.62	117.61	123.70
27	B8	2686	G	C5-C6-O6	-7.62	124.03	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BG	93	TYR	CB-CG-CD1	-7.62	116.43	121.00
27	B8	1499	C	O4'-C1'-N1	7.61	114.29	108.20
27	B8	2394	C	O4'-C1'-N1	7.61	114.29	108.20
27	B8	2165	C	P-O3'-C3'	7.61	128.83	119.70
27	B8	2442	C	O4'-C1'-N1	7.61	114.29	108.20
27	B8	2844	G	O4'-C1'-N9	7.61	114.29	108.20
1	AA	348	G	C5-C6-O6	-7.61	124.03	128.60
27	B8	1416	G	C5-C6-O6	-7.61	124.03	128.60
27	B8	1992	G	C5-C6-O6	-7.61	124.04	128.60
1	AA	1070	U	O4'-C1'-N1	7.61	114.28	108.20
27	B8	698	C	O4'-C1'-N1	7.61	114.28	108.20
27	B8	1411	U	O4'-C1'-N1	7.61	114.28	108.20
27	B8	79	C	O4'-C1'-N1	7.60	114.28	108.20
27	B8	1096	A	O4'-C1'-N9	7.60	114.28	108.20
27	B8	2330	G	C5-C6-O6	-7.60	124.04	128.60
1	AA	929	G	C5-C6-O6	-7.60	124.04	128.60
1	AA	1356	G	C5-C6-O6	-7.60	124.04	128.60
1	AA	1481	U	O4'-C1'-N1	7.60	114.28	108.20
27	B8	959	A	C5-C6-N6	-7.60	117.62	123.70
27	B8	1062	G	C5-C6-O6	-7.60	124.04	128.60
27	B8	1007	C	O4'-C1'-N1	7.60	114.28	108.20
27	B8	1708	C	O4'-C1'-N1	7.60	114.28	108.20
27	B8	2123	G	C5-C6-O6	-7.60	124.04	128.60
1	AA	277	C	O4'-C1'-N1	7.60	114.28	108.20
27	B8	122	G	C5-C6-O6	-7.60	124.04	128.60
1	AA	1183	U	O4'-C1'-N1	7.59	114.28	108.20
27	B8	810	U	O4'-C1'-N1	7.59	114.28	108.20
27	B8	1641	A	C4-C5-C6	7.59	120.80	117.00
27	B8	2514	U	O4'-C1'-N1	7.59	114.28	108.20
1	AA	659	U	O4'-C1'-N1	7.59	114.27	108.20
27	B8	2427	C	O4'-C1'-N1	7.59	114.27	108.20
1	AA	1353	G	C5-C6-O6	-7.59	124.05	128.60
1	AA	1536	C	O4'-C1'-N1	7.59	114.27	108.20
27	B8	674	G	C5-C6-O6	-7.59	124.05	128.60
27	B8	1064	C	O4'-C1'-N1	7.59	114.27	108.20
27	B8	1974	C	O4'-C1'-N1	7.59	114.27	108.20
27	B8	2875	C	O4'-C1'-N1	7.59	114.27	108.20
1	AA	474	G	C5-C6-O6	-7.59	124.05	128.60
1	AA	1373	G	C5-C6-O6	-7.59	124.05	128.60
27	B8	1052	C	O4'-C1'-N1	7.59	114.27	108.20
27	B8	1933	G	C5-C6-O6	-7.59	124.05	128.60
1	AA	29	U	O4'-C1'-N1	7.59	114.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	123	U	O4'-C1'-N1	7.59	114.27	108.20
26	B7	19	C	O4'-C1'-N1	7.59	114.27	108.20
27	B8	2621	G	C5-C6-O6	-7.59	124.05	128.60
1	AA	1341	U	O4'-C1'-N1	7.59	114.27	108.20
1	AA	1367	C	O4'-C1'-N1	7.59	114.27	108.20
27	B8	441	U	O4'-C1'-N1	7.59	114.27	108.20
1	AA	1100	C	O4'-C1'-N1	7.58	114.27	108.20
27	B8	1833	C	O4'-C1'-N1	7.58	114.27	108.20
27	B8	1861	G	C5-C6-O6	-7.58	124.05	128.60
27	B8	314	C	O4'-C1'-N1	7.58	114.27	108.20
27	B8	1019	U	O4'-C1'-N1	7.58	114.27	108.20
27	B8	1190	G	C5-C6-O6	-7.58	124.05	128.60
1	AA	671	G	C5-C6-O6	-7.58	124.05	128.60
27	B8	1675	C	O4'-C1'-N1	7.58	114.26	108.20
27	B8	2047	C	O4'-C1'-N1	7.58	114.26	108.20
1	AA	342	C	O4'-C1'-N1	7.58	114.26	108.20
1	AA	1027	C	O4'-C1'-N1	7.58	114.26	108.20
1	AA	1114	C	O4'-C1'-N1	7.58	114.26	108.20
27	B8	1771	C	O4'-C1'-N1	7.58	114.26	108.20
1	AA	615	G	O4'-C1'-N9	7.58	114.26	108.20
27	B8	1097	U	O4'-C1'-N1	7.58	114.26	108.20
27	B8	2840	C	O4'-C1'-N1	7.58	114.26	108.20
1	AA	233	C	O4'-C1'-N1	7.58	114.26	108.20
27	B8	1707	G	C5-C6-O6	-7.58	124.06	128.60
27	B8	2672	U	O4'-C1'-N1	7.58	114.26	108.20
1	AA	811	C	O4'-C1'-N1	7.57	114.26	108.20
27	B8	1537	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	1941	C	O4'-C1'-N1	7.57	114.26	108.20
1	AA	1457	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	2012	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	406	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	994	C	O4'-C1'-N1	7.57	114.26	108.20
27	B8	2702	G	C5-C6-O6	-7.57	124.06	128.60
1	AA	396	C	O4'-C1'-N1	7.57	114.25	108.20
1	AA	1119	C	O4'-C1'-N1	7.57	114.25	108.20
1	AA	436	C	O4'-C1'-N1	7.57	114.25	108.20
26	B7	64	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	560	C	O4'-C1'-N1	7.57	114.25	108.20
27	B8	2878	U	O4'-C1'-N1	7.57	114.25	108.20
27	B8	760	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	1241	A	O4'-C1'-N9	7.57	114.25	108.20
27	B8	1533	C	O4'-C1'-N1	7.57	114.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1984	G	C5-C6-O6	-7.57	124.06	128.60
27	B8	2456	C	O4'-C1'-N1	7.57	114.25	108.20
27	B8	420	C	O4'-C1'-N1	7.56	114.25	108.20
27	B8	2313	C	O4'-C1'-N1	7.56	114.25	108.20
27	B8	2440	C	O4'-C1'-N1	7.56	114.25	108.20
1	AA	545	C	O4'-C1'-N1	7.56	114.25	108.20
27	B8	2888	C	O4'-C1'-N1	7.56	114.25	108.20
1	AA	1412	C	O4'-C1'-N1	7.56	114.25	108.20
27	B8	1624	U	O4'-C1'-N1	7.56	114.25	108.20
27	B8	2150	C	O4'-C1'-N1	7.56	114.25	108.20
27	B8	2235	G	C5-C6-O6	-7.56	124.06	128.60
1	AA	221	C	O4'-C1'-N1	7.56	114.25	108.20
3	AV	41	U	O4'-C1'-N1	7.56	114.25	108.20
27	B8	1081	U	O4'-C1'-N1	7.56	114.25	108.20
27	B8	2247	A	O4'-C1'-N9	7.56	114.25	108.20
27	B8	2293	G	C5-C6-O6	-7.56	124.06	128.60
27	B8	1158	C	O4'-C1'-N1	7.56	114.25	108.20
1	AA	249	U	O4'-C1'-N1	7.55	114.24	108.20
27	B8	873	C	O4'-C1'-N1	7.55	114.24	108.20
27	B8	2004	G	C5-C6-O6	-7.55	124.07	128.60
1	AA	786	G	O4'-C1'-N9	7.55	114.24	108.20
27	B8	1808	A	O4'-C1'-N9	7.55	114.24	108.20
27	B8	1976	U	O4'-C1'-N1	7.55	114.24	108.20
1	AA	395	C	O4'-C1'-N1	7.55	114.24	108.20
3	AV	24	C	O4'-C1'-N1	7.55	114.24	108.20
26	B7	16	G	O4'-C1'-N9	7.55	114.24	108.20
26	B7	83	G	C5-C6-O6	-7.55	124.07	128.60
27	B8	786	C	O4'-C1'-N1	7.55	114.24	108.20
1	AA	737	C	O4'-C1'-N1	7.55	114.24	108.20
1	AA	766	A	O4'-C1'-N9	7.55	114.24	108.20
1	AA	805	C	O4'-C1'-N1	7.55	114.24	108.20
26	B7	108	A	C5-C6-N6	-7.55	117.66	123.70
27	B8	738	G	C5-C6-O6	-7.55	124.07	128.60
27	B8	2026	U	O4'-C1'-N1	7.55	114.24	108.20
27	B8	2650	U	O4'-C1'-N1	7.55	114.24	108.20
1	AA	656	G	O4'-C1'-N9	7.54	114.23	108.20
1	AA	1468	A	C4-C5-C6	7.54	120.77	117.00
27	B8	1220	G	O4'-C1'-N9	7.54	114.23	108.20
27	B8	1438	U	O4'-C1'-N1	7.54	114.23	108.20
27	B8	1560	G	C5-C6-O6	-7.54	124.07	128.60
27	B8	1564	C	O4'-C1'-N1	7.54	114.24	108.20
27	B8	1881	C	O4'-C1'-N1	7.54	114.23	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2322	A	O4'-C1'-N9	7.54	114.23	108.20
27	B8	1430	G	C5-C6-O6	-7.54	124.08	128.60
35	BG	93	TYR	CB-CG-CD2	7.54	125.52	121.00
1	AA	1444	U	O4'-C1'-N1	7.54	114.23	108.20
27	B8	1535	A	O4'-C1'-N9	7.54	114.23	108.20
27	B8	2567	G	C5-C6-O6	-7.54	124.08	128.60
1	AA	795	C	O4'-C1'-N1	7.54	114.23	108.20
1	AA	984	C	O4'-C1'-N1	7.54	114.23	108.20
1	AA	1078	U	O4'-C1'-N1	7.54	114.23	108.20
27	B8	2903	U	C2-N1-C1'	7.54	126.74	117.70
1	AA	1232	U	O4'-C1'-N1	7.53	114.23	108.20
27	B8	1195	G	C5-C6-O6	-7.53	124.08	128.60
27	B8	1330	C	O4'-C1'-N1	7.53	114.23	108.20
1	AA	916	U	O4'-C1'-N1	7.53	114.22	108.20
27	B8	1653	G	C5-C6-O6	-7.53	124.08	128.60
27	B8	2569	G	C5-C6-O6	-7.53	124.08	128.60
27	B8	2583	G	C5-C6-O6	-7.53	124.08	128.60
27	B8	2303	G	C5-C6-O6	-7.53	124.08	128.60
1	AA	110	C	O4'-C1'-N1	7.53	114.22	108.20
1	AA	709	U	O4'-C1'-N1	7.53	114.22	108.20
1	AA	1351	U	O4'-C1'-N1	7.53	114.22	108.20
27	B8	358	U	O4'-C1'-N1	7.53	114.22	108.20
27	B8	380	G	C5-C6-O6	-7.53	124.08	128.60
27	B8	681	G	C5-C6-O6	-7.53	124.08	128.60
27	B8	865	C	O4'-C1'-N1	7.53	114.22	108.20
27	B8	908	C	O4'-C1'-N1	7.53	114.22	108.20
1	AA	1056	U	O4'-C1'-N1	7.53	114.22	108.20
27	B8	1764	C	O4'-C1'-N1	7.53	114.22	108.20
27	B8	45	G	C5-C6-O6	-7.52	124.09	128.60
27	B8	281	C	O4'-C1'-N1	7.52	114.22	108.20
27	B8	554	U	O4'-C1'-N1	7.52	114.22	108.20
27	B8	1486	U	O4'-C1'-N1	7.52	114.22	108.20
1	AA	1348	U	O4'-C1'-N1	7.52	114.22	108.20
27	B8	2087	G	C5-C6-O6	-7.52	124.09	128.60
1	AA	1472	U	O4'-C1'-N1	7.52	114.22	108.20
27	B8	2006	C	O4'-C1'-N1	7.52	114.22	108.20
27	B8	2316	G	C5-C6-O6	-7.52	124.09	128.60
1	AA	521	G	C5-C6-O6	-7.52	124.09	128.60
27	B8	906	U	O4'-C1'-N1	7.52	114.21	108.20
27	B8	1043	C	O4'-C1'-N1	7.52	114.21	108.20
1	AA	953	G	C5-C6-O6	-7.52	124.09	128.60
27	B8	145	C	O4'-C1'-N1	7.52	114.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1441	G	C5-C6-O6	-7.52	124.09	128.60
1	AA	720	C	O4'-C1'-N1	7.51	114.21	108.20
1	AA	1207	G	C5-C6-O6	-7.51	124.09	128.60
27	B8	271	G	C5-C6-O6	-7.51	124.09	128.60
27	B8	2413	G	C5-C6-O6	-7.51	124.09	128.60
1	AA	200	G	C5-C6-O6	-7.51	124.09	128.60
3	AV	28	C	O4'-C1'-N1	7.51	114.21	108.20
1	AA	276	G	C5-C6-O6	-7.51	124.09	128.60
27	B8	691	C	O4'-C1'-N1	7.51	114.21	108.20
27	B8	1500	G	C5-C6-O6	-7.51	124.09	128.60
27	B8	2428	G	C5-C6-O6	-7.51	124.09	128.60
27	B8	141	G	O4'-C1'-N9	7.51	114.21	108.20
27	B8	1216	G	C5-C6-O6	-7.51	124.10	128.60
27	B8	2606	C	O4'-C1'-N1	7.51	114.20	108.20
27	B8	498	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	588	U	O4'-C1'-N1	7.50	114.20	108.20
27	B8	1175	A	O4'-C1'-N9	7.50	114.20	108.20
27	B8	1208	C	O4'-C1'-N1	7.50	114.20	108.20
1	AA	1043	G	C5-C6-O6	-7.50	124.10	128.60
1	AA	1187	G	C5-C6-O6	-7.50	124.10	128.60
1	AA	1370	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	60	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	2341	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	2389	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	335	C	O4'-C1'-N1	7.50	114.20	108.20
27	B8	2788	C	O4'-C1'-N1	7.50	114.20	108.20
27	B8	1337	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	1368	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	1382	G	N1-C6-O6	7.50	124.40	119.90
27	B8	2246	G	C5-C6-O6	-7.50	124.10	128.60
1	AA	1423	G	C5-C6-O6	-7.50	124.10	128.60
27	B8	2619	C	O4'-C1'-N1	7.50	114.20	108.20
27	B8	2126	A	O4'-C1'-N9	7.50	114.20	108.20
1	AA	804	U	O4'-C1'-N1	7.49	114.19	108.20
1	AA	885	G	C5-C6-O6	-7.49	124.11	128.60
27	B8	2633	G	C5-C6-O6	-7.49	124.11	128.60
1	AA	548	G	C5-C6-O6	-7.49	124.11	128.60
1	AA	643	C	O4'-C1'-N1	7.49	114.19	108.20
27	B8	229	C	O4'-C1'-N1	7.49	114.19	108.20
27	B8	839	U	O4'-C1'-N1	7.49	114.19	108.20
27	B8	1017	G	O4'-C1'-N9	7.49	114.19	108.20
27	B8	1185	G	C5-C6-O6	-7.49	124.11	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1663	G	C5-C6-O6	-7.49	124.11	128.60
1	AA	293	G	C5-C6-O6	-7.49	124.11	128.60
1	AA	937	A	C5-C6-N6	-7.49	117.71	123.70
27	B8	944	C	O4'-C1'-N1	7.49	114.19	108.20
27	B8	1390	U	O4'-C1'-N1	7.49	114.19	108.20
27	B8	2709	G	C5-C6-O6	-7.49	124.11	128.60
27	B8	1303	G	C5-C6-O6	-7.49	124.11	128.60
27	B8	1555	G	C5-C6-O6	-7.49	124.11	128.60
27	B8	2661	G	C5-C6-O6	-7.49	124.11	128.60
26	B7	65	U	O4'-C1'-N1	7.49	114.19	108.20
27	B8	1491	G	C5-C6-O6	-7.49	124.11	128.60
27	B8	2337	G	C5-C6-O6	-7.49	124.11	128.60
1	AA	611	C	O4'-C1'-N1	7.48	114.19	108.20
1	AA	943	U	O4'-C1'-N1	7.48	114.19	108.20
27	B8	82	U	O4'-C1'-N1	7.48	114.19	108.20
27	B8	2064	C	O4'-C1'-N1	7.48	114.19	108.20
27	B8	2167	U	O4'-C1'-N1	7.48	114.19	108.20
1	AA	493	A	O4'-C1'-N9	7.48	114.18	108.20
3	AV	17	C	O4'-C1'-N1	7.48	114.19	108.20
27	B8	1873	G	C5-C6-O6	-7.48	124.11	128.60
27	B8	640	C	O4'-C1'-N1	7.48	114.18	108.20
1	AA	227	G	C5-C6-O6	-7.48	124.11	128.60
27	B8	132	G	C5-C6-O6	-7.48	124.11	128.60
27	B8	2454	G	C5-C6-O6	-7.47	124.12	128.60
1	AA	911	U	O4'-C1'-N1	7.47	114.18	108.20
1	AA	1327	C	O4'-C1'-N1	7.47	114.18	108.20
27	B8	2272	U	O4'-C1'-N1	7.47	114.18	108.20
27	B8	2642	G	C5-C6-O6	-7.47	124.12	128.60
27	B8	76	C	O4'-C1'-N1	7.47	114.17	108.20
27	B8	553	G	C5-C6-O6	-7.47	124.12	128.60
27	B8	2152	G	N1-C6-O6	7.47	124.38	119.90
27	B8	2334	U	O4'-C1'-N1	7.47	114.18	108.20
1	AA	37	U	O4'-C1'-N1	7.47	114.17	108.20
1	AA	68	G	N1-C6-O6	7.47	124.38	119.90
27	B8	410	G	C5-C6-O6	-7.47	124.12	128.60
1	AA	697	U	O4'-C1'-N1	7.47	114.17	108.20
1	AA	1442	G	C5-C6-O6	-7.47	124.12	128.60
26	B7	89	U	O4'-C1'-N1	7.47	114.17	108.20
27	B8	848	C	O4'-C1'-N1	7.47	114.17	108.20
27	B8	697	G	C5-C6-O6	-7.46	124.12	128.60
27	B8	1202	G	C5-C6-O6	-7.46	124.12	128.60
27	B8	2669	G	C5-C6-O6	-7.46	124.12	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2710	C	O4'-C1'-N1	7.46	114.17	108.20
1	AA	590	U	O4'-C1'-N1	7.46	114.17	108.20
26	B7	117	G	C5-C6-O6	-7.46	124.12	128.60
27	B8	1443	U	O4'-C1'-N1	7.46	114.17	108.20
27	B8	1474	U	O4'-C1'-N1	7.46	114.17	108.20
27	B8	2818	U	O4'-C1'-N1	7.46	114.17	108.20
1	AA	903	G	C5-C6-O6	-7.46	124.12	128.60
1	AA	955	U	O4'-C1'-N1	7.46	114.17	108.20
1	AA	1339	A	C4-C5-C6	7.46	120.73	117.00
27	B8	1868	C	O4'-C1'-N1	7.46	114.17	108.20
27	B8	484	C	O4'-C1'-N1	7.46	114.17	108.20
27	B8	1894	C	O4'-C1'-N1	7.46	114.17	108.20
27	B8	536	G	C5-C6-O6	-7.46	124.12	128.60
1	AA	485	U	O4'-C1'-N1	7.46	114.17	108.20
27	B8	1295	C	O4'-C1'-N1	7.46	114.17	108.20
27	B8	1112	G	O4'-C1'-N9	7.46	114.16	108.20
26	B7	48	U	O4'-C1'-N1	7.45	114.16	108.20
27	B8	1740	G	C5-C6-O6	-7.45	124.13	128.60
1	AA	678	U	O4'-C1'-N1	7.45	114.16	108.20
1	AA	1186	G	C5-C6-O6	-7.45	124.13	128.60
1	AA	1208	C	O4'-C1'-N1	7.45	114.16	108.20
1	AA	1376	U	O4'-C1'-N1	7.45	114.16	108.20
26	B7	116	G	C5-C6-O6	-7.45	124.13	128.60
27	B8	134	G	C5-C6-O6	-7.45	124.13	128.60
27	B8	2180	U	O4'-C1'-N1	7.45	114.16	108.20
27	B8	2495	G	C5-C6-O6	-7.45	124.13	128.60
27	B8	2528	U	O4'-C1'-N1	7.45	114.16	108.20
27	B8	80	G	C5-C6-O6	-7.45	124.13	128.60
27	B8	2762	C	O4'-C1'-N1	7.45	114.16	108.20
1	AA	73	C	O4'-C1'-N1	7.45	114.16	108.20
27	B8	1761	C	O4'-C1'-N1	7.45	114.16	108.20
1	AA	372	C	O4'-C1'-N1	7.44	114.16	108.20
27	B8	1576	U	O4'-C1'-N1	7.44	114.16	108.20
27	B8	2241	A	O4'-C1'-N9	7.44	114.16	108.20
27	B8	856	G	C5-C6-O6	-7.44	124.13	128.60
27	B8	1409	U	O4'-C1'-N1	7.44	114.15	108.20
1	AA	1131	G	N1-C6-O6	7.44	124.36	119.90
27	B8	852	U	O4'-C1'-N1	7.44	114.15	108.20
27	B8	2395	C	O4'-C1'-N1	7.44	114.15	108.20
27	B8	2525	G	C5-C6-O6	-7.44	124.14	128.60
1	AA	877	G	C5-C6-O6	-7.44	124.14	128.60
1	AA	1354	U	O4'-C1'-N1	7.44	114.15	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1335	C	O4'-C1'-N1	7.44	114.15	108.20
27	B8	510	C	O4'-C1'-N1	7.44	114.15	108.20
27	B8	1660	G	C5-C6-O6	-7.44	124.14	128.60
1	AA	391	G	C5-C6-O6	-7.43	124.14	128.60
1	AA	847	G	O4'-C1'-N9	7.43	114.15	108.20
27	B8	774	G	C5-C6-O6	-7.43	124.14	128.60
1	AA	920	U	O4'-C1'-N1	7.43	114.15	108.20
26	B7	21	G	C5-C6-O6	-7.43	124.14	128.60
27	B8	70	G	C5-C6-O6	-7.43	124.14	128.60
27	B8	1813	G	C5-C6-O6	-7.43	124.14	128.60
27	B8	2367	G	C5-C6-O6	-7.43	124.14	128.60
1	AA	1264	U	O4'-C1'-N1	7.43	114.14	108.20
27	B8	37	C	O4'-C1'-N1	7.43	114.14	108.20
27	B8	702	U	O4'-C1'-N1	7.43	114.14	108.20
27	B8	1923	U	O4'-C1'-N1	7.43	114.14	108.20
27	B8	993	G	C5-C6-O6	-7.43	124.14	128.60
27	B8	1055	G	C5-C6-O6	-7.43	124.14	128.60
1	AA	577	G	C5-C6-O6	-7.42	124.14	128.60
26	B7	98	G	C5-C6-O6	-7.42	124.14	128.60
1	AA	1342	C	O4'-C1'-N1	7.42	114.14	108.20
26	B7	32	U	O4'-C1'-N1	7.42	114.14	108.20
27	B8	304	U	O4'-C1'-N1	7.42	114.14	108.20
27	B8	1722	A	C4-C5-C6	7.42	120.71	117.00
27	B8	35	G	C5-C6-O6	-7.42	124.15	128.60
27	B8	2212	A	O4'-C1'-N9	7.42	114.14	108.20
27	B8	2219	U	O4'-C1'-N1	7.42	114.14	108.20
1	AA	453	G	N1-C6-O6	7.42	124.35	119.90
1	AA	1300	G	C5-C6-O6	-7.42	124.15	128.60
27	B8	1282	U	O4'-C1'-N1	7.42	114.13	108.20
27	B8	2290	G	C5-C6-O6	-7.42	124.15	128.60
1	AA	144	G	C5-C6-O6	-7.41	124.15	128.60
1	AA	40	C	O4'-C1'-N1	7.41	114.13	108.20
1	AA	837	U	O4'-C1'-N1	7.41	114.13	108.20
1	AA	1198	G	C5-C6-O6	-7.41	124.15	128.60
27	B8	1449	G	C5-C6-O6	-7.41	124.15	128.60
1	AA	1233	G	C5-C6-O6	-7.41	124.16	128.60
27	B8	178	G	C5-C6-O6	-7.41	124.16	128.60
27	B8	683	U	O4'-C1'-N1	7.41	114.13	108.20
27	B8	1887	C	O4'-C1'-N1	7.41	114.12	108.20
1	AA	1314	C	O4'-C1'-N1	7.41	114.12	108.20
27	B8	877	A	C4-C5-C6	7.41	120.70	117.00
27	B8	1011	G	C5-C6-O6	-7.41	124.16	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1574	C	O4'-C1'-N1	7.41	114.12	108.20
27	B8	2487	G	C5-C6-O6	-7.41	124.16	128.60
1	AA	491	G	C5-C6-O6	-7.40	124.16	128.60
1	AA	791	G	C5-C6-O6	-7.40	124.16	128.60
1	AA	1243	C	O4'-C1'-N1	7.40	114.12	108.20
27	B8	296	U	O4'-C1'-N1	7.40	114.12	108.20
27	B8	708	G	C5-C6-O6	-7.40	124.16	128.60
27	B8	1846	G	C5-C6-O6	-7.40	124.16	128.60
27	B8	1867	G	C5-C6-O6	-7.40	124.16	128.60
1	AA	550	G	C5-C6-O6	-7.40	124.16	128.60
1	AA	1538	C	O4'-C1'-N1	7.40	114.12	108.20
27	B8	884	U	O4'-C1'-N1	7.40	114.12	108.20
1	AA	1307	U	O4'-C1'-N1	7.40	114.12	108.20
27	B8	934	U	O4'-C1'-N1	7.40	114.12	108.20
27	B8	1053	C	O4'-C1'-N1	7.40	114.12	108.20
27	B8	1628	G	C5-C6-O6	-7.40	124.16	128.60
1	AA	896	C	O4'-C1'-N1	7.39	114.11	108.20
1	AA	1159	U	O4'-C1'-N1	7.39	114.11	108.20
26	B7	70	C	O4'-C1'-N1	7.39	114.11	108.20
27	B8	378	C	O4'-C1'-N1	7.39	114.12	108.20
27	B8	449	A	C5-C6-N6	-7.39	117.79	123.70
27	B8	2251	G	C5-C6-O6	-7.39	124.17	128.60
1	AA	967	C	O4'-C1'-N1	7.39	114.11	108.20
27	B8	301	G	C5-C6-O6	-7.39	124.17	128.60
1	AA	119	A	C4-C5-C6	7.39	120.69	117.00
27	B8	1897	G	C5-C6-O6	-7.39	124.17	128.60
1	AA	212	G	C5-C6-O6	-7.39	124.17	128.60
27	B8	464	U	O4'-C1'-N1	7.39	114.11	108.20
27	B8	773	U	O4'-C1'-N1	7.39	114.11	108.20
26	B7	30	C	O4'-C1'-N1	7.39	114.11	108.20
27	B8	805	G	C5-C6-O6	-7.39	124.17	128.60
27	B8	1136	G	C5-C6-O6	-7.39	124.17	128.60
27	B8	1388	G	C5-C6-O6	-7.39	124.17	128.60
27	B8	1747	U	O4'-C1'-N1	7.39	114.11	108.20
1	AA	410	G	N1-C6-O6	7.38	124.33	119.90
27	B8	1013	C	O4'-C1'-N1	7.38	114.11	108.20
27	B8	2187	U	O4'-C1'-N1	7.38	114.11	108.20
27	B8	585	G	C5-C6-O6	-7.38	124.17	128.60
1	AA	316	C	O4'-C1'-N1	7.38	114.11	108.20
1	AA	1535	C	O4'-C1'-N1	7.38	114.11	108.20
27	B8	1161	C	O4'-C1'-N1	7.38	114.10	108.20
27	B8	1659	G	C5-C6-O6	-7.38	124.17	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1725	U	O4'-C1'-N1	7.38	114.10	108.20
27	B8	2555	U	O4'-C1'-N1	7.38	114.10	108.20
1	AA	783	C	O4'-C1'-N1	7.37	114.10	108.20
1	AA	836	G	C5-C6-O6	-7.37	124.18	128.60
27	B8	392	U	O4'-C1'-N1	7.37	114.10	108.20
1	AA	1270	G	C5-C6-O6	-7.37	124.18	128.60
27	B8	1037	G	C5-C6-O6	-7.37	124.18	128.60
27	B8	2036	C	O4'-C1'-N1	7.37	114.10	108.20
1	AA	154	U	O4'-C1'-N1	7.37	114.10	108.20
1	AA	1142	G	P-O3'-C3'	7.37	128.54	119.70
27	B8	1666	G	C5-C6-O6	-7.37	124.18	128.60
1	AA	406	G	C5-C6-O6	-7.37	124.18	128.60
1	AA	723	U	O4'-C1'-N1	7.37	114.09	108.20
1	AA	893	C	O4'-C1'-N1	7.37	114.09	108.20
1	AA	765	G	O4'-C1'-N9	7.37	114.09	108.20
27	B8	2445	G	C5-C6-O6	-7.37	124.18	128.60
1	AA	515	G	C5-C6-O6	-7.37	124.18	128.60
1	AA	1316	G	N3-C2-N2	7.37	125.06	119.90
27	B8	656	G	C5-C6-O6	-7.37	124.18	128.60
27	B8	1608	A	C4-C5-C6	7.37	120.68	117.00
1	AA	839	C	O4'-C1'-N1	7.36	114.09	108.20
1	AA	1312	G	C5-C6-O6	-7.36	124.18	128.60
27	B8	1360	G	N1-C6-O6	7.36	124.32	119.90
27	B8	1444	G	C5-C6-O6	-7.36	124.18	128.60
27	B8	1450	G	C5-C6-O6	-7.36	124.18	128.60
1	AA	1228	C	O4'-C1'-N1	7.36	114.09	108.20
27	B8	1228	G	C5-C6-O6	-7.36	124.18	128.60
27	B8	1446	C	O4'-C1'-N1	7.36	114.09	108.20
27	B8	1748	C	O4'-C1'-N1	7.36	114.09	108.20
1	AA	665	A	O4'-C1'-N9	7.36	114.09	108.20
1	AA	612	C	O4'-C1'-N1	7.36	114.09	108.20
27	B8	1050	A	O4'-C1'-N9	7.36	114.09	108.20
27	B8	1645	G	C5-C6-O6	-7.36	124.19	128.60
27	B8	2815	C	O4'-C1'-N1	7.36	114.09	108.20
1	AA	388	G	C5-C6-O6	-7.36	124.19	128.60
1	AA	529	G	C5-C6-O6	-7.36	124.19	128.60
1	AA	813	U	O4'-C1'-N1	7.36	114.08	108.20
1	AA	1329	A	O4'-C1'-N9	7.36	114.08	108.20
27	B8	2687	U	O4'-C1'-N1	7.36	114.08	108.20
27	B8	2760	C	O4'-C1'-N1	7.36	114.08	108.20
27	B8	2862	G	C5-C6-O6	-7.36	124.19	128.60
27	B8	1139	G	C5-C6-O6	-7.35	124.19	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	444	G	C5-C6-O6	-7.35	124.19	128.60
1	AA	863	U	O4'-C1'-N1	7.35	114.08	108.20
1	AA	925	G	C5-C6-O6	-7.35	124.19	128.60
26	B7	16	G	C5-C6-O6	-7.35	124.19	128.60
27	B8	890	C	O4'-C1'-N1	7.35	114.08	108.20
27	B8	2373	G	C5-C6-O6	-7.35	124.19	128.60
1	AA	69	G	C5-C6-O6	-7.35	124.19	128.60
27	B8	840	C	O4'-C1'-N1	7.35	114.08	108.20
27	B8	862	G	C5-C6-O6	-7.35	124.19	128.60
27	B8	2401	U	O4'-C1'-N1	7.35	114.08	108.20
27	B8	2892	G	C5-C6-O6	-7.35	124.19	128.60
1	AA	254	G	O4'-C1'-N9	7.35	114.08	108.20
1	AA	698	G	C5-C6-O6	-7.35	124.19	128.60
1	AA	987	G	C5-C6-O6	-7.35	124.19	128.60
27	B8	967	U	O4'-C1'-N1	7.35	114.08	108.20
27	B8	1003	G	C5-C6-O6	-7.35	124.19	128.60
1	AA	355	C	O4'-C1'-N1	7.35	114.08	108.20
27	B8	1995	U	O4'-C1'-N1	7.34	114.08	108.20
27	B8	2178	C	O4'-C1'-N1	7.34	114.08	108.20
27	B8	2585	U	P-O3'-C3'	7.34	128.51	119.70
1	AA	776	G	C5-C6-O6	-7.34	124.19	128.60
27	B8	657	U	O4'-C1'-N1	7.34	114.07	108.20
27	B8	1172	C	O4'-C1'-N1	7.34	114.07	108.20
27	B8	171	U	O4'-C1'-N1	7.34	114.07	108.20
1	AA	423	G	O4'-C1'-N9	7.34	114.07	108.20
1	AA	631	C	O4'-C1'-N1	7.34	114.07	108.20
1	AA	1522	U	O4'-C1'-N1	7.34	114.07	108.20
3	AV	13	C	O4'-C1'-N1	7.34	114.07	108.20
2	AX	16	C	O4'-C1'-N1	7.34	114.07	108.20
27	B8	364	C	O4'-C1'-N1	7.34	114.07	108.20
27	B8	2008	C	O4'-C1'-N1	7.34	114.07	108.20
27	B8	2845	U	O4'-C1'-N1	7.33	114.07	108.20
26	B7	43	C	O4'-C1'-N1	7.33	114.07	108.20
27	B8	516	C	O4'-C1'-N1	7.33	114.07	108.20
3	AV	48	U	O4'-C1'-N1	7.33	114.06	108.20
27	B8	187	G	C5-C6-O6	-7.33	124.20	128.60
27	B8	694	U	O4'-C1'-N1	7.33	114.06	108.20
27	B8	1638	C	O4'-C1'-N1	7.33	114.06	108.20
1	AA	1073	U	O4'-C1'-N1	7.33	114.06	108.20
27	B8	2001	C	O4'-C1'-N1	7.33	114.06	108.20
1	AA	1315	U	O4'-C1'-N1	7.33	114.06	108.20
27	B8	1688	U	O4'-C1'-N1	7.33	114.06	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1479	C	O4'-C1'-N1	7.33	114.06	108.20
1	AA	213	G	C5-C6-O6	-7.32	124.21	128.60
1	AA	549	C	O4'-C1'-N1	7.32	114.06	108.20
27	B8	408	G	C5-C6-O6	-7.32	124.21	128.60
27	B8	2755	C	O4'-C1'-N1	7.32	114.06	108.20
1	AA	56	U	O4'-C1'-N1	7.32	114.06	108.20
1	AA	140	U	O4'-C1'-N1	7.32	114.06	108.20
1	AA	770	C	O4'-C1'-N1	7.32	114.06	108.20
27	B8	259	G	C5-C6-O6	-7.32	124.21	128.60
27	B8	1280	G	C5-C6-O6	-7.32	124.21	128.60
27	B8	1423	G	O4'-C1'-N9	7.32	114.06	108.20
27	B8	837	C	O4'-C1'-N1	7.32	114.06	108.20
26	B7	44	G	C5-C6-O6	-7.32	124.21	128.60
27	B8	154	U	O4'-C1'-N1	7.32	114.05	108.20
27	B8	2616	C	O4'-C1'-N1	7.32	114.06	108.20
27	B8	1336	A	O4'-C1'-N9	7.32	114.05	108.20
1	AA	358	U	O4'-C1'-N1	7.31	114.05	108.20
27	B8	235	U	O4'-C1'-N1	7.31	114.05	108.20
27	B8	2869	G	C5-C6-O6	-7.31	124.21	128.60
1	AA	330	C	O4'-C1'-N1	7.31	114.05	108.20
1	AA	828	U	O4'-C1'-N1	7.31	114.05	108.20
1	AA	1153	G	C5-C6-O6	-7.31	124.21	128.60
27	B8	518	G	C5-C6-O6	-7.31	124.21	128.60
27	B8	826	U	O4'-C1'-N1	7.31	114.05	108.20
1	AA	670	G	C5-C6-O6	-7.31	124.21	128.60
1	AA	218	U	O4'-C1'-N1	7.31	114.05	108.20
1	AA	1459	G	C5-C6-O6	-7.31	124.22	128.60
27	B8	196	A	O4'-C1'-N9	7.31	114.05	108.20
27	B8	1863	G	C5-C6-O6	-7.31	124.22	128.60
1	AA	1301	U	O4'-C1'-N1	7.31	114.05	108.20
27	B8	494	G	O4'-C1'-N9	7.31	114.05	108.20
27	B8	638	G	C5-C6-O6	-7.31	124.22	128.60
27	B8	771	G	O4'-C1'-N9	7.31	114.05	108.20
27	B8	2225	A	C4-C5-C6	7.31	120.65	117.00
27	B8	2256	G	C5-C6-O6	-7.31	124.22	128.60
27	B8	2352	A	C4-C5-C6	7.31	120.65	117.00
27	B8	2674	G	C5-C6-O6	-7.31	124.22	128.60
27	B8	2836	U	O4'-C1'-N1	7.31	114.05	108.20
26	B7	80	U	O4'-C1'-N1	7.31	114.05	108.20
27	B8	567	U	O4'-C1'-N1	7.31	114.05	108.20
27	B8	2646	C	O4'-C1'-N1	7.31	114.05	108.20
1	AA	516	U	O4'-C1'-N1	7.30	114.04	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	638	U	O4'-C1'-N1	7.30	114.04	108.20
27	B8	11	C	O4'-C1'-N1	7.30	114.04	108.20
27	B8	1623	G	C5-C6-O6	-7.30	124.22	128.60
27	B8	1943	U	O4'-C1'-N1	7.30	114.04	108.20
27	B8	2196	C	O4'-C1'-N1	7.30	114.04	108.20
27	B8	135	U	O4'-C1'-N1	7.30	114.04	108.20
1	AA	666	G	C5-C6-O6	-7.30	124.22	128.60
3	AV	63	C	O4'-C1'-N1	7.30	114.04	108.20
27	B8	2552	U	O4'-C1'-N1	7.30	114.04	108.20
1	AA	801	U	O4'-C1'-N1	7.30	114.04	108.20
1	AA	1465	A	C5-C6-N6	-7.30	117.86	123.70
27	B8	1063	G	C5-C6-O6	-7.30	124.22	128.60
1	AA	506	G	C5-C6-O6	-7.30	124.22	128.60
27	B8	320	A	P-O3'-C3'	7.30	128.46	119.70
27	B8	2103	C	O4'-C1'-N1	7.30	114.04	108.20
27	B8	2143	C	O4'-C1'-N1	7.30	114.04	108.20
1	AA	562	U	P-O3'-C3'	7.30	128.46	119.70
1	AA	347	G	O4'-C1'-N9	7.29	114.04	108.20
1	AA	371	A	O4'-C1'-N9	7.29	114.04	108.20
26	B7	95	U	O4'-C1'-N1	7.29	114.03	108.20
27	B8	658	U	O4'-C1'-N1	7.29	114.03	108.20
27	B8	939	G	C5-C6-O6	-7.29	124.23	128.60
27	B8	1453	A	O4'-C1'-N9	7.29	114.03	108.20
1	AA	971	G	C5-C6-O6	-7.29	124.23	128.60
27	B8	1016	G	O4'-C1'-N9	7.29	114.03	108.20
27	B8	1035	U	O4'-C1'-N1	7.29	114.03	108.20
27	B8	1847	A	O4'-C1'-N9	7.29	114.03	108.20
27	B8	2585	U	O4'-C1'-N1	7.29	114.03	108.20
1	AA	833	G	C5-C6-O6	-7.29	124.23	128.60
1	AA	887	G	C5-C6-O6	-7.29	124.23	128.60
26	B7	2	G	C5-C6-O6	-7.29	124.23	128.60
1	AA	103	U	O4'-C1'-N1	7.29	114.03	108.20
1	AA	526	C	O4'-C1'-N1	7.29	114.03	108.20
27	B8	962	G	C5-C6-O6	-7.29	124.23	128.60
27	B8	1292	G	C5-C6-O6	-7.29	124.23	128.60
27	B8	1484	U	O4'-C1'-N1	7.29	114.03	108.20
1	AA	11	G	C5-C6-O6	-7.29	124.23	128.60
1	AA	93	U	O4'-C1'-N1	7.29	114.03	108.20
27	B8	177	G	O4'-C1'-N9	7.29	114.03	108.20
27	B8	289	G	C5-C6-O6	-7.29	124.23	128.60
27	B8	1220	G	C5-C6-O6	-7.28	124.23	128.60
27	B8	1859	U	O4'-C1'-N1	7.28	114.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	133	U	O4'-C1'-N1	7.28	114.02	108.20
27	B8	156	A	O4'-C1'-N9	7.28	114.02	108.20
27	B8	375	G	C5-C6-O6	-7.28	124.23	128.60
27	B8	2242	G	C5-C6-O6	-7.28	124.23	128.60
27	B8	220	G	C5-C6-O6	-7.28	124.23	128.60
27	B8	370	G	C5-C6-O6	-7.28	124.23	128.60
27	B8	660	C	O4'-C1'-N1	7.28	114.02	108.20
27	B8	2511	U	O4'-C1'-N1	7.28	114.02	108.20
27	B8	2617	U	O4'-C1'-N1	7.28	114.02	108.20
1	AA	318	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	297	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	768	G	O4'-C1'-N9	7.27	114.02	108.20
27	B8	2573	C	C2-N1-C1'	7.27	126.80	118.80
1	AA	21	G	O4'-C1'-N9	7.27	114.02	108.20
27	B8	8	C	N3-C4-N4	7.27	123.09	118.00
27	B8	193	U	O4'-C1'-N1	7.27	114.02	108.20
27	B8	2860	A	C5-C6-N1	-7.27	114.06	117.70
27	B8	249	C	O4'-C1'-N1	7.27	114.02	108.20
27	B8	1041	G	C5-C6-O6	-7.27	124.24	128.60
1	AA	230	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	543	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	610	C	O4'-C1'-N1	7.27	114.02	108.20
27	B8	874	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	1234	U	O4'-C1'-N1	7.27	114.02	108.20
27	B8	1487	U	O4'-C1'-N1	7.27	114.02	108.20
1	AA	94	G	C5-C6-O6	-7.27	124.24	128.60
1	AA	830	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	1719	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	2062	A	O4'-C1'-N9	7.27	114.01	108.20
27	B8	2455	G	C5-C6-O6	-7.27	124.24	128.60
27	B8	4	U	O4'-C1'-N1	7.27	114.01	108.20
27	B8	1696	G	C5-C6-O6	-7.26	124.24	128.60
27	B8	1878	G	C5-C6-O6	-7.26	124.24	128.60
27	B8	2767	C	O4'-C1'-N1	7.26	114.01	108.20
1	AA	564	C	O4'-C1'-N1	7.26	114.01	108.20
1	AA	1124	G	C5-C6-O6	-7.26	124.24	128.60
1	AA	1175	G	C5-C6-O6	-7.26	124.24	128.60
1	AA	1221	G	C5-C6-O6	-7.26	124.24	128.60
27	B8	965	C	O4'-C1'-N1	7.26	114.01	108.20
27	B8	1617	C	O4'-C1'-N1	7.26	114.01	108.20
27	B8	2110	G	C5-C6-O6	-7.26	124.24	128.60
1	AA	1527	U	O4'-C1'-N1	7.26	114.01	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	712	G	C5-C6-O6	-7.26	124.24	128.60
27	B8	1117	C	O4'-C1'-N1	7.26	114.01	108.20
27	B8	2561	U	O4'-C1'-N1	7.26	114.01	108.20
1	AA	1106	G	C5-C6-O6	-7.26	124.25	128.60
27	B8	377	G	C5-C6-O6	-7.26	124.25	128.60
27	B8	1895	C	O4'-C1'-N1	7.26	114.00	108.20
27	B8	923	G	C5-C6-O6	-7.25	124.25	128.60
27	B8	2458	G	C5-C6-O6	-7.25	124.25	128.60
1	AA	625	U	O4'-C1'-N1	7.25	114.00	108.20
27	B8	1744	A	C4-C5-C6	7.25	120.63	117.00
27	B8	2137	U	O4'-C1'-N1	7.25	114.00	108.20
1	AA	126	G	C5-C6-O6	-7.25	124.25	128.60
1	AA	719	C	O4'-C1'-N1	7.25	114.00	108.20
1	AA	912	C	O4'-C1'-N1	7.25	114.00	108.20
27	B8	419	U	O4'-C1'-N1	7.25	114.00	108.20
27	B8	2106	U	O4'-C1'-N1	7.25	114.00	108.20
27	B8	2492	U	O4'-C1'-N1	7.25	114.00	108.20
27	B8	2707	U	O4'-C1'-N1	7.25	114.00	108.20
1	AA	751	U	O4'-C1'-N1	7.25	114.00	108.20
1	AA	1241	G	C5-C6-O6	-7.25	124.25	128.60
1	AA	684	U	O4'-C1'-N1	7.25	114.00	108.20
1	AA	866	C	O4'-C1'-N1	7.25	114.00	108.20
27	B8	1922	G	C5-C6-O6	-7.25	124.25	128.60
26	B7	103	U	O4'-C1'-N1	7.25	114.00	108.20
27	B8	1702	G	C5-C6-O6	-7.25	124.25	128.60
27	B8	2102	G	C5-C6-O6	-7.25	124.25	128.60
1	AA	947	G	C5-C6-O6	-7.25	124.25	128.60
27	B8	1137	G	C5-C6-O6	-7.25	124.25	128.60
1	AA	224	U	O4'-C1'-N1	7.24	113.99	108.20
3	AV	53	G	O4'-C1'-N9	7.24	114.00	108.20
27	B8	646	U	O4'-C1'-N1	7.24	113.99	108.20
27	B8	1078	U	O4'-C1'-N1	7.24	113.99	108.20
27	B8	216	A	C4-C5-C6	7.24	120.62	117.00
1	AA	980	C	O4'-C1'-N1	7.24	113.99	108.20
1	AA	1419	G	C5-C6-O6	-7.24	124.25	128.60
26	B7	105	G	C5-C6-O6	-7.24	124.26	128.60
27	B8	283	G	C5-C6-O6	-7.24	124.25	128.60
27	B8	591	U	O4'-C1'-N1	7.24	113.99	108.20
27	B8	710	U	O4'-C1'-N1	7.24	113.99	108.20
27	B8	1074	G	C5-C6-O6	-7.24	124.26	128.60
27	B8	1963	U	O4'-C1'-N1	7.24	113.99	108.20
27	B8	2112	G	N1-C6-O6	7.24	124.24	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	780	A	C5-C6-N6	-7.24	117.91	123.70
1	AA	1036	A	C5-C6-N6	-7.24	117.91	123.70
27	B8	2415	G	C5-C6-O6	-7.24	124.26	128.60
1	AA	157	U	O4'-C1'-N1	7.24	113.99	108.20
27	B8	1797	G	C5-C6-O6	-7.24	124.26	128.60
1	AA	874	G	C5-C6-O6	-7.24	124.26	128.60
27	B8	993	G	O4'-C1'-N9	7.24	113.99	108.20
27	B8	1229	C	O4'-C1'-N1	7.24	113.99	108.20
27	B8	1834	U	O4'-C1'-N1	7.24	113.99	108.20
1	AA	941	G	C5-C6-O6	-7.23	124.26	128.60
1	AA	1467	C	O4'-C1'-N1	7.23	113.99	108.20
1	AA	1496	C	O4'-C1'-N1	7.23	113.99	108.20
26	B7	31	C	O4'-C1'-N1	7.23	113.99	108.20
1	AA	31	G	C5-C6-O6	-7.23	124.26	128.60
1	AA	288	A	C5-C6-N6	-7.23	117.91	123.70
1	AA	757	U	O4'-C1'-N1	7.23	113.98	108.20
27	B8	1506	U	O4'-C1'-N1	7.23	113.99	108.20
27	B8	1840	G	C5-C6-O6	-7.23	124.26	128.60
27	B8	2179	C	O4'-C1'-N1	7.23	113.99	108.20
1	AA	841	C	O4'-C1'-N1	7.23	113.98	108.20
1	AA	873	A	C4-C5-C6	7.23	120.61	117.00
27	B8	2399	G	C5-C6-O6	-7.23	124.26	128.60
1	AA	1402	C	O4'-C1'-N1	7.23	113.98	108.20
27	B8	2549	G	C5-C6-O6	-7.23	124.26	128.60
1	AA	615	G	C5-C6-O6	-7.23	124.26	128.60
1	AA	1116	U	O4'-C1'-N1	7.23	113.98	108.20
27	B8	1279	G	C5-C6-O6	-7.23	124.26	128.60
27	B8	766	U	O4'-C1'-N1	7.23	113.98	108.20
1	AA	399	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	549	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	808	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	1377	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	1662	U	O4'-C1'-N1	7.22	113.98	108.20
1	AA	1083	U	O4'-C1'-N1	7.22	113.98	108.20
26	B7	61	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	447	A	N1-C6-N6	7.22	122.93	118.60
27	B8	2236	U	O4'-C1'-N1	7.22	113.98	108.20
1	AA	1313	U	O4'-C1'-N1	7.22	113.97	108.20
27	B8	1346	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	2412	A	C4-C5-C6	7.22	120.61	117.00
27	B8	2470	G	C5-C6-O6	-7.22	124.27	128.60
3	AV	29	C	O4'-C1'-N1	7.22	113.97	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2578	G	C5-C6-O6	-7.22	124.27	128.60
1	AA	46	G	C5-C6-O6	-7.22	124.27	128.60
1	AA	1104	G	C5-C6-O6	-7.22	124.27	128.60
1	AA	1244	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	29	U	O4'-C1'-N1	7.22	113.97	108.20
27	B8	439	A	O4'-C1'-N9	7.22	113.97	108.20
27	B8	500	G	C5-C6-O6	-7.22	124.27	128.60
27	B8	542	C	O4'-C1'-N1	7.22	113.97	108.20
27	B8	868	U	O4'-C1'-N1	7.22	113.97	108.20
1	AA	1168	U	O4'-C1'-N1	7.21	113.97	108.20
27	B8	52	A	C4-C5-C6	7.21	120.61	117.00
27	B8	2305	U	O4'-C1'-N1	7.21	113.97	108.20
27	B8	2536	G	C5-C6-O6	-7.21	124.27	128.60
27	B8	2759	G	C5-C6-O6	-7.21	124.27	128.60
27	B8	962	G	O4'-C1'-N9	7.21	113.97	108.20
27	B8	1469	A	C4-C5-C6	7.21	120.61	117.00
1	AA	1047	G	C5-C6-O6	-7.21	124.27	128.60
1	AA	1182	G	C5-C6-O6	-7.21	124.28	128.60
27	B8	1310	G	C5-C6-O6	-7.21	124.28	128.60
1	AA	1202	U	O4'-C1'-N1	7.21	113.97	108.20
1	AA	1360	A	C4-C5-C6	7.21	120.60	117.00
1	AA	1518	A	O4'-C1'-N9	7.21	113.97	108.20
27	B8	629	G	C5-C6-O6	-7.21	124.28	128.60
27	B8	1410	G	C5-C6-O6	-7.21	124.28	128.60
27	B8	438	G	C5-C6-O6	-7.21	124.28	128.60
27	B8	2087	G	O4'-C1'-N9	7.21	113.96	108.20
1	AA	255	G	C5-C6-O6	-7.20	124.28	128.60
1	AA	289	G	O4'-C1'-N9	7.20	113.96	108.20
1	AA	537	G	C5-C6-O6	-7.20	124.28	128.60
1	AA	1192	C	O4'-C1'-N1	7.20	113.96	108.20
27	B8	124	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	346	A	O4'-C1'-N9	7.20	113.96	108.20
27	B8	1324	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	1393	A	O4'-C1'-N9	7.20	113.96	108.20
27	B8	2061	G	C5-C6-O6	-7.20	124.28	128.60
1	AA	881	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	1959	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	2109	U	O4'-C1'-N1	7.20	113.96	108.20
1	AA	736	C	O4'-C1'-N1	7.20	113.96	108.20
1	AA	923	A	C5-C6-N6	-7.20	117.94	123.70
27	B8	189	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	647	G	C5-C6-O6	-7.20	124.28	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	734	A	C5-C6-N6	-7.20	117.94	123.70
27	B8	841	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	1165	A	O4'-C1'-N9	7.20	113.96	108.20
27	B8	30	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	1160	G	C5-C6-O6	-7.20	124.28	128.60
1	AA	1135	U	O4'-C1'-N1	7.20	113.96	108.20
27	B8	1899	A	C5-C6-N6	-7.20	117.94	123.70
27	B8	2223	G	C5-C6-O6	-7.20	124.28	128.60
27	B8	2385	C	O4'-C1'-N1	7.20	113.96	108.20
27	B8	1588	G	C5-C6-O6	-7.19	124.28	128.60
27	B8	1620	G	C5-C6-O6	-7.19	124.28	128.60
27	B8	1720	U	O4'-C1'-N1	7.19	113.95	108.20
27	B8	2044	C	O4'-C1'-N1	7.19	113.95	108.20
27	B8	956	G	C5-C6-O6	-7.19	124.28	128.60
27	B8	2318	G	C5-C6-O6	-7.19	124.28	128.60
27	B8	2869	G	O4'-C1'-N9	7.19	113.95	108.20
1	AA	333	U	O4'-C1'-N1	7.19	113.95	108.20
1	AA	1532	U	O4'-C1'-N1	7.19	113.95	108.20
27	B8	201	C	N3-C4-N4	7.19	123.03	118.00
27	B8	206	U	O4'-C1'-N1	7.19	113.95	108.20
1	AA	1322	C	O4'-C1'-N1	7.19	113.95	108.20
27	B8	926	G	C5-C6-O6	-7.19	124.29	128.60
1	AA	929	G	O4'-C1'-N9	7.19	113.95	108.20
1	AA	1249	C	O4'-C1'-N1	7.19	113.95	108.20
27	B8	1379	U	O4'-C1'-N1	7.19	113.95	108.20
27	B8	1459	G	O4'-C1'-N9	7.19	113.95	108.20
27	B8	2218	G	C5-C6-O6	-7.19	124.29	128.60
27	B8	2490	G	C5-C6-O6	-7.19	124.29	128.60
1	AA	952	U	O4'-C1'-N1	7.19	113.95	108.20
27	B8	989	G	C5-C6-O6	-7.19	124.29	128.60
27	B8	2737	G	C5-C6-O6	-7.19	124.29	128.60
27	B8	1513	U	O4'-C1'-N1	7.18	113.95	108.20
27	B8	1095	A	O4'-C1'-N9	7.18	113.95	108.20
27	B8	1742	U	O4'-C1'-N1	7.18	113.95	108.20
27	B8	1750	G	O4'-C1'-N9	7.18	113.95	108.20
27	B8	1849	G	C5-C6-O6	-7.18	124.29	128.60
27	B8	2354	C	O4'-C1'-N1	7.18	113.95	108.20
27	B8	2457	U	O4'-C1'-N1	7.18	113.95	108.20
1	AA	95	C	N3-C4-N4	7.18	123.03	118.00
27	B8	1836	C	O4'-C1'-N1	7.18	113.94	108.20
1	AA	137	U	O4'-C1'-N1	7.18	113.94	108.20
1	AA	181	A	C5-C6-N6	-7.18	117.96	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B7	5	U	O4'-C1'-N1	7.18	113.94	108.20
26	B7	18	G	C5-C6-O6	-7.18	124.29	128.60
27	B8	437	U	O4'-C1'-N1	7.18	113.94	108.20
27	B8	643	A	O4'-C1'-N9	7.18	113.94	108.20
27	B8	740	C	O4'-C1'-N1	7.18	113.94	108.20
1	AA	108	G	O4'-C1'-N9	7.18	113.94	108.20
27	B8	2696	U	O4'-C1'-N1	7.18	113.94	108.20
27	B8	1309	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	1373	A	C4-C5-C6	7.17	120.59	117.00
1	AA	957	U	O4'-C1'-N1	7.17	113.94	108.20
1	AA	423	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	107	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	578	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	2398	U	O4'-C1'-N1	7.17	113.94	108.20
27	B8	2693	G	C5-C6-O6	-7.17	124.30	128.60
26	B7	12	C	O4'-C1'-N1	7.17	113.94	108.20
1	AA	299	G	C5-C6-O6	-7.17	124.30	128.60
1	AA	1084	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	2605	U	O4'-C1'-N1	7.17	113.94	108.20
1	AA	906	A	C5-C6-N6	-7.17	117.97	123.70
26	B7	120	U	O4'-C1'-N1	7.17	113.93	108.20
27	B8	27	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	771	G	C5-C6-O6	-7.17	124.30	128.60
27	B8	2586	U	O4'-C1'-N1	7.17	113.93	108.20
27	B8	2881	U	O4'-C1'-N1	7.17	113.93	108.20
27	B8	96	C	O4'-C1'-N1	7.17	113.93	108.20
27	B8	1209	U	O4'-C1'-N1	7.17	113.93	108.20
1	AA	569	C	O4'-C1'-N1	7.16	113.93	108.20
1	AA	979	C	O4'-C1'-N1	7.16	113.93	108.20
1	AA	132	C	O4'-C1'-N1	7.16	113.93	108.20
1	AA	462	G	C5-C6-O6	-7.16	124.30	128.60
1	AA	900	A	O4'-C1'-N9	7.16	113.93	108.20
27	B8	24	G	C5-C6-O6	-7.16	124.30	128.60
27	B8	636	G	C5-C6-O6	-7.16	124.30	128.60
27	B8	2245	U	O4'-C1'-N1	7.16	113.93	108.20
1	AA	514	C	O4'-C1'-N1	7.16	113.93	108.20
1	AA	1404	C	O4'-C1'-N1	7.16	113.93	108.20
27	B8	2000	C	O4'-C1'-N1	7.16	113.93	108.20
27	B8	2259	U	O4'-C1'-N1	7.16	113.93	108.20
27	B8	2846	G	C5-C6-O6	-7.16	124.31	128.60
1	AA	295	C	O4'-C1'-N1	7.16	113.93	108.20
27	B8	136	G	C5-C6-O6	-7.16	124.31	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	357	C	O4'-C1'-N1	7.16	113.93	108.20
1	AA	442	G	C5-C6-O6	-7.16	124.31	128.60
3	AV	51	G	C5-C6-O6	-7.16	124.31	128.60
27	B8	511	U	O4'-C1'-N1	7.16	113.92	108.20
27	B8	1053	C	N3-C4-N4	7.16	123.01	118.00
27	B8	2204	G	C5-C6-O6	-7.15	124.31	128.60
1	AA	210	C	O4'-C1'-N1	7.15	113.92	108.20
1	AA	1463	U	O4'-C1'-N1	7.15	113.92	108.20
1	AA	445	G	C5-C6-O6	-7.15	124.31	128.60
27	B8	1148	U	O4'-C1'-N1	7.15	113.92	108.20
27	B8	2668	G	C5-C6-O6	-7.15	124.31	128.60
1	AA	24	U	O4'-C1'-N1	7.15	113.92	108.20
27	B8	1249	U	O4'-C1'-N1	7.15	113.92	108.20
27	B8	2685	G	C5-C6-O6	-7.15	124.31	128.60
1	AA	79	G	C5-C6-O6	-7.15	124.31	128.60
1	AA	799	G	C5-C6-O6	-7.15	124.31	128.60
1	AA	1138	G	C5-C6-O6	-7.15	124.31	128.60
1	AA	42	G	C5-C6-O6	-7.14	124.31	128.60
1	AA	644	U	O4'-C1'-N1	7.14	113.92	108.20
1	AA	711	G	C5-C6-O6	-7.14	124.31	128.60
1	AA	904	U	O4'-C1'-N1	7.14	113.92	108.20
27	B8	1509	A	O4'-C1'-N9	7.14	113.92	108.20
27	B8	1680	U	O4'-C1'-N1	7.14	113.92	108.20
27	B8	2243	U	O4'-C1'-N1	7.14	113.92	108.20
27	B8	2680	U	O4'-C1'-N1	7.14	113.92	108.20
1	AA	39	G	O4'-C1'-N9	7.14	113.92	108.20
26	B7	75	G	C5-C6-O6	-7.14	124.31	128.60
27	B8	1380	G	C5-C6-O6	-7.14	124.31	128.60
27	B8	2496	C	O4'-C1'-N1	7.14	113.91	108.20
1	AA	375	U	O4'-C1'-N1	7.14	113.91	108.20
27	B8	2593	U	O4'-C1'-N1	7.14	113.91	108.20
27	B8	269	C	O4'-C1'-N1	7.14	113.91	108.20
27	B8	1632	A	O4'-C1'-N9	7.14	113.91	108.20
27	B8	2216	G	C5-C6-O6	-7.14	124.32	128.60
27	B8	2277	G	O4'-C1'-N9	7.14	113.91	108.20
1	AA	741	G	O4'-C1'-N9	7.14	113.91	108.20
1	AA	1308	U	O4'-C1'-N1	7.14	113.91	108.20
27	B8	1222	U	O4'-C1'-N1	7.14	113.91	108.20
27	B8	1714	U	O4'-C1'-N1	7.14	113.91	108.20
27	B8	2826	A	C5-C6-N6	-7.14	117.99	123.70
1	AA	1397	C	O4'-C1'-N1	7.13	113.91	108.20
26	B7	109	A	C5-C6-N6	-7.13	117.99	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	23	G	C5-C6-O6	-7.13	124.32	128.60
27	B8	705	A	C4-C5-C6	7.13	120.57	117.00
27	B8	1993	U	O4'-C1'-N1	7.13	113.91	108.20
1	AA	524	G	C5-C6-O6	-7.13	124.32	128.60
1	AA	425	G	O4'-C1'-N9	7.13	113.91	108.20
1	AA	921	U	O4'-C1'-N1	7.13	113.91	108.20
27	B8	150	U	O4'-C1'-N1	7.13	113.91	108.20
27	B8	1266	G	C5-C6-O6	-7.13	124.32	128.60
27	B8	1891	G	C5-C6-O6	-7.13	124.32	128.60
27	B8	2387	U	O4'-C1'-N1	7.13	113.90	108.20
27	B8	2884	U	O4'-C1'-N1	7.13	113.90	108.20
1	AA	993	G	O4'-C1'-N9	7.13	113.90	108.20
27	B8	618	G	C5-C6-O6	-7.13	124.32	128.60
27	B8	1128	G	C5-C6-O6	-7.13	124.32	128.60
27	B8	1231	U	O4'-C1'-N1	7.13	113.90	108.20
27	B8	2293	G	O4'-C1'-N9	7.13	113.90	108.20
1	AA	1005	A	C4-C5-C6	7.12	120.56	117.00
27	B8	205	G	C5-C6-O6	-7.12	124.33	128.60
27	B8	1199	U	O4'-C1'-N1	7.12	113.90	108.20
27	B8	1451	C	O4'-C1'-N1	7.12	113.90	108.20
1	AA	64	G	C5-C6-O6	-7.12	124.33	128.60
1	AA	468	A	C4-C5-C6	7.12	120.56	117.00
1	AA	682	G	C5-C6-O6	-7.12	124.33	128.60
1	AA	961	U	O4'-C1'-N1	7.12	113.90	108.20
27	B8	1036	G	O4'-C1'-N9	7.12	113.90	108.20
27	B8	1862	G	C5-C6-O6	-7.12	124.33	128.60
1	AA	533	A	C4-C5-C6	7.12	120.56	117.00
27	B8	49	A	C4-C5-C6	7.12	120.56	117.00
27	B8	89	A	O4'-C1'-N9	7.12	113.89	108.20
27	B8	1137	G	O4'-C1'-N9	7.12	113.89	108.20
1	AA	674	G	O4'-C1'-N9	7.11	113.89	108.20
1	AA	762	U	O4'-C1'-N1	7.11	113.89	108.20
1	AA	809	G	C5-C6-O6	-7.11	124.33	128.60
27	B8	614	A	O4'-C1'-N9	7.11	113.89	108.20
27	B8	1257	C	O4'-C1'-N1	7.11	113.89	108.20
1	AA	121	U	O4'-C1'-N1	7.11	113.89	108.20
1	AA	1464	U	O4'-C1'-N1	7.11	113.89	108.20
1	AA	505	G	C5-C6-O6	-7.11	124.33	128.60
26	B7	79	G	C5-C6-O6	-7.11	124.34	128.60
27	B8	34	U	O4'-C1'-N1	7.11	113.89	108.20
1	AA	1160	G	N1-C6-O6	7.11	124.16	119.90
27	B8	315	G	O4'-C1'-N9	7.11	113.89	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	639	U	O4'-C1'-N1	7.11	113.89	108.20
27	B8	1004	U	O4'-C1'-N1	7.11	113.89	108.20
27	B8	2074	U	O4'-C1'-N1	7.11	113.89	108.20
1	AA	292	G	C5-C6-O6	-7.10	124.34	128.60
1	AA	353	A	O4'-C1'-N9	7.10	113.88	108.20
1	AA	1361	G	O4'-C1'-N9	7.10	113.88	108.20
3	AV	55	U	O4'-C1'-N1	7.10	113.88	108.20
27	B8	2085	U	O4'-C1'-N1	7.10	113.88	108.20
1	AA	891	U	O4'-C1'-N1	7.10	113.88	108.20
27	B8	1079	C	O4'-C1'-N1	7.10	113.88	108.20
27	B8	1582	C	O4'-C1'-N1	7.10	113.88	108.20
27	B8	2580	U	O4'-C1'-N1	7.10	113.88	108.20
1	AA	661	G	C5-C6-O6	-7.10	124.34	128.60
27	B8	1711	A	O4'-C1'-N9	7.10	113.88	108.20
27	B8	1882	U	O4'-C1'-N1	7.10	113.88	108.20
27	B8	2231	U	O4'-C1'-N1	7.10	113.88	108.20
27	B8	2800	A	C4-C5-C6	7.10	120.55	117.00
1	AA	88	U	O4'-C1'-N1	7.10	113.88	108.20
27	B8	860	U	O4'-C1'-N1	7.10	113.88	108.20
27	B8	686	U	O4'-C1'-N1	7.09	113.88	108.20
1	AA	809	G	O4'-C1'-N9	7.09	113.87	108.20
1	AA	1504	G	C5-C6-O6	-7.09	124.34	128.60
26	B7	102	G	C5-C6-O6	-7.09	124.34	128.60
27	B8	5	A	C5-C6-N6	-7.09	118.03	123.70
27	B8	495	G	C5-C6-O6	-7.09	124.34	128.60
27	B8	2612	C	O4'-C1'-N1	7.09	113.87	108.20
1	AA	982	U	O4'-C1'-N1	7.09	113.87	108.20
1	AA	1387	G	C5-C6-O6	-7.09	124.35	128.60
27	B8	323	C	C2-N1-C1'	7.09	126.60	118.80
27	B8	1255	U	O4'-C1'-N1	7.09	113.87	108.20
27	B8	2366	A	C4-C5-C6	7.09	120.54	117.00
27	B8	2768	U	O4'-C1'-N1	7.09	113.87	108.20
3	AV	15	G	C5-C6-O6	-7.09	124.35	128.60
1	AA	1194	U	O4'-C1'-N1	7.09	113.87	108.20
1	AA	1448	C	N3-C4-N4	7.09	122.96	118.00
3	AV	40	G	C5-C6-O6	-7.09	124.35	128.60
27	B8	59	U	O4'-C1'-N1	7.09	113.87	108.20
1	AA	672	U	O4'-C1'-N1	7.08	113.87	108.20
27	B8	1926	U	O4'-C1'-N1	7.08	113.87	108.20
27	B8	2186	G	C5-C6-O6	-7.08	124.35	128.60
1	AA	605	U	O4'-C1'-N1	7.08	113.87	108.20
27	B8	612	G	C5-C6-O6	-7.08	124.35	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	915	C	O4'-C1'-N1	7.08	113.87	108.20
1	AA	446	G	C5-C6-O6	-7.08	124.35	128.60
1	AA	1526	G	C5-C6-O6	-7.08	124.35	128.60
27	B8	459	U	O4'-C1'-N1	7.08	113.86	108.20
27	B8	952	G	C5-C6-O6	-7.08	124.35	128.60
27	B8	1475	G	C5-C6-O6	-7.08	124.35	128.60
27	B8	2771	C	O4'-C1'-N1	7.08	113.86	108.20
27	B8	310	A	C4-C5-C6	7.08	120.54	117.00
27	B8	1069	A	O4'-C1'-N9	7.08	113.86	108.20
27	B8	1358	G	C5-C6-O6	-7.08	124.35	128.60
27	B8	1398	C	O4'-C1'-N1	7.08	113.86	108.20
27	B8	1765	U	O4'-C1'-N1	7.08	113.86	108.20
27	B8	1845	G	C5-C6-O6	-7.08	124.35	128.60
27	B8	2107	G	C5-C6-O6	-7.08	124.35	128.60
1	AA	495	A	C4-C5-C6	7.08	120.54	117.00
27	B8	1225	G	C5-C6-O6	-7.08	124.36	128.60
27	B8	1709	U	O4'-C1'-N1	7.08	113.86	108.20
27	B8	864	G	O4'-C1'-N9	7.07	113.86	108.20
27	B8	2647	U	O4'-C1'-N1	7.07	113.86	108.20
1	AA	460	A	O4'-C1'-N9	7.07	113.86	108.20
27	B8	1210	G	C5-C6-O6	-7.07	124.36	128.60
27	B8	1767	G	C5-C6-O6	-7.07	124.36	128.60
27	B8	2286	G	C5-C6-O6	-7.07	124.36	128.60
27	B8	2405	G	C5-C6-O6	-7.07	124.36	128.60
1	AA	1393	U	O4'-C1'-N1	7.07	113.86	108.20
1	AA	1378	C	O4'-C1'-N1	7.07	113.85	108.20
27	B8	2541	A	C4-C5-C6	7.07	120.53	117.00
1	AA	198	G	C5-C6-O6	-7.07	124.36	128.60
1	AA	1306	A	O4'-C1'-N9	7.07	113.85	108.20
27	B8	8	C	O4'-C1'-N1	7.07	113.85	108.20
27	B8	1431	A	C5-C6-N6	-7.07	118.05	123.70
1	AA	1422	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	2452	C	O4'-C1'-N1	7.06	113.85	108.20
1	AA	1365	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	803	U	O4'-C1'-N1	7.06	113.85	108.20
27	B8	1350	C	O4'-C1'-N1	7.06	113.85	108.20
27	B8	1633	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	1842	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	2489	U	O4'-C1'-N1	7.06	113.85	108.20
1	AA	331	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	169	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	463	G	C5-C6-O6	-7.06	124.36	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	776	G	C5-C6-O6	-7.06	124.36	128.60
1	AA	745	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	576	U	O4'-C1'-N1	7.06	113.84	108.20
27	B8	695	G	C5-C6-O6	-7.06	124.36	128.60
27	B8	769	U	O4'-C1'-N1	7.06	113.84	108.20
1	AA	127	G	C5-C6-O6	-7.06	124.37	128.60
1	AA	193	C	N3-C4-N4	7.05	122.94	118.00
1	AA	274	A	P-O3'-C3'	7.05	128.16	119.70
1	AA	822	U	O4'-C1'-N1	7.05	113.84	108.20
3	AV	8	U	O4'-C1'-N1	7.05	113.84	108.20
3	AV	44	G	C5-C6-O6	-7.05	124.37	128.60
1	AA	1529	G	O4'-C1'-N9	7.05	113.84	108.20
1	AA	381	C	O4'-C1'-N1	7.05	113.84	108.20
27	B8	688	U	O4'-C1'-N1	7.05	113.84	108.20
1	AA	773	G	C5-C6-O6	-7.05	124.37	128.60
1	AA	945	G	C5-C6-O6	-7.05	124.37	128.60
27	B8	78	U	O4'-C1'-N1	7.05	113.84	108.20
27	B8	323	C	O4'-C1'-N1	7.05	113.84	108.20
27	B8	583	G	C5-C6-O6	-7.05	124.37	128.60
27	B8	1930	G	P-O3'-C3'	7.05	128.16	119.70
27	B8	2378	A	C5-C6-N1	-7.05	114.17	117.70
1	AA	571	U	O4'-C1'-N1	7.05	113.84	108.20
1	AA	1525	G	O4'-C1'-N9	7.05	113.84	108.20
27	B8	1507	C	O4'-C1'-N1	7.05	113.84	108.20
1	AA	1258	G	C5-C6-O6	-7.05	124.37	128.60
27	B8	1982	U	O4'-C1'-N1	7.05	113.84	108.20
27	B8	2852	G	O4'-C1'-N9	7.05	113.84	108.20
1	AA	1023	U	O4'-C1'-N1	7.04	113.84	108.20
1	AA	416	G	C5-C6-O6	-7.04	124.37	128.60
1	AA	993	G	C5-C6-O6	-7.04	124.37	128.60
27	B8	2	G	C5-C6-O6	-7.04	124.37	128.60
27	B8	265	A	C5-C6-N6	-7.04	118.06	123.70
26	B7	56	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	90	U	O4'-C1'-N1	7.04	113.83	108.20
27	B8	295	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	1125	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	1292	G	O4'-C1'-N9	7.04	113.83	108.20
27	B8	1401	G	C5-C6-O6	-7.04	124.38	128.60
1	AA	1474	U	O4'-C1'-N1	7.04	113.83	108.20
27	B8	469	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	1116	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	2335	A	C4-C5-C6	7.04	120.52	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2669	G	O4'-C1'-N9	7.04	113.83	108.20
27	B8	926	G	O4'-C1'-N9	7.04	113.83	108.20
27	B8	942	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	969	G	C5-C6-O6	-7.04	124.38	128.60
27	B8	975	A	C4-C5-C6	7.04	120.52	117.00
1	AA	72	A	O4'-C1'-N9	7.04	113.83	108.20
1	AA	1359	C	O4'-C1'-N1	7.04	113.83	108.20
27	B8	620	G	C5-C6-O6	-7.04	124.38	128.60
1	AA	1242	G	C5-C6-O6	-7.03	124.38	128.60
1	AA	905	U	O4'-C1'-N1	7.03	113.83	108.20
1	AA	339	C	O4'-C1'-N1	7.03	113.83	108.20
27	B8	427	U	O4'-C1'-N1	7.03	113.83	108.20
27	B8	1825	U	O4'-C1'-N1	7.03	113.82	108.20
27	B8	2326	C	O4'-C1'-N1	7.03	113.82	108.20
1	AA	203	G	C5-C6-O6	-7.03	124.38	128.60
1	AA	597	G	C5-C6-O6	-7.03	124.38	128.60
1	AA	1064	G	C5-C6-O6	-7.03	124.38	128.60
3	AV	69	U	O4'-C1'-N1	7.03	113.82	108.20
27	B8	1024	G	C5-C6-O6	-7.03	124.38	128.60
27	B8	535	G	C5-C6-O6	-7.03	124.39	128.60
27	B8	1831	G	C5-C6-O6	-7.03	124.39	128.60
1	AA	310	G	O4'-C1'-N9	7.02	113.82	108.20
1	AA	829	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	303	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	930	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	974	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	1456	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	1860	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	2244	U	O4'-C1'-N1	7.02	113.82	108.20
1	AA	802	A	O4'-C1'-N9	7.02	113.82	108.20
26	B7	37	C	O4'-C1'-N1	7.02	113.82	108.20
27	B8	514	A	O4'-C1'-N9	7.02	113.82	108.20
27	B8	2645	G	C5-C6-O6	-7.02	124.39	128.60
3	AV	35	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	573	U	O4'-C1'-N1	7.02	113.82	108.20
27	B8	891	G	C1'-O4'-C4'	-7.02	104.28	109.90
27	B8	2848	G	O4'-C1'-N9	7.02	113.82	108.20
1	AA	699	C	O4'-C1'-N1	7.02	113.82	108.20
27	B8	188	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	1018	U	O4'-C1'-N1	7.02	113.82	108.20
27	B8	1441	G	O4'-C1'-N9	7.02	113.82	108.20
27	B8	2695	U	O4'-C1'-N1	7.02	113.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	770	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	1567	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	2002	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	2543	G	O4'-C1'-N9	7.02	113.81	108.20
1	AA	1530	G	C5-C6-O6	-7.02	124.39	128.60
27	B8	2307	G	N1-C6-O6	7.02	124.11	119.90
27	B8	2584	U	O4'-C1'-N1	7.02	113.81	108.20
27	B8	2828	G	C5-C6-O6	-7.02	124.39	128.60
1	AA	542	G	C5-C6-O6	-7.01	124.39	128.60
27	B8	1349	C	O4'-C1'-N1	7.01	113.81	108.20
27	B8	1219	U	O4'-C1'-N1	7.01	113.81	108.20
27	B8	1699	G	C5-C6-O6	-7.01	124.39	128.60
27	B8	2267	A	C4-C5-C6	7.01	120.50	117.00
27	B8	2292	U	O4'-C1'-N1	7.01	113.81	108.20
27	B8	2488	G	C5-C6-O6	-7.01	124.39	128.60
1	AA	775	G	C5-C6-O6	-7.01	124.39	128.60
1	AA	1032	G	C5-C6-O6	-7.01	124.39	128.60
27	B8	361	G	C5-C6-O6	-7.01	124.39	128.60
27	B8	475	C	O4'-C1'-N1	7.01	113.81	108.20
27	B8	2697	G	C5-C6-O6	-7.01	124.39	128.60
1	AA	928	G	C5-C6-O6	-7.01	124.39	128.60
27	B8	2547	A	O4'-C1'-N9	7.01	113.81	108.20
1	AA	451	A	C5-C6-N6	-7.01	118.09	123.70
27	B8	364	C	N3-C4-N4	7.01	122.90	118.00
27	B8	1516	G	C5-C6-O6	-7.01	124.40	128.60
27	B8	1070	A	O4'-C1'-N9	7.00	113.80	108.20
27	B8	1410	G	O4'-C1'-N9	7.00	113.80	108.20
27	B8	2082	A	C4-C5-C6	7.00	120.50	117.00
26	B7	66	A	C5-C6-N6	-7.00	118.10	123.70
27	B8	521	U	O4'-C1'-N1	7.00	113.80	108.20
27	B8	1286	A	C4-C5-C6	7.00	120.50	117.00
27	B8	1374	G	C5-C6-O6	-7.00	124.40	128.60
1	AA	725	G	O4'-C1'-N9	7.00	113.80	108.20
1	AA	1304	G	C5-C6-O6	-7.00	124.40	128.60
1	AA	48	C	O4'-C1'-N1	7.00	113.80	108.20
27	B8	254	G	C5-C6-O6	-7.00	124.40	128.60
27	B8	2406	A	O4'-C1'-N9	7.00	113.80	108.20
1	AA	447	G	N3-C2-N2	7.00	124.80	119.90
1	AA	792	A	O4'-C1'-N9	7.00	113.80	108.20
1	AA	1252	A	C4-C5-C6	7.00	120.50	117.00
27	B8	457	A	O4'-C1'-N9	7.00	113.80	108.20
27	B8	630	G	C5-C6-O6	-7.00	124.40	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1149	G	C5-C6-O6	-7.00	124.40	128.60
27	B8	2545	G	C5-C6-O6	-7.00	124.40	128.60
1	AA	155	A	C5-C6-N6	-7.00	118.10	123.70
1	AA	1439	G	C5-C6-O6	-7.00	124.40	128.60
27	B8	1402	U	O4'-C1'-N1	7.00	113.80	108.20
27	B8	1823	G	O4'-C1'-N9	7.00	113.80	108.20
1	AA	237	G	C5-C6-O6	-6.99	124.40	128.60
27	B8	1432	G	C5-C6-O6	-6.99	124.40	128.60
27	B8	2700	A	O4'-C1'-N9	6.99	113.80	108.20
1	AA	1295	U	O4'-C1'-N1	6.99	113.79	108.20
26	B7	51	G	C5-C6-O6	-6.99	124.41	128.60
1	AA	327	A	C4-C5-C6	6.99	120.50	117.00
1	AA	713	G	C5-C6-O6	-6.99	124.41	128.60
1	AA	1190	G	C5-C6-O6	-6.99	124.41	128.60
27	B8	785	G	C5-C6-O6	-6.99	124.41	128.60
27	B8	1466	U	O4'-C1'-N1	6.99	113.79	108.20
27	B8	2188	U	O4'-C1'-N1	6.99	113.79	108.20
26	B7	96	G	C5-C6-O6	-6.99	124.41	128.60
27	B8	1407	G	O4'-C1'-N9	6.99	113.79	108.20
1	AA	273	U	O4'-C1'-N1	6.99	113.79	108.20
3	AV	2	G	C5-C6-O6	-6.99	124.41	128.60
27	B8	753	A	C4-C5-C6	6.99	120.49	117.00
27	B8	1767	G	O4'-C1'-N9	6.99	113.79	108.20
27	B8	2393	U	O4'-C1'-N1	6.99	113.79	108.20
1	AA	251	G	C5-C6-O6	-6.98	124.41	128.60
1	AA	100	G	C5-C6-O6	-6.98	124.41	128.60
1	AA	1035	A	C5-C6-N6	-6.98	118.11	123.70
1	AA	1477	U	O4'-C1'-N1	6.98	113.79	108.20
27	B8	306	U	O4'-C1'-N1	6.98	113.79	108.20
27	B8	770	G	O4'-C1'-N9	6.98	113.79	108.20
27	B8	997	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	1087	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	1120	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	1332	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	2877	G	C5-C6-O6	-6.98	124.41	128.60
1	AA	383	A	C4-C5-C6	6.98	120.49	117.00
27	B8	263	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	918	A	C4-C5-C6	6.98	120.49	117.00
27	B8	1619	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	2471	A	O4'-C1'-N9	6.98	113.78	108.20
27	B8	327	G	C5-C6-O6	-6.98	124.41	128.60
1	AA	55	A	C4-C5-C6	6.98	120.49	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1255	G	O4'-C1'-N9	6.98	113.78	108.20
27	B8	1163	G	C5-C6-O6	-6.98	124.41	128.60
27	B8	2049	G	C5-C6-O6	-6.98	124.41	128.60
1	AA	72	A	C4-C5-C6	6.98	120.49	117.00
27	B8	1666	G	O4'-C1'-N9	6.98	113.78	108.20
27	B8	1848	A	C4-C5-C6	6.98	120.49	117.00
27	B8	648	G	C5-C6-O6	-6.97	124.42	128.60
27	B8	2148	G	C5-C6-O6	-6.97	124.42	128.60
1	AA	530	G	C5-C6-O6	-6.97	124.42	128.60
1	AA	402	G	O4'-C1'-N9	6.97	113.77	108.20
1	AA	1200	C	N3-C4-N4	6.97	122.88	118.00
27	B8	396	G	O4'-C1'-N9	6.97	113.77	108.20
27	B8	525	U	O4'-C1'-N1	6.97	113.77	108.20
27	B8	537	G	C5-C6-O6	-6.97	124.42	128.60
27	B8	2174	C	O4'-C1'-N1	6.97	113.77	108.20
1	AA	710	G	O4'-C1'-N9	6.96	113.77	108.20
27	B8	215	G	C5-C6-O6	-6.96	124.42	128.60
27	B8	1363	C	O4'-C1'-N1	6.96	113.77	108.20
1	AA	265	G	N1-C6-O6	6.96	124.08	119.90
27	B8	431	U	O4'-C1'-N1	6.96	113.77	108.20
27	B8	397	U	O4'-C1'-N1	6.96	113.77	108.20
27	B8	1029	A	C4-C5-C6	6.96	120.48	117.00
1	AA	932	C	O4'-C1'-N1	6.96	113.77	108.20
27	B8	407	G	O4'-C1'-N9	6.96	113.77	108.20
1	AA	54	C	O4'-C1'-N1	6.96	113.77	108.20
1	AA	491	G	O4'-C1'-N9	6.96	113.77	108.20
27	B8	1147	A	O4'-C1'-N9	6.96	113.77	108.20
27	B8	1733	G	C5-C6-O6	-6.96	124.42	128.60
1	AA	771	G	C5-C6-O6	-6.96	124.43	128.60
1	AA	1134	G	C5-C6-O6	-6.96	124.43	128.60
27	B8	1205	A	O4'-C1'-N9	6.96	113.77	108.20
27	B8	1371	G	C5-C6-O6	-6.96	124.43	128.60
27	B8	1621	U	O4'-C1'-N1	6.96	113.77	108.20
27	B8	2152	G	O4'-C1'-N9	6.96	113.77	108.20
27	B8	2852	G	C5-C6-O6	-6.96	124.43	128.60
1	AA	1024	G	O4'-C1'-N9	6.96	113.76	108.20
27	B8	506	G	C5-C6-O6	-6.96	124.43	128.60
27	B8	733	G	C5-C6-O6	-6.96	124.43	128.60
26	B7	77	U	O4'-C1'-N1	6.95	113.76	108.20
27	B8	1056	G	C5-C6-O6	-6.95	124.43	128.60
27	B8	2297	A	C4-C5-C6	6.95	120.48	117.00
27	B8	2484	G	O4'-C1'-N9	6.95	113.76	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AX	18	C	O4'-C1'-N1	6.95	113.76	108.20
27	B8	2111	U	O4'-C1'-N1	6.95	113.76	108.20
1	AA	1400	C	O4'-C1'-N1	6.95	113.76	108.20
27	B8	2493	U	O4'-C1'-N1	6.95	113.76	108.20
1	AA	278	G	C5-C6-O6	-6.95	124.43	128.60
27	B8	551	G	C5-C6-O6	-6.95	124.43	128.60
27	B8	877	A	C5-C6-N1	-6.95	114.22	117.70
27	B8	1568	G	C5-C6-O6	-6.95	124.43	128.60
27	B8	2291	U	O4'-C1'-N1	6.95	113.76	108.20
27	B8	2379	G	C5-C6-O6	-6.95	124.43	128.60
27	B8	2633	G	O4'-C1'-N9	6.95	113.76	108.20
1	AA	729	A	O4'-C1'-N9	6.95	113.76	108.20
27	B8	580	U	O4'-C1'-N1	6.95	113.76	108.20
1	AA	1379	G	O4'-C1'-N9	6.94	113.75	108.20
3	AV	30	G	C5-C6-O6	-6.94	124.43	128.60
1	AA	966	G	C5-C6-O6	-6.94	124.44	128.60
1	AA	1267	C	O4'-C1'-N1	6.94	113.75	108.20
27	B8	2786	U	O4'-C1'-N1	6.94	113.75	108.20
1	AA	1235	U	O4'-C1'-N1	6.94	113.75	108.20
1	AA	46	G	O4'-C1'-N9	6.94	113.75	108.20
1	AA	656	G	C5-C6-O6	-6.94	124.44	128.60
1	AA	1395	C	O4'-C1'-N1	6.94	113.75	108.20
27	B8	794	A	C5-C6-N6	-6.94	118.15	123.70
1	AA	716	A	O4'-C1'-N9	6.94	113.75	108.20
27	B8	519	U	O4'-C1'-N1	6.94	113.75	108.20
27	B8	1866	A	C4-C5-C6	6.94	120.47	117.00
27	B8	2361	G	O4'-C1'-N9	6.94	113.75	108.20
27	B8	278	A	C4-C5-C6	6.93	120.47	117.00
27	B8	2193	G	C5-C6-O6	-6.93	124.44	128.60
27	B8	2571	U	O4'-C1'-N1	6.93	113.75	108.20
27	B8	2663	G	C5-C6-O6	-6.93	124.44	128.60
1	AA	175	C	N3-C4-N4	6.93	122.85	118.00
1	AA	1468	A	O4'-C1'-N9	6.93	113.75	108.20
27	B8	1473	G	C5-C6-O6	-6.93	124.44	128.60
27	B8	628	G	O4'-C1'-N9	6.93	113.75	108.20
27	B8	2864	G	C5-C6-O6	-6.93	124.44	128.60
27	B8	471	A	C4-C5-C6	6.93	120.46	117.00
27	B8	780	G	C5-C6-O6	-6.93	124.44	128.60
27	B8	928	A	C5-C6-N6	-6.93	118.16	123.70
27	B8	1750	G	C5-C6-O6	-6.93	124.44	128.60
27	B8	2077	A	C4-C5-C6	6.93	120.47	117.00
1	AA	703	G	C5-C6-O6	-6.93	124.44	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1177	G	C5-C6-O6	-6.93	124.44	128.60
1	AA	563	A	C4-C5-C6	6.93	120.46	117.00
27	B8	494	G	C5-C6-O6	-6.93	124.44	128.60
27	B8	2834	G	C5-C6-O6	-6.93	124.44	128.60
1	AA	71	A	C5-C6-N6	-6.92	118.16	123.70
1	AA	796	C	O4'-C1'-N1	6.92	113.74	108.20
1	AA	1139	G	C5-C6-O6	-6.92	124.45	128.60
1	AA	1438	G	C5-C6-O6	-6.92	124.44	128.60
27	B8	286	U	O4'-C1'-N1	6.92	113.74	108.20
27	B8	1753	G	C5-C6-O6	-6.92	124.44	128.60
27	B8	1903	G	C5-C6-O6	-6.92	124.44	128.60
1	AA	603	U	O4'-C1'-N1	6.92	113.74	108.20
1	AA	1088	G	C5-C6-O6	-6.92	124.45	128.60
1	AA	1241	G	O4'-C1'-N9	6.92	113.74	108.20
1	AA	310	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	2157	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	2371	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	474	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	1322	A	O4'-C1'-N9	6.92	113.74	108.20
27	B8	1814	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	2178	C	C2-N1-C1'	6.92	126.41	118.80
1	AA	721	G	C5-C6-O6	-6.92	124.45	128.60
26	B7	100	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	373	U	O4'-C1'-N1	6.92	113.73	108.20
27	B8	1816	C	C6-N1-C1'	-6.92	112.50	120.80
27	B8	2499	C	O4'-C1'-N1	6.92	113.73	108.20
27	B8	2770	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	667	U	O4'-C1'-N1	6.92	113.73	108.20
27	B8	1425	G	C5-C6-O6	-6.92	124.45	128.60
27	B8	2161	C	O4'-C1'-N1	6.92	113.73	108.20
1	AA	91	U	O4'-C1'-N1	6.91	113.73	108.20
27	B8	889	C	O4'-C1'-N1	6.91	113.73	108.20
27	B8	1178	C	O4'-C1'-N1	6.91	113.73	108.20
27	B8	2570	G	C5-C6-O6	-6.91	124.45	128.60
1	AA	194	C	O4'-C1'-N1	6.91	113.73	108.20
27	B8	1133	A	P-O3'-C3'	6.91	127.99	119.70
27	B8	1369	G	C5-C6-O6	-6.91	124.45	128.60
27	B8	51	G	C5-C6-O6	-6.91	124.45	128.60
27	B8	1516	G	O4'-C1'-N9	6.91	113.73	108.20
27	B8	1763	G	C5-C6-O6	-6.91	124.45	128.60
27	B8	1841	U	O4'-C1'-N1	6.91	113.73	108.20
27	B8	2135	A	O4'-C1'-N9	6.91	113.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1156	G	C5-C6-O6	-6.91	124.45	128.60
1	AA	1492	A	C5-C6-N6	-6.91	118.17	123.70
26	B7	7	G	O4'-C1'-N9	6.91	113.73	108.20
27	B8	191	A	C4-C5-C6	6.91	120.45	117.00
27	B8	586	A	N1-C6-N6	6.91	122.75	118.60
27	B8	2372	U	O4'-C1'-N1	6.91	113.73	108.20
27	B8	1361	G	C5-C6-O6	-6.91	124.46	128.60
27	B8	1851	U	O4'-C1'-N1	6.90	113.72	108.20
1	AA	384	G	C5-C6-O6	-6.90	124.46	128.60
1	AA	601	G	O4'-C1'-N9	6.90	113.72	108.20
1	AA	753	A	C4-C5-C6	6.90	120.45	117.00
1	AA	860	A	O4'-C1'-N9	6.90	113.72	108.20
1	AA	1473	G	C5-C6-O6	-6.90	124.46	128.60
27	B8	2429	G	C5-C6-O6	-6.90	124.46	128.60
27	B8	2662	A	C4-C5-C6	6.90	120.45	117.00
27	B8	904	G	C5-C6-O6	-6.90	124.46	128.60
27	B8	1355	G	O4'-C1'-N9	6.90	113.72	108.20
27	B8	2697	G	O4'-C1'-N9	6.90	113.72	108.20
1	AA	287	U	O4'-C1'-N1	6.90	113.72	108.20
1	AA	988	G	C5-C6-O6	-6.90	124.46	128.60
1	AA	1185	G	C5-C6-O6	-6.90	124.46	128.60
27	B8	214	G	O4'-C1'-N9	6.90	113.72	108.20
27	B8	1168	G	C5-C6-O6	-6.90	124.46	128.60
1	AA	568	G	C5-C6-O6	-6.90	124.46	128.60
27	B8	1400	U	O4'-C1'-N1	6.90	113.72	108.20
27	B8	515	A	O4'-C1'-N9	6.89	113.72	108.20
27	B8	545	U	O4'-C1'-N1	6.89	113.72	108.20
27	B8	1776	G	C5-C6-O6	-6.89	124.46	128.60
1	AA	714	G	C5-C6-O6	-6.89	124.47	128.60
26	B7	96	G	O4'-C1'-N9	6.89	113.71	108.20
27	B8	15	G	C5-C6-O6	-6.89	124.46	128.60
27	B8	1831	G	O4'-C1'-N9	6.89	113.72	108.20
27	B8	2374	C	O4'-C1'-N1	6.89	113.71	108.20
27	B8	389	G	C5-C6-O6	-6.89	124.47	128.60
27	B8	2031	A	O4'-C1'-N9	6.89	113.71	108.20
1	AA	683	G	O4'-C1'-N9	6.89	113.71	108.20
27	B8	158	U	O4'-C1'-N1	6.89	113.71	108.20
27	B8	718	A	C5-C6-N6	-6.89	118.19	123.70
27	B8	2162	G	C5-C6-O6	-6.89	124.47	128.60
27	B8	2302	U	O4'-C1'-N1	6.89	113.71	108.20
27	B8	1830	C	N3-C4-N4	6.89	122.82	118.00
27	B8	651	G	C5-C6-O6	-6.89	124.47	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1958	C	O4'-C1'-N1	6.89	113.71	108.20
1	AA	151	A	C4-C5-C6	6.88	120.44	117.00
27	B8	1721	G	C5-C6-O6	-6.88	124.47	128.60
1	AA	1322	C	C2-N1-C1'	6.88	126.37	118.80
27	B8	1143	A	O4'-C1'-N9	6.88	113.71	108.20
27	B8	2751	G	C5-C6-O6	-6.88	124.47	128.60
27	B8	2763	G	C5-C6-O6	-6.88	124.47	128.60
1	AA	618	C	O4'-C1'-N1	6.88	113.71	108.20
1	AA	1310	G	O4'-C1'-N9	6.88	113.70	108.20
27	B8	268	C	N3-C4-N4	6.88	122.82	118.00
27	B8	2016	U	O4'-C1'-N1	6.88	113.71	108.20
27	B8	2340	A	O4'-C1'-N9	6.88	113.71	108.20
27	B8	2900	A	O4'-C1'-N9	6.88	113.71	108.20
1	AA	1512	U	O4'-C1'-N1	6.88	113.70	108.20
27	B8	727	A	O4'-C1'-N9	6.88	113.70	108.20
27	B8	1789	A	C4-C5-C6	6.88	120.44	117.00
1	AA	1505	G	C5-C6-O6	-6.88	124.47	128.60
1	AA	1529	G	C5'-C4'-O4'	6.88	117.35	109.10
1	AA	430	A	N1-C6-N6	6.88	122.73	118.60
1	AA	1137	C	O4'-C1'-N1	6.88	113.70	108.20
1	AA	1368	A	O4'-C1'-N9	6.88	113.70	108.20
27	B8	169	G	O4'-C1'-N9	6.88	113.70	108.20
27	B8	1888	G	C5-C6-O6	-6.88	124.47	128.60
27	B8	2116	G	C5-C6-O6	-6.88	124.47	128.60
1	AA	903	G	O4'-C1'-N9	6.88	113.70	108.20
27	B8	353	C	O4'-C1'-N1	6.88	113.70	108.20
27	B8	2163	A	C4-C5-C6	6.88	120.44	117.00
1	AA	340	U	O4'-C1'-N1	6.87	113.70	108.20
1	AA	673	A	C4-C5-C6	6.87	120.44	117.00
1	AA	1108	G	C5-C6-O6	-6.87	124.47	128.60
27	B8	251	A	C4-C5-C6	6.87	120.44	117.00
27	B8	1777	U	O4'-C1'-N1	6.87	113.70	108.20
27	B8	2159	G	C5-C6-O6	-6.87	124.48	128.60
27	B8	2181	U	O4'-C1'-N1	6.87	113.70	108.20
27	B8	67	U	O4'-C1'-N1	6.87	113.70	108.20
27	B8	411	G	C5-C6-O6	-6.87	124.48	128.60
27	B8	604	G	C5-C6-O6	-6.87	124.48	128.60
27	B8	1730	C	O4'-C1'-N1	6.87	113.70	108.20
27	B8	2721	A	O4'-C1'-N9	6.87	113.70	108.20
27	B8	1600	C	O4'-C1'-N1	6.87	113.70	108.20
27	B8	1757	A	O4'-C1'-N9	6.87	113.70	108.20
1	AA	558	G	C5-C6-O6	-6.87	124.48	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1000	A	O4'-C1'-N9	6.87	113.69	108.20
27	B8	2811	G	C5-C6-O6	-6.87	124.48	128.60
1	AA	71	A	O4'-C1'-N9	6.87	113.69	108.20
1	AA	346	G	C5-C6-O6	-6.87	124.48	128.60
1	AA	464	U	O4'-C1'-N1	6.87	113.69	108.20
1	AA	803	G	C5-C6-O6	-6.87	124.48	128.60
1	AA	824	G	O4'-C1'-N9	6.87	113.69	108.20
27	B8	544	C	O4'-C1'-N1	6.87	113.69	108.20
27	B8	2615	U	O4'-C1'-N1	6.87	113.69	108.20
27	B8	2734	A	C5-C6-N6	-6.87	118.21	123.70
1	AA	220	G	C5-C6-O6	-6.86	124.48	128.60
1	AA	1294	G	C5-C6-O6	-6.86	124.48	128.60
27	B8	2587	A	C4-C5-C6	6.86	120.43	117.00
27	B8	2871	U	O4'-C1'-N1	6.86	113.69	108.20
1	AA	1044	A	C5-C6-N6	-6.86	118.21	123.70
3	AV	36	G	C5-C6-O6	-6.86	124.48	128.60
27	B8	75	G	C5-C6-O6	-6.86	124.48	128.60
27	B8	330	A	C5-C6-N6	-6.86	118.21	123.70
27	B8	625	G	C5-C6-O6	-6.86	124.48	128.60
1	AA	593	U	O4'-C1'-N1	6.86	113.69	108.20
27	B8	917	A	C4-C5-C6	6.86	120.43	117.00
27	B8	1198	U	O4'-C1'-N1	6.86	113.69	108.20
27	B8	2097	A	O4'-C1'-N9	6.86	113.69	108.20
1	AA	95	C	O4'-C1'-N1	6.86	113.69	108.20
27	B8	824	U	O4'-C1'-N1	6.86	113.69	108.20
27	B8	1551	A	O4'-C1'-N9	6.86	113.69	108.20
27	B8	2139	U	O4'-C1'-N1	6.86	113.69	108.20
27	B8	2728	U	O4'-C1'-N1	6.86	113.69	108.20
1	AA	174	A	C5-C6-N6	-6.86	118.22	123.70
27	B8	1782	U	O4'-C1'-N1	6.86	113.68	108.20
27	B8	2601	C	N3-C4-N4	6.86	122.80	118.00
1	AA	116	A	C4-C5-C6	6.85	120.43	117.00
1	AA	610	U	C2-N1-C1'	6.85	125.92	117.70
1	AA	935	A	C4-C5-C6	6.85	120.43	117.00
27	B8	912	C	O4'-C1'-N1	6.85	113.68	108.20
27	B8	2217	G	O4'-C1'-N9	6.85	113.68	108.20
27	B8	2532	G	C5-C6-O6	-6.85	124.49	128.60
27	B8	2575	C	O4'-C1'-N1	6.85	113.68	108.20
27	B8	2825	G	C5-C6-O6	-6.85	124.49	128.60
27	B8	48	G	C5-C6-O6	-6.85	124.49	128.60
27	B8	1598	A	C5-C6-N6	-6.85	118.22	123.70
1	AA	1115	U	O4'-C1'-N1	6.85	113.68	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	242	G	O4'-C1'-N9	6.85	113.68	108.20
27	B8	744	U	O4'-C1'-N1	6.85	113.68	108.20
27	B8	1556	C	O4'-C1'-N1	6.85	113.68	108.20
27	B8	1603	A	C5-C6-N6	-6.85	118.22	123.70
27	B8	2129	C	O4'-C1'-N1	6.85	113.68	108.20
1	AA	924	C	N3-C4-N4	6.85	122.79	118.00
1	AA	1294	G	O4'-C1'-N9	6.85	113.68	108.20
27	B8	340	A	C4-C5-C6	6.85	120.42	117.00
27	B8	1369	G	O4'-C1'-N9	6.85	113.68	108.20
27	B8	2438	U	O4'-C1'-N1	6.85	113.68	108.20
1	AA	591	U	O4'-C1'-N1	6.85	113.68	108.20
27	B8	1984	G	O4'-C1'-N9	6.85	113.68	108.20
1	AA	1453	G	C5-C6-O6	-6.84	124.49	128.60
27	B8	489	G	C5-C6-O6	-6.84	124.49	128.60
27	B8	971	G	C5-C6-O6	-6.84	124.49	128.60
27	B8	1539	U	O4'-C1'-N1	6.84	113.67	108.20
27	B8	277	G	C5-C6-O6	-6.84	124.49	128.60
27	B8	704	G	C5-C6-O6	-6.84	124.49	128.60
1	AA	437	U	O4'-C1'-N1	6.84	113.67	108.20
26	B7	24	G	C5-C6-O6	-6.84	124.50	128.60
26	B7	33	G	O4'-C1'-N9	6.84	113.67	108.20
27	B8	2025	C	O4'-C1'-N1	6.84	113.67	108.20
27	B8	2067	G	C5-C6-O6	-6.84	124.50	128.60
1	AA	107	G	C5-C6-O6	-6.84	124.50	128.60
1	AA	710	G	C5-C6-O6	-6.84	124.50	128.60
1	AA	1489	G	C5-C6-O6	-6.84	124.50	128.60
1	AA	1003	G	C5-C6-O6	-6.84	124.50	128.60
1	AA	1177	G	C5-C6-O6	-6.84	124.50	128.60
27	B8	356	G	C5-C6-O6	-6.84	124.50	128.60
27	B8	1120	G	O4'-C1'-N9	6.84	113.67	108.20
27	B8	2253	G	C5-C6-O6	-6.84	124.50	128.60
1	AA	1131	G	O4'-C1'-N9	6.84	113.67	108.20
27	B8	2280	G	C5-C6-O6	-6.84	124.50	128.60
27	B8	2604	U	O4'-C1'-N1	6.84	113.67	108.20
1	AA	606	G	C5-C6-O6	-6.83	124.50	128.60
27	B8	221	A	C4-C5-C6	6.83	120.42	117.00
27	B8	367	G	C5-C6-O6	-6.83	124.50	128.60
1	AA	528	C	O4'-C1'-N1	6.83	113.67	108.20
1	AA	1046	A	O4'-C1'-N9	6.83	113.67	108.20
27	B8	178	G	O4'-C1'-N9	6.83	113.67	108.20
27	B8	190	A	C4-C5-C6	6.83	120.42	117.00
27	B8	279	A	C4-C5-C6	6.83	120.42	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	939	G	O4'-C1'-N9	6.83	113.67	108.20
1	AA	2	A	O4'-C1'-N9	6.83	113.67	108.20
27	B8	1915	U	O4'-C1'-N1	6.83	113.67	108.20
27	B8	2479	U	O4'-C1'-N1	6.83	113.67	108.20
1	AA	20	U	O4'-C1'-N1	6.83	113.66	108.20
27	B8	303	G	O4'-C1'-N9	6.83	113.66	108.20
27	B8	787	C	N3-C4-N4	6.83	122.78	118.00
27	B8	1277	G	C5-C6-O6	-6.83	124.50	128.60
1	AA	67	C	O4'-C1'-N1	6.83	113.66	108.20
1	AA	690	G	C5-C6-O6	-6.83	124.50	128.60
27	B8	971	G	O4'-C1'-N9	6.83	113.66	108.20
1	AA	420	U	O4'-C1'-N1	6.83	113.66	108.20
1	AA	730	G	O4'-C1'-N9	6.83	113.66	108.20
27	B8	1027	A	C4-C5-C6	6.83	120.41	117.00
27	B8	2110	G	O4'-C1'-N9	6.83	113.66	108.20
1	AA	976	G	C5-C6-O6	-6.82	124.50	128.60
27	B8	12	U	O4'-C1'-N1	6.82	113.66	108.20
27	B8	669	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1464	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1853	A	O4'-C1'-N9	6.82	113.66	108.20
27	B8	2018	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	2242	G	O4'-C1'-N9	6.82	113.66	108.20
27	B8	2271	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	2813	A	O4'-C1'-N9	6.82	113.66	108.20
1	AA	589	U	O4'-C1'-N1	6.82	113.66	108.20
27	B8	2867	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1104	C	N3-C4-N4	6.82	122.78	118.00
27	B8	2249	U	O4'-C1'-N1	6.82	113.66	108.20
27	B8	2789	C	N3-C4-N4	6.82	122.77	118.00
1	AA	350	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1807	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1968	G	C5-C6-O6	-6.82	124.51	128.60
3	AV	53	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1110	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	1989	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	2255	G	C5-C6-O6	-6.82	124.51	128.60
27	B8	2163	A	C5-C6-N6	-6.81	118.25	123.70
27	B8	2769	U	O4'-C1'-N1	6.81	113.65	108.20
1	AA	761	G	C5-C6-O6	-6.81	124.51	128.60
3	AV	38	G	N1-C6-O6	6.81	123.99	119.90
26	B7	55	U	O4'-C1'-N1	6.81	113.65	108.20
27	B8	39	G	C5-C6-O6	-6.81	124.51	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	596	U	O4'-C1'-N1	6.81	113.65	108.20
27	B8	1149	G	O4'-C1'-N9	6.81	113.65	108.20
27	B8	1407	G	C5-C6-O6	-6.81	124.51	128.60
27	B8	2847	U	O4'-C1'-N1	6.81	113.65	108.20
1	AA	1111	A	C5-C6-N6	-6.81	118.25	123.70
27	B8	2169	A	O4'-C1'-N9	6.81	113.65	108.20
1	AA	257	G	C5-C6-O6	-6.81	124.51	128.60
1	AA	1016	A	C5-C6-N1	-6.81	114.30	117.70
27	B8	376	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	555	G	C5-C6-O6	-6.81	124.51	128.60
27	B8	1364	G	C5-C6-O6	-6.81	124.51	128.60
1	AA	814	A	C5-C6-N6	-6.81	118.25	123.70
1	AA	1379	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	98	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	859	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	1112	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	1217	U	O4'-C1'-N1	6.81	113.65	108.20
27	B8	1333	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	1452	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	2168	G	C5-C6-O6	-6.81	124.52	128.60
27	B8	2661	G	O4'-C1'-N9	6.81	113.65	108.20
27	B8	2898	U	O4'-C1'-N1	6.81	113.64	108.20
1	AA	479	U	O4'-C1'-N1	6.81	113.64	108.20
27	B8	1354	A	C4-C5-C6	6.81	120.40	117.00
27	B8	2120	G	C5-C6-O6	-6.81	124.52	128.60
1	AA	229	U	O4'-C1'-N1	6.80	113.64	108.20
1	AA	296	U	O4'-C1'-N1	6.80	113.64	108.20
3	AV	73	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	595	C	O4'-C1'-N1	6.80	113.64	108.20
27	B8	1481	U	O4'-C1'-N1	6.80	113.64	108.20
27	B8	1552	A	C4-C5-C6	6.80	120.40	117.00
27	B8	1883	U	O4'-C1'-N1	6.80	113.64	108.20
27	B8	2607	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	2784	U	O4'-C1'-N1	6.80	113.64	108.20
1	AA	250	A	O4'-C1'-N9	6.80	113.64	108.20
3	AV	43	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	2348	U	O4'-C1'-N1	6.80	113.64	108.20
1	AA	41	G	O4'-C1'-N9	6.80	113.64	108.20
1	AA	844	G	C5-C6-O6	-6.80	124.52	128.60
1	AA	1403	C	N3-C4-N4	6.80	122.76	118.00
27	B8	1212	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	1710	G	C5-C6-O6	-6.80	124.52	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1794	A	O4'-C1'-N9	6.80	113.64	108.20
27	B8	1884	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	772	C	O4'-C1'-N1	6.80	113.64	108.20
27	B8	1684	G	O4'-C1'-N9	6.80	113.64	108.20
27	B8	2644	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	2848	G	C5-C6-O6	-6.80	124.52	128.60
1	AA	319	G	O4'-C1'-N9	6.80	113.64	108.20
1	AA	1036	A	C4-C5-C6	6.80	120.40	117.00
27	B8	512	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	1025	G	C5-C6-O6	-6.80	124.52	128.60
27	B8	1598	A	C4-C5-C6	6.80	120.40	117.00
27	B8	1784	A	P-O3'-C3'	6.80	127.86	119.70
27	B8	2868	A	C4-C5-C6	6.80	120.40	117.00
27	B8	911	A	C5-C6-N6	-6.79	118.26	123.70
1	AA	362	G	C5-C6-O6	-6.79	124.52	128.60
1	AA	1231	G	O4'-C1'-N9	6.79	113.64	108.20
27	B8	462	C	O4'-C1'-N1	6.79	113.64	108.20
27	B8	775	G	C5-C6-O6	-6.79	124.52	128.60
27	B8	1461	C	O4'-C1'-N1	6.79	113.63	108.20
1	AA	1260	G	C5-C6-O6	-6.79	124.53	128.60
27	B8	1138	G	C5-C6-O6	-6.79	124.53	128.60
27	B8	1420	A	O4'-C1'-N9	6.79	113.63	108.20
1	AA	850	U	O4'-C1'-N1	6.79	113.63	108.20
1	AA	1330	U	O4'-C1'-N1	6.79	113.63	108.20
27	B8	1743	G	N3-C2-N2	6.79	124.65	119.90
27	B8	2214	C	N3-C4-N4	6.79	122.75	118.00
1	AA	1401	G	O4'-C1'-N9	6.79	113.63	108.20
27	B8	2144	G	C5-C6-O6	-6.79	124.53	128.60
1	AA	380	G	C5-C6-O6	-6.79	124.53	128.60
1	AA	1436	U	O4'-C1'-N1	6.79	113.63	108.20
1	AA	1273	C	N3-C4-N4	6.79	122.75	118.00
27	B8	199	A	C5-C6-N6	-6.79	118.27	123.70
27	B8	313	G	C5-C6-O6	-6.79	124.53	128.60
27	B8	1681	G	C5-C6-O6	-6.79	124.53	128.60
27	B8	1745	A	C5-C6-N6	-6.79	118.27	123.70
1	AA	652	U	O4'-C1'-N1	6.78	113.63	108.20
1	AA	1024	G	C5-C6-O6	-6.78	124.53	128.60
1	AA	1297	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	2459	A	C4-C5-C6	6.78	120.39	117.00
27	B8	2897	U	O4'-C1'-N1	6.78	113.63	108.20
1	AA	901	A	C4-C5-C6	6.78	120.39	117.00
27	B8	955	U	O4'-C1'-N1	6.78	113.62	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	338	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	947	A	C5-C6-N6	-6.78	118.28	123.70
27	B8	1869	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	1904	G	O4'-C1'-N9	6.78	113.62	108.20
27	B8	2102	G	O4'-C1'-N9	6.78	113.62	108.20
27	B8	2553	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	1533	C	N3-C4-N4	6.78	122.75	118.00
27	B8	2204	G	O4'-C1'-N9	6.78	113.62	108.20
1	AA	134	G	C5-C6-O6	-6.78	124.53	128.60
1	AA	390	U	O4'-C1'-N1	6.78	113.62	108.20
1	AA	496	A	C5-C6-N6	-6.78	118.28	123.70
26	B7	20	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	219	A	C5-C6-N6	-6.78	118.28	123.70
27	B8	1115	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	1467	U	O4'-C1'-N1	6.78	113.62	108.20
27	B8	1584	U	O4'-C1'-N1	6.78	113.62	108.20
1	AA	875	U	O4'-C1'-N1	6.78	113.62	108.20
1	AA	1278	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	443	A	O4'-C1'-N9	6.78	113.62	108.20
27	B8	1051	G	C5-C6-O6	-6.78	124.53	128.60
27	B8	1775	U	O4'-C1'-N1	6.78	113.62	108.20
1	AA	1017	U	O4'-C1'-N1	6.77	113.62	108.20
27	B8	569	U	O4'-C1'-N1	6.77	113.62	108.20
1	AA	303	A	O4'-C1'-N9	6.77	113.62	108.20
1	AA	354	G	C5-C6-O6	-6.77	124.54	128.60
1	AA	817	C	O4'-C1'-N1	6.77	113.62	108.20
27	B8	175	G	C5-C6-O6	-6.77	124.54	128.60
27	B8	232	G	C5-C6-O6	-6.77	124.54	128.60
27	B8	1159	U	O4'-C1'-N1	6.77	113.62	108.20
27	B8	1423	G	C5-C6-O6	-6.77	124.54	128.60
27	B8	1842	G	O4'-C1'-N9	6.77	113.62	108.20
2	AX	14	G	C5-C6-O6	-6.77	124.54	128.60
27	B8	1202	G	O4'-C1'-N9	6.77	113.62	108.20
27	B8	1644	C	O4'-C1'-N1	6.77	113.62	108.20
27	B8	899	A	O4'-C1'-N9	6.77	113.61	108.20
27	B8	997	G	O4'-C1'-N9	6.77	113.62	108.20
27	B8	2171	A	C5-C6-N6	-6.77	118.28	123.70
1	AA	500	G	O4'-C1'-N9	6.77	113.61	108.20
27	B8	1622	G	C5-C6-O6	-6.77	124.54	128.60
27	B8	1687	G	O4'-C1'-N9	6.77	113.61	108.20
27	B8	1872	A	O4'-C1'-N9	6.77	113.61	108.20
27	B8	372	G	C5-C6-O6	-6.77	124.54	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1355	G	O4'-C1'-N9	6.76	113.61	108.20
2	AX	20	G	C5-C6-O6	-6.76	124.54	128.60
27	B8	1245	G	O4'-C1'-N9	6.76	113.61	108.20
27	B8	1734	G	O4'-C1'-N9	6.76	113.61	108.20
27	B8	2049	G	O4'-C1'-N9	6.76	113.61	108.20
27	B8	2748	A	C4-C5-C6	6.76	120.38	117.00
27	B8	561	G	C5-C6-O6	-6.76	124.54	128.60
27	B8	2825	G	O4'-C1'-N9	6.76	113.61	108.20
1	AA	847	G	C5-C6-O6	-6.76	124.54	128.60
1	AA	827	U	O4'-C1'-N1	6.76	113.61	108.20
1	AA	1197	A	C5-C6-N6	-6.76	118.29	123.70
1	AA	1454	G	O4'-C1'-N9	6.76	113.61	108.20
27	B8	470	A	C4-C5-C6	6.76	120.38	117.00
27	B8	2357	G	C5-C6-O6	-6.76	124.55	128.60
1	AA	1381	U	O4'-C1'-N1	6.76	113.61	108.20
27	B8	1857	G	C5-C6-O6	-6.76	124.55	128.60
27	B8	2395	C	N3-C4-N4	6.76	122.73	118.00
1	AA	1375	A	C4-C5-C6	6.76	120.38	117.00
27	B8	1703	G	C5-C6-O6	-6.76	124.55	128.60
27	B8	1873	G	O4'-C1'-N9	6.76	113.61	108.20
27	B8	56	A	C5-C6-N6	-6.75	118.30	123.70
27	B8	458	G	C5-C6-O6	-6.75	124.55	128.60
27	B8	2435	A	C4-C5-C6	6.75	120.38	117.00
3	AV	14	A	C4-C5-C6	6.75	120.38	117.00
27	B8	2360	G	C5-C6-O6	-6.75	124.55	128.60
27	B8	2656	U	O4'-C1'-N1	6.75	113.60	108.20
27	B8	2844	G	C5-C6-O6	-6.75	124.55	128.60
27	B8	2857	G	C5-C6-O6	-6.75	124.55	128.60
1	AA	205	A	C5-C6-N6	-6.75	118.30	123.70
1	AA	561	U	O4'-C1'-N1	6.75	113.60	108.20
1	AA	642	A	C4-C5-C6	6.75	120.38	117.00
27	B8	221	A	C5-C6-N6	-6.75	118.30	123.70
27	B8	371	A	C4-C5-C6	6.75	120.38	117.00
27	B8	2073	C	O4'-C1'-N1	6.75	113.60	108.20
1	AA	881	G	O4'-C1'-N9	6.75	113.60	108.20
1	AA	1529	G	C5-C6-O6	-6.75	124.55	128.60
27	B8	2083	G	C5-C6-O6	-6.75	124.55	128.60
1	AA	148	G	O4'-C1'-N9	6.75	113.60	108.20
1	AA	714	G	O4'-C1'-N9	6.75	113.60	108.20
1	AA	752	G	C5-C6-O6	-6.75	124.55	128.60
1	AA	781	A	C4-C5-C6	6.75	120.38	117.00
27	B8	473	G	C5-C6-O6	-6.75	124.55	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2893	A	C4-C5-C6	6.75	120.37	117.00
1	AA	230	G	O4'-C1'-N9	6.75	113.60	108.20
1	AA	919	A	C4-C5-C6	6.75	120.37	117.00
27	B8	49	A	O4'-C1'-N9	6.75	113.60	108.20
27	B8	456	C	O4'-C1'-N1	6.75	113.60	108.20
27	B8	513	A	C4-C5-C6	6.75	120.37	117.00
27	B8	1697	G	C5-C6-O6	-6.75	124.55	128.60
1	AA	1398	A	C5-C6-N6	-6.75	118.30	123.70
3	AV	45	G	C5-C6-O6	-6.74	124.55	128.60
27	B8	633	A	C5-C6-N1	-6.74	114.33	117.70
27	B8	1498	C	O4'-C1'-N1	6.74	113.59	108.20
27	B8	2100	G	C5-C6-O6	-6.74	124.55	128.60
1	AA	332	G	C5-C6-O6	-6.74	124.56	128.60
1	AA	555	U	O4'-C1'-N1	6.74	113.59	108.20
27	B8	256	A	C4-C5-C6	6.74	120.37	117.00
27	B8	1468	U	O4'-C1'-N1	6.74	113.59	108.20
27	B8	1977	A	C4-C5-C6	6.74	120.37	117.00
1	AA	735	C	O4'-C1'-N1	6.74	113.59	108.20
1	AA	950	U	O4'-C1'-N1	6.74	113.59	108.20
1	AA	1060	U	O4'-C1'-N1	6.74	113.59	108.20
1	AA	1516	G	C5-C6-O6	-6.74	124.56	128.60
27	B8	1071	G	C5-C6-O6	-6.74	124.56	128.60
27	B8	2349	G	N1-C6-O6	6.74	123.94	119.90
1	AA	108	G	C5-C6-O6	-6.74	124.56	128.60
1	AA	412	A	O4'-C1'-N9	6.74	113.59	108.20
1	AA	1094	G	C5-C6-O6	-6.74	124.56	128.60
1	AA	1316	G	C5-C6-O6	-6.74	124.56	128.60
27	B8	491	G	C5-C6-O6	-6.74	124.56	128.60
27	B8	835	C	N3-C4-N4	6.74	122.72	118.00
1	AA	282	A	N1-C6-N6	6.74	122.64	118.60
1	AA	700	G	C5-C6-O6	-6.74	124.56	128.60
1	AA	1068	G	C5-C6-O6	-6.74	124.56	128.60
1	AA	1458	G	C5-C6-O6	-6.74	124.56	128.60
27	B8	1339	G	C5-C6-O6	-6.74	124.56	128.60
27	B8	2754	U	O4'-C1'-N1	6.74	113.59	108.20
27	B8	2810	A	O4'-C1'-N9	6.74	113.59	108.20
1	AA	907	A	C4-C5-C6	6.74	120.37	117.00
27	B8	1091	G	N1-C6-O6	6.74	123.94	119.90
27	B8	2476	A	C4-C5-C6	6.74	120.37	117.00
1	AA	769	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	446	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	819	A	C4-C5-C6	6.73	120.37	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	281	G	C5-C6-O6	-6.73	124.56	128.60
3	AV	20	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	363	G	O4'-C1'-N9	6.73	113.59	108.20
27	B8	2341	G	O4'-C1'-N9	6.73	113.58	108.20
27	B8	2701	U	O4'-C1'-N1	6.73	113.58	108.20
27	B8	1593	A	O4'-C1'-N9	6.73	113.58	108.20
27	B8	1865	U	O4'-C1'-N1	6.73	113.58	108.20
27	B8	2319	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	2436	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	2831	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	652	U	O4'-C1'-N1	6.73	113.58	108.20
27	B8	1311	G	C5-C6-O6	-6.73	124.56	128.60
1	AA	1103	C	O4'-C1'-N1	6.73	113.58	108.20
27	B8	359	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	608	A	C4-C5-C6	6.73	120.36	117.00
27	B8	1067	A	O4'-C1'-N9	6.73	113.58	108.20
27	B8	1227	G	O4'-C1'-N9	6.73	113.58	108.20
27	B8	1313	U	C2-N1-C1'	6.73	125.77	117.70
27	B8	1955	U	O4'-C1'-N1	6.73	113.58	108.20
27	B8	1715	G	C5-C6-O6	-6.73	124.56	128.60
27	B8	2090	A	C5-C6-N6	-6.73	118.32	123.70
1	AA	352	C	O4'-C1'-N1	6.72	113.58	108.20
26	B7	107	G	C5-C6-O6	-6.72	124.56	128.60
27	B8	426	C	N3-C4-N4	6.72	122.71	118.00
27	B8	747	U	O4'-C1'-N1	6.72	113.58	108.20
27	B8	1434	A	O4'-C1'-N9	6.72	113.58	108.20
27	B8	1807	G	O4'-C1'-N9	6.72	113.58	108.20
27	B8	2742	G	C5-C6-O6	-6.72	124.56	128.60
27	B8	704	G	O4'-C1'-N9	6.72	113.58	108.20
1	AA	1076	U	O4'-C1'-N1	6.72	113.58	108.20
1	AA	405	U	O4'-C1'-N1	6.72	113.58	108.20
1	AA	1066	C	O4'-C1'-N1	6.72	113.58	108.20
1	AA	1397	C	C2-N1-C1'	6.72	126.19	118.80
27	B8	332	A	C4-C5-C6	6.72	120.36	117.00
27	B8	381	G	C5-C6-O6	-6.72	124.57	128.60
27	B8	642	U	O4'-C1'-N1	6.72	113.58	108.20
27	B8	1382	G	C5-C6-O6	-6.72	124.57	128.60
27	B8	2408	U	O4'-C1'-N1	6.72	113.58	108.20
1	AA	211	G	O4'-C1'-N9	6.72	113.57	108.20
1	AA	262	A	C4-C5-C6	6.72	120.36	117.00
27	B8	720	U	O4'-C1'-N1	6.72	113.57	108.20
27	B8	1746	A	O4'-C1'-N9	6.72	113.58	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2670	A	O4'-C1'-N9	6.72	113.57	108.20
1	AA	102	G	C5-C6-O6	-6.72	124.57	128.60
1	AA	1165	U	O4'-C1'-N1	6.72	113.57	108.20
27	B8	280	U	O4'-C1'-N1	6.72	113.57	108.20
27	B8	480	A	C4-C5-C6	6.72	120.36	117.00
27	B8	594	U	O4'-C1'-N1	6.72	113.57	108.20
27	B8	842	U	O4'-C1'-N1	6.72	113.57	108.20
1	AA	297	G	C5-C6-O6	-6.71	124.57	128.60
1	AA	453	G	C5-C6-O6	-6.71	124.57	128.60
1	AA	834	U	O4'-C1'-N1	6.71	113.57	108.20
1	AA	1261	A	C4-C5-C6	6.71	120.36	117.00
27	B8	721	A	C5-C6-N1	-6.71	114.34	117.70
27	B8	2353	G	C5-C6-O6	-6.71	124.57	128.60
27	B8	2373	G	O4'-C1'-N9	6.71	113.57	108.20
1	AA	10	A	O4'-C1'-N9	6.71	113.57	108.20
27	B8	551	G	O4'-C1'-N9	6.71	113.57	108.20
27	B8	556	A	C4-C5-C6	6.71	120.36	117.00
27	B8	2465	C	N3-C4-N4	6.71	122.70	118.00
1	AA	369	G	C5-C6-O6	-6.71	124.57	128.60
3	AV	25	G	C5-C6-O6	-6.71	124.57	128.60
27	B8	741	U	O4'-C1'-N1	6.71	113.57	108.20
27	B8	1001	A	C4-C5-C6	6.71	120.36	117.00
27	B8	1573	G	O4'-C1'-N9	6.71	113.57	108.20
27	B8	1724	G	C5-C6-O6	-6.71	124.57	128.60
27	B8	2708	G	C5-C6-O6	-6.71	124.57	128.60
27	B8	2199	A	C4-C5-C6	6.71	120.36	117.00
1	AA	662	U	O4'-C1'-N1	6.71	113.57	108.20
1	AA	1013	G	C5-C6-O6	-6.71	124.57	128.60
27	B8	96	C	N3-C4-N4	6.71	122.70	118.00
27	B8	527	C	O4'-C1'-N1	6.71	113.57	108.20
27	B8	1002	G	C5-C6-O6	-6.71	124.58	128.60
27	B8	2517	C	O4'-C1'-N1	6.71	113.57	108.20
1	AA	746	A	C5-C6-N6	-6.71	118.33	123.70
3	AV	68	G	C5-C6-O6	-6.71	124.58	128.60
27	B8	374	A	C4-C5-C6	6.71	120.35	117.00
27	B8	467	G	O4'-C1'-N9	6.71	113.57	108.20
27	B8	1254	A	C4-C5-C6	6.71	120.35	117.00
27	B8	1267	U	O4'-C1'-N1	6.71	113.56	108.20
27	B8	2886	A	C4-C5-C6	6.71	120.35	117.00
1	AA	1028	C	O4'-C1'-N1	6.71	113.56	108.20
27	B8	1130	U	O4'-C1'-N1	6.71	113.56	108.20
27	B8	2356	U	O4'-C1'-N1	6.71	113.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	575	G	C5-C6-O6	-6.70	124.58	128.60
27	B8	1839	G	C5-C6-O6	-6.70	124.58	128.60
1	AA	76	G	O4'-C1'-N9	6.70	113.56	108.20
26	B7	25	U	O4'-C1'-N1	6.70	113.56	108.20
27	B8	175	G	O4'-C1'-N9	6.70	113.56	108.20
27	B8	1248	G	C5-C6-O6	-6.70	124.58	128.60
27	B8	1501	G	C5-C6-O6	-6.70	124.58	128.60
27	B8	1664	A	C4-C5-C6	6.70	120.35	117.00
27	B8	1669	A	C4-C5-C6	6.70	120.35	117.00
1	AA	772	U	O4'-C1'-N1	6.70	113.56	108.20
1	AA	909	A	C4-C5-C6	6.70	120.35	117.00
26	B7	52	A	O4'-C1'-N9	6.70	113.56	108.20
27	B8	547	A	O4'-C1'-N9	6.70	113.56	108.20
27	B8	2526	G	C5-C6-O6	-6.70	124.58	128.60
27	B8	2808	G	C5-C6-O6	-6.70	124.58	128.60
1	AA	1500	A	C5-C6-N6	-6.70	118.34	123.70
27	B8	1096	A	C4-C5-C6	6.70	120.35	117.00
27	B8	1674	G	C5-C6-O6	-6.70	124.58	128.60
27	B8	1269	A	C5-C6-N6	-6.69	118.34	123.70
27	B8	2017	U	O4'-C1'-N1	6.69	113.56	108.20
27	B8	2086	U	O4'-C1'-N1	6.69	113.56	108.20
1	AA	1439	G	O4'-C1'-N9	6.69	113.55	108.20
27	B8	2720	U	O4'-C1'-N1	6.69	113.55	108.20
27	B8	2007	U	O4'-C1'-N1	6.69	113.55	108.20
27	B8	2803	G	O4'-C1'-N9	6.69	113.55	108.20
27	B8	2843	G	C5-C6-O6	-6.69	124.58	128.60
1	AA	1252	A	O4'-C1'-N9	6.69	113.55	108.20
27	B8	256	A	O4'-C1'-N9	6.69	113.55	108.20
27	B8	1310	G	O4'-C1'-N9	6.69	113.55	108.20
1	AA	324	G	C5-C6-O6	-6.69	124.59	128.60
26	B7	41	G	C5-C6-O6	-6.69	124.59	128.60
27	B8	820	A	C4-C5-C6	6.69	120.34	117.00
27	B8	1347	A	O4'-C1'-N9	6.69	113.55	108.20
27	B8	1802	A	C4-C5-C6	6.69	120.34	117.00
1	AA	653	U	O4'-C1'-N1	6.69	113.55	108.20
27	B8	308	G	C5-C6-O6	-6.69	124.59	128.60
27	B8	941	A	O4'-C1'-N9	6.69	113.55	108.20
1	AA	1129	C	O4'-C1'-N1	6.68	113.55	108.20
27	B8	1683	U	O4'-C1'-N1	6.68	113.55	108.20
1	AA	927	G	C5-C6-O6	-6.68	124.59	128.60
27	B8	907	G	C5-C6-O6	-6.68	124.59	128.60
27	B8	1355	G	C5-C6-O6	-6.68	124.59	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	787	A	O4'-C1'-N9	6.68	113.54	108.20
1	AA	944	G	N3-C2-N2	6.68	124.58	119.90
1	AA	1089	G	C5-C6-O6	-6.68	124.59	128.60
27	B8	622	G	C5-C6-O6	-6.68	124.59	128.60
27	B8	1068	G	C5-C6-O6	-6.68	124.59	128.60
28	BA	79	ALA	N-CA-CB	6.68	119.45	110.10
1	AA	539	A	O4'-C1'-N9	6.68	113.54	108.20
27	B8	1439	A	C4-C5-C6	6.68	120.34	117.00
27	B8	2797	U	O4'-C1'-N1	6.68	113.54	108.20
1	AA	923	A	C4-C5-C6	6.68	120.34	117.00
26	B7	13	G	C5-C6-O6	-6.68	124.59	128.60
27	B8	1036	G	C5-C6-O6	-6.68	124.59	128.60
1	AA	563	A	C5-C6-N6	-6.67	118.36	123.70
27	B8	830	G	C5-C6-O6	-6.67	124.60	128.60
27	B8	1395	A	C4-C5-C6	6.67	120.34	117.00
27	B8	1572	A	C4-C5-C6	6.67	120.34	117.00
27	B8	1920	C	N3-C4-N4	6.67	122.67	118.00
1	AA	1528	U	O4'-C1'-N1	6.67	113.54	108.20
27	B8	2618	G	C5-C6-O6	-6.67	124.60	128.60
1	AA	81	A	C5-C6-N6	-6.67	118.36	123.70
27	B8	2775	G	C5-C6-O6	-6.67	124.60	128.60
27	B8	2885	G	C5-C6-O6	-6.67	124.60	128.60
1	AA	1452	C	O4'-C1'-N1	6.67	113.54	108.20
27	B8	709	U	O4'-C1'-N1	6.67	113.54	108.20
27	B8	2566	A	C4-C5-C6	6.67	120.33	117.00
1	AA	534	U	O4'-C1'-N1	6.67	113.53	108.20
1	AA	963	G	C5-C6-O6	-6.67	124.60	128.60
27	B8	924	G	O4'-C1'-N9	6.67	113.53	108.20
27	B8	2416	C	N3-C4-N4	6.67	122.67	118.00
27	B8	2809	A	O4'-C1'-N9	6.67	113.53	108.20
27	B8	725	G	C5-C6-O6	-6.67	124.60	128.60
27	B8	1242	U	O4'-C1'-N1	6.67	113.53	108.20
27	B8	2133	G	C5-C6-O6	-6.67	124.60	128.60
27	B8	2239	G	C5-C6-O6	-6.67	124.60	128.60
1	AA	1166	G	C5-C6-O6	-6.67	124.60	128.60
1	AA	717	U	O4'-C1'-N1	6.66	113.53	108.20
1	AA	888	G	C5-C6-O6	-6.66	124.60	128.60
1	AA	1065	U	O4'-C1'-N1	6.66	113.53	108.20
1	AA	1374	A	O4'-C1'-N9	6.66	113.53	108.20
1	AA	1453	G	O4'-C1'-N9	6.66	113.53	108.20
27	B8	950	G	C5-C6-O6	-6.66	124.60	128.60
27	B8	1360	G	O4'-C1'-N9	6.66	113.53	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1459	G	C5-C6-O6	-6.66	124.60	128.60
27	B8	2524	G	C5-C6-O6	-6.66	124.60	128.60
1	AA	1431	A	P-O3'-C3'	6.66	127.69	119.70
1	AA	1534	A	O4'-C1'-N9	6.66	113.53	108.20
27	B8	126	A	O4'-C1'-N9	6.66	113.53	108.20
27	B8	665	U	O4'-C1'-N1	6.66	113.53	108.20
27	B8	2780	G	C5-C6-O6	-6.66	124.60	128.60
1	AA	621	A	O4'-C1'-N9	6.66	113.53	108.20
1	AA	673	A	C5-C6-N6	-6.66	118.37	123.70
26	B7	105	G	O4'-C1'-N9	6.66	113.53	108.20
27	B8	159	G	C5-C6-O6	-6.66	124.61	128.60
27	B8	528	A	O4'-C1'-N9	6.66	113.53	108.20
27	B8	2192	U	O4'-C1'-N1	6.66	113.53	108.20
1	AA	506	G	O4'-C1'-N9	6.66	113.53	108.20
1	AA	646	G	C5-C6-O6	-6.66	124.61	128.60
27	B8	161	A	O4'-C1'-N9	6.66	113.52	108.20
27	B8	969	G	O4'-C1'-N9	6.66	113.53	108.20
27	B8	1824	G	C5-C6-O6	-6.66	124.61	128.60
27	B8	1970	A	C4-C5-C6	6.66	120.33	117.00
1	AA	1009	U	O4'-C1'-N1	6.65	113.52	108.20
1	AA	696	A	C4-C5-C6	6.65	120.33	117.00
1	AA	733	G	C5-C6-O6	-6.65	124.61	128.60
27	B8	1057	A	C4-C5-C6	6.65	120.33	117.00
27	B8	2284	A	C4-C5-C6	6.65	120.33	117.00
1	AA	63	C	N3-C4-N4	6.65	122.66	118.00
1	AA	520	A	C4-C5-C6	6.65	120.33	117.00
27	B8	1631	G	C5-C6-O6	-6.65	124.61	128.60
1	AA	1170	A	C4-C5-C6	6.65	120.32	117.00
27	B8	2227	A	O4'-C1'-N9	6.65	113.52	108.20
1	AA	444	G	O4'-C1'-N9	6.65	113.52	108.20
26	B7	99	A	C4-C5-C6	6.65	120.32	117.00
1	AA	991	U	O4'-C1'-N1	6.65	113.52	108.20
27	B8	548	G	C5-C6-O6	-6.65	124.61	128.60
27	B8	664	G	C5-C6-O6	-6.65	124.61	128.60
1	AA	797	C	N3-C4-N4	6.64	122.65	118.00
26	B7	72	G	C5-C6-O6	-6.64	124.61	128.60
27	B8	2569	G	O4'-C1'-N9	6.64	113.52	108.20
27	B8	99	U	C2-N1-C1'	6.64	125.67	117.70
27	B8	425	G	O4'-C1'-N9	6.64	113.51	108.20
27	B8	821	A	O4'-C1'-N9	6.64	113.51	108.20
27	B8	1015	U	O4'-C1'-N1	6.64	113.51	108.20
27	B8	1026	G	C5-C6-O6	-6.64	124.61	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1559	U	O4'-C1'-N1	6.64	113.52	108.20
27	B8	1634	A	C4-C5-C6	6.64	120.32	117.00
27	B8	1643	G	O4'-C1'-N9	6.64	113.51	108.20
1	AA	1483	A	C4-C5-C6	6.64	120.32	117.00
1	AA	1057	G	O4'-C1'-N9	6.64	113.51	108.20
1	AA	1312	G	O4'-C1'-N9	6.64	113.51	108.20
27	B8	869	G	C5-C6-O6	-6.64	124.62	128.60
1	AA	194	C	N3-C4-N4	6.64	122.64	118.00
1	AA	270	A	O4'-C1'-N9	6.64	113.51	108.20
1	AA	1400	C	C2-N1-C1'	6.64	126.10	118.80
26	B7	110	C	N3-C4-N4	6.64	122.64	118.00
27	B8	1828	G	C5-C6-O6	-6.64	124.62	128.60
27	B8	2285	C	N3-C4-N4	6.64	122.65	118.00
1	AA	254	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	166	U	O4'-C1'-N1	6.63	113.51	108.20
27	B8	1935	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	2477	U	O4'-C1'-N1	6.63	113.51	108.20
27	B8	2638	G	C5-C6-O6	-6.63	124.62	128.60
1	AA	1178	G	C5-C6-O6	-6.63	124.62	128.60
1	AA	1362	A	O4'-C1'-N9	6.63	113.51	108.20
1	AA	1531	A	C4-C5-C6	6.63	120.32	117.00
27	B8	1791	A	C5-C6-N6	-6.63	118.39	123.70
27	B8	900	A	O4'-C1'-N9	6.63	113.50	108.20
27	B8	2032	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	2351	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	2890	G	C5-C6-O6	-6.63	124.62	128.60
1	AA	180	U	O4'-C1'-N1	6.63	113.50	108.20
1	AA	394	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	2551	C	O4'-C1'-N1	6.63	113.50	108.20
27	B8	247	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	1017	G	C5-C6-O6	-6.63	124.62	128.60
27	B8	1528	A	C4-C5-C6	6.63	120.31	117.00
27	B8	2800	A	C5-C6-N6	-6.63	118.40	123.70
1	AA	270	A	C4-C5-C6	6.63	120.31	117.00
1	AA	908	A	C4-C5-C6	6.63	120.31	117.00
27	B8	3	U	O4'-C1'-N1	6.63	113.50	108.20
27	B8	1406	U	O4'-C1'-N1	6.63	113.50	108.20
27	B8	379	G	C5-C6-O6	-6.62	124.62	128.60
27	B8	2044	C	N3-C4-N4	6.62	122.64	118.00
27	B8	1089	A	C4-C5-C6	6.62	120.31	117.00
27	B8	2118	U	O4'-C1'-N1	6.62	113.50	108.20
1	AA	480	U	O4'-C1'-N1	6.62	113.50	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1282	C	N3-C4-N4	6.62	122.64	118.00
27	B8	2648	G	O4'-C1'-N9	6.62	113.50	108.20
27	B8	413	C	N3-C4-N4	6.62	122.63	118.00
27	B8	1326	U	O4'-C1'-N1	6.62	113.50	108.20
1	AA	818	G	O4'-C1'-N9	6.62	113.49	108.20
26	B7	69	G	N1-C6-O6	6.62	123.87	119.90
27	B8	1473	G	O4'-C1'-N9	6.62	113.49	108.20
27	B8	2684	U	O4'-C1'-N1	6.62	113.49	108.20
1	AA	429	U	P-O3'-C3'	6.62	127.64	119.70
27	B8	1271	G	C5-C6-O6	-6.62	124.63	128.60
27	B8	1426	G	C5-C6-O6	-6.62	124.63	128.60
1	AA	596	A	O4'-C1'-N9	6.62	113.49	108.20
1	AA	1517	G	C5-C6-O6	-6.62	124.63	128.60
3	AV	5	A	O4'-C1'-N9	6.62	113.49	108.20
27	B8	493	G	C5-C6-O6	-6.62	124.63	128.60
27	B8	343	C	O4'-C1'-N1	6.61	113.49	108.20
27	B8	1832	C	N3-C4-N4	6.61	122.63	118.00
27	B8	2435	A	C5-C6-N1	-6.61	114.39	117.70
27	B8	2608	G	C5-C6-O6	-6.61	124.63	128.60
1	AA	1035	A	O4'-C1'-N9	6.61	113.49	108.20
27	B8	2315	G	O4'-C1'-N9	6.61	113.49	108.20
1	AA	49	U	O4'-C1'-N1	6.61	113.49	108.20
1	AA	231	U	O4'-C1'-N1	6.61	113.49	108.20
1	AA	587	G	C5-C6-O6	-6.61	124.63	128.60
1	AA	1370	G	O4'-C1'-N9	6.61	113.49	108.20
27	B8	176	A	O4'-C1'-N9	6.61	113.49	108.20
27	B8	745	G	C5-C6-O6	-6.61	124.63	128.60
27	B8	1611	C	O4'-C1'-N1	6.61	113.49	108.20
1	AA	481	G	C5-C6-O6	-6.61	124.64	128.60
1	AA	628	G	O4'-C1'-N9	6.61	113.49	108.20
27	B8	1376	C	O4'-C1'-N1	6.61	113.49	108.20
27	B8	1852	U	O4'-C1'-N1	6.61	113.49	108.20
1	AA	1413	A	O4'-C1'-N9	6.61	113.49	108.20
27	B8	228	C	O4'-C1'-N1	6.61	113.48	108.20
27	B8	849	A	C5-C6-N6	-6.61	118.41	123.70
27	B8	1100	C	N3-C4-N4	6.61	122.63	118.00
27	B8	1387	A	O4'-C1'-N9	6.61	113.49	108.20
27	B8	1470	A	C4-C5-C6	6.61	120.30	117.00
27	B8	1543	G	C5-C6-O6	-6.61	124.64	128.60
27	B8	597	G	C5-C6-O6	-6.61	124.64	128.60
27	B8	1965	C	O4'-C1'-N1	6.61	113.48	108.20
1	AA	1213	A	C4-C5-C6	6.60	120.30	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	149	A	C4-C5-C6	6.60	120.30	117.00
27	B8	1501	G	O4'-C1'-N9	6.60	113.48	108.20
27	B8	2842	G	C5-C6-O6	-6.60	124.64	128.60
1	AA	145	G	O4'-C1'-N9	6.60	113.48	108.20
1	AA	1014	A	C5-C6-N6	-6.60	118.42	123.70
1	AA	1259	C	N3-C4-N4	6.60	122.62	118.00
27	B8	159	G	O4'-C1'-N9	6.60	113.48	108.20
27	B8	522	A	C5-C6-N6	-6.60	118.42	123.70
27	B8	728	G	C5-C6-O6	-6.60	124.64	128.60
27	B8	1690	A	C4-C5-C6	6.60	120.30	117.00
27	B8	1798	U	O4'-C1'-N1	6.60	113.48	108.20
27	B8	2220	U	O4'-C1'-N1	6.60	113.48	108.20
27	B8	2533	U	O4'-C1'-N1	6.60	113.48	108.20
1	AA	1171	A	O4'-C1'-N9	6.60	113.48	108.20
27	B8	180	G	C5-C6-O6	-6.60	124.64	128.60
27	B8	1032	A	O4'-C1'-N9	6.60	113.48	108.20
1	AA	118	U	O4'-C1'-N1	6.60	113.48	108.20
27	B8	2289	G	C5-C6-O6	-6.60	124.64	128.60
1	AA	96	U	O4'-C1'-N1	6.60	113.48	108.20
1	AA	478	A	O4'-C1'-N9	6.60	113.48	108.20
1	AA	502	A	C5-C6-N6	-6.60	118.42	123.70
1	AA	843	U	O4'-C1'-N1	6.59	113.47	108.20
1	AA	927	G	O4'-C1'-N9	6.59	113.48	108.20
1	AA	1490	U	O4'-C1'-N1	6.59	113.47	108.20
27	B8	998	C	N3-C4-N4	6.59	122.62	118.00
27	B8	1493	C	C6-N1-C1'	-6.59	112.89	120.80
27	B8	2877	G	O4'-C1'-N9	6.59	113.47	108.20
27	B8	2879	A	C5-C6-N6	-6.59	118.42	123.70
1	AA	1347	G	C5-C6-O6	-6.59	124.64	128.60
27	B8	327	G	O4'-C1'-N9	6.59	113.47	108.20
27	B8	756	A	C5-C6-N6	-6.59	118.43	123.70
27	B8	891	G	C5-C6-O6	-6.59	124.64	128.60
27	B8	1477	A	C4-C5-C6	6.59	120.30	117.00
27	B8	1549	A	O4'-C1'-N9	6.59	113.47	108.20
27	B8	2504	U	O4'-C1'-N1	6.59	113.47	108.20
1	AA	1197	A	C4-C5-C6	6.59	120.30	117.00
27	B8	2048	G	C5-C6-O6	-6.59	124.65	128.60
1	AA	696	A	O4'-C1'-N9	6.59	113.47	108.20
1	AA	860	A	C4-C5-C6	6.59	120.30	117.00
1	AA	1418	A	C4-C5-C6	6.59	120.30	117.00
27	B8	1716	U	O4'-C1'-N1	6.59	113.47	108.20
27	B8	2478	A	C4-C5-C6	6.59	120.30	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2668	G	O4'-C1'-N9	6.59	113.47	108.20
27	B8	530	G	C5-C6-O6	-6.59	124.65	128.60
27	B8	1182	G	O4'-C1'-N9	6.59	113.47	108.20
27	B8	2149	U	O4'-C1'-N1	6.59	113.47	108.20
27	B8	2865	U	O4'-C1'-N1	6.59	113.47	108.20
1	AA	126	G	O4'-C1'-N9	6.59	113.47	108.20
1	AA	158	G	C5-C6-O6	-6.59	124.65	128.60
1	AA	1279	G	C5-C6-O6	-6.59	124.65	128.60
27	B8	408	G	O4'-C1'-N9	6.59	113.47	108.20
27	B8	827	U	O4'-C1'-N1	6.59	113.47	108.20
27	B8	1283	G	C5-C6-O6	-6.59	124.65	128.60
27	B8	1299	G	C5-C6-O6	-6.59	124.65	128.60
27	B8	1383	A	O4'-C1'-N9	6.59	113.47	108.20
27	B8	1485	U	O4'-C1'-N1	6.59	113.47	108.20
27	B8	1514	G	C5-C6-O6	-6.59	124.65	128.60
27	B8	1590	A	O4'-C1'-N9	6.59	113.47	108.20
27	B8	2444	G	O4'-C1'-N9	6.59	113.47	108.20
27	B8	1420	A	C4-C5-C6	6.58	120.29	117.00
27	B8	1774	C	O4'-C1'-N1	6.58	113.47	108.20
1	AA	377	G	O4'-C1'-N9	6.58	113.47	108.20
1	AA	588	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	74	A	C4-C5-C6	6.58	120.29	117.00
27	B8	443	A	C4-C5-C6	6.58	120.29	117.00
27	B8	577	G	C5-C6-O6	-6.58	124.65	128.60
1	AA	595	A	C5-C6-N6	-6.58	118.43	123.70
1	AA	1144	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	2119	A	C4-C5-C6	6.58	120.29	117.00
27	B8	2121	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	2194	U	O4'-C1'-N1	6.58	113.47	108.20
27	B8	2294	G	C5-C6-O6	-6.58	124.65	128.60
1	AA	730	G	C5-C6-O6	-6.58	124.65	128.60
1	AA	971	G	O4'-C1'-N9	6.58	113.46	108.20
1	AA	1225	A	C4-C5-C6	6.58	120.29	117.00
3	AV	13	C	N3-C4-N4	6.58	122.61	118.00
27	B8	307	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	2494	G	C5-C6-O6	-6.58	124.65	128.60
1	AA	267	C	N3-C4-N4	6.58	122.60	118.00
27	B8	198	C	N3-C4-N4	6.58	122.61	118.00
27	B8	402	A	C4-C5-C6	6.58	120.29	117.00
27	B8	493	G	O4'-C1'-N9	6.58	113.46	108.20
27	B8	1223	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	1352	U	O4'-C1'-N1	6.58	113.46	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1521	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	2370	G	C5-C6-O6	-6.58	124.65	128.60
1	AA	1258	G	O4'-C1'-N9	6.58	113.46	108.20
27	B8	1936	A	C4-C5-C6	6.58	120.29	117.00
1	AA	253	A	O4'-C1'-N9	6.58	113.46	108.20
27	B8	1047	G	C5-C6-O6	-6.58	124.65	128.60
27	B8	1213	A	C5-C6-N1	-6.58	114.41	117.70
27	B8	1766	G	O4'-C1'-N9	6.58	113.46	108.20
27	B8	2092	U	O4'-C1'-N1	6.58	113.46	108.20
27	B8	2802	G	O4'-C1'-N9	6.58	113.46	108.20
1	AA	149	A	C4-C5-C6	6.57	120.29	117.00
1	AA	865	A	C4-C5-C6	6.57	120.29	117.00
1	AA	1416	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	443	A	C5-C6-N6	-6.57	118.44	123.70
27	B8	1031	G	O4'-C1'-N9	6.57	113.46	108.20
27	B8	983	A	C4-C5-C6	6.57	120.29	117.00
27	B8	1045	C	N3-C4-N4	6.57	122.60	118.00
1	AA	315	A	O4'-C1'-N9	6.57	113.46	108.20
1	AA	566	G	N1-C6-O6	6.57	123.84	119.90
1	AA	890	G	C5-C6-O6	-6.57	124.66	128.60
1	AA	1432	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	359	G	O4'-C1'-N9	6.57	113.46	108.20
27	B8	879	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	1604	C	N3-C4-N4	6.57	122.60	118.00
27	B8	2529	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	36	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	117	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	233	A	C4-C5-C6	6.57	120.28	117.00
27	B8	333	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	1378	A	C4-C5-C6	6.57	120.28	117.00
3	AV	7	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	388	G	C5-C6-O6	-6.57	124.66	128.60
27	B8	696	G	O4'-C1'-N9	6.57	113.45	108.20
27	B8	2817	U	O4'-C1'-N1	6.57	113.45	108.20
1	AA	360	G	C5-C6-O6	-6.56	124.66	128.60
1	AA	3	A	C4-C5-C6	6.56	120.28	117.00
1	AA	768	A	O4'-C1'-N9	6.56	113.45	108.20
1	AA	994	A	C4-C5-C6	6.56	120.28	117.00
3	AV	49	C	O4'-C1'-N1	6.56	113.45	108.20
27	B8	488	G	C5-C6-O6	-6.56	124.66	128.60
27	B8	1186	G	O4'-C1'-N9	6.56	113.45	108.20
27	B8	1508	A	O4'-C1'-N9	6.56	113.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1571	A	C5-C6-N1	-6.56	114.42	117.70
27	B8	2174	C	N3-C4-N4	6.56	122.59	118.00
27	B8	2190	G	O4'-C1'-N9	6.56	113.45	108.20
27	B8	2740	A	O4'-C1'-N9	6.56	113.45	108.20
1	AA	338	A	O4'-C1'-N9	6.56	113.45	108.20
1	AA	780	A	O4'-C1'-N9	6.56	113.45	108.20
1	AA	1440	U	O4'-C1'-N1	6.56	113.45	108.20
1	AA	14	U	O4'-C1'-N1	6.56	113.45	108.20
1	AA	1001	C	N3-C4-N4	6.56	122.59	118.00
27	B8	53	A	C4-C5-C6	6.56	120.28	117.00
27	B8	113	U	O4'-C1'-N1	6.56	113.45	108.20
27	B8	195	A	C4-C5-C6	6.56	120.28	117.00
27	B8	2659	G	C5-C6-O6	-6.56	124.66	128.60
1	AA	63	C	O4'-C1'-N1	6.56	113.45	108.20
1	AA	1355	G	C5-C6-O6	-6.56	124.67	128.60
27	B8	664	G	O4'-C1'-N9	6.56	113.45	108.20
27	B8	1073	A	C5-C6-N6	-6.56	118.45	123.70
1	AA	16	A	C5-C6-N6	-6.55	118.46	123.70
1	AA	504	C	N3-C4-N4	6.55	122.59	118.00
1	AA	598	U	O4'-C1'-N1	6.55	113.44	108.20
1	AA	1303	C	O4'-C1'-N1	6.55	113.44	108.20
27	B8	225	C	O4'-C1'-N1	6.55	113.44	108.20
27	B8	2115	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	2862	G	O4'-C1'-N9	6.55	113.44	108.20
27	B8	414	C	N3-C4-N4	6.55	122.59	118.00
27	B8	421	C	O4'-C1'-N1	6.55	113.44	108.20
1	AA	1426	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	233	A	C5-C6-N6	-6.55	118.46	123.70
27	B8	399	U	O4'-C1'-N1	6.55	113.44	108.20
27	B8	503	A	C5-C6-N6	-6.55	118.46	123.70
27	B8	1021	A	C4-C5-C6	6.55	120.28	117.00
27	B8	2822	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	1987	A	O4'-C1'-N9	6.55	113.44	108.20
27	B8	95	A	C4-C5-C6	6.55	120.27	117.00
27	B8	298	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	880	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	1945	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	2237	G	C5-C6-O6	-6.55	124.67	128.60
27	B8	2311	A	C4-C5-C6	6.55	120.27	117.00
27	B8	2400	G	O4'-C1'-N9	6.55	113.44	108.20
27	B8	2597	G	C5-C6-O6	-6.55	124.67	128.60
1	AA	944	G	C5-C6-O6	-6.54	124.67	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1305	G	C5-C6-O6	-6.54	124.67	128.60
1	AA	1386	G	O4'-C1'-N9	6.54	113.44	108.20
1	AA	1542	A	C4-C5-C6	6.54	120.27	117.00
27	B8	191	A	O4'-C1'-N9	6.54	113.44	108.20
27	B8	2842	G	O4'-C1'-N9	6.54	113.44	108.20
27	B8	1175	A	C4-C5-C6	6.54	120.27	117.00
27	B8	1419	A	C4-C5-C6	6.54	120.27	117.00
27	B8	2328	A	C4-C5-C6	6.54	120.27	117.00
1	AA	35	G	C5-C6-O6	-6.54	124.67	128.60
1	AA	307	C	O4'-C1'-N1	6.54	113.43	108.20
27	B8	831	G	O4'-C1'-N9	6.54	113.43	108.20
27	B8	1671	U	O4'-C1'-N1	6.54	113.43	108.20
27	B8	2681	C	O4'-C1'-N1	6.54	113.43	108.20
1	AA	1222	G	C5-C6-O6	-6.54	124.68	128.60
3	AV	9	A	C4-C5-C6	6.54	120.27	117.00
27	B8	619	G	C5-C6-O6	-6.54	124.68	128.60
27	B8	2872	A	C4-C5-C6	6.54	120.27	117.00
1	AA	226	G	C5-C6-O6	-6.54	124.68	128.60
1	AA	691	G	C5-C6-O6	-6.54	124.68	128.60
1	AA	693	G	C5-C6-O6	-6.54	124.68	128.60
1	AA	1055	A	C4-C5-C6	6.54	120.27	117.00
1	AA	1149	C	N3-C4-N4	6.54	122.58	118.00
26	B7	15	A	C4-C5-C6	6.54	120.27	117.00
27	B8	731	C	N3-C4-N4	6.54	122.58	118.00
27	B8	927	A	O4'-C1'-N9	6.54	113.43	108.20
27	B8	1252	G	C5-C6-O6	-6.54	124.68	128.60
27	B8	1946	U	O4'-C1'-N1	6.54	113.43	108.20
27	B8	253	C	N3-C4-N4	6.54	122.58	118.00
27	B8	434	U	O4'-C1'-N1	6.54	113.43	108.20
27	B8	1226	A	C4-C5-C6	6.54	120.27	117.00
27	B8	2112	G	O4'-C1'-N9	6.54	113.43	108.20
1	AA	1077	G	C5-C6-O6	-6.54	124.68	128.60
27	B8	174	U	O4'-C1'-N1	6.54	113.43	108.20
27	B8	1412	U	O4'-C1'-N1	6.54	113.43	108.20
27	B8	2010	G	C5-C6-O6	-6.54	124.68	128.60
27	B8	2040	G	O4'-C1'-N9	6.54	113.43	108.20
27	B8	2068	U	O4'-C1'-N1	6.54	113.43	108.20
27	B8	2268	A	C4-C5-C6	6.54	120.27	117.00
27	B8	2611	C	O4'-C1'-N1	6.54	113.43	108.20
1	AA	190	A	C5-C6-N1	-6.53	114.43	117.70
1	AA	260	G	C5-C6-O6	-6.53	124.68	128.60
27	B8	1911	U	O4'-C1'-N1	6.53	113.43	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	43	G	C5-C6-O6	-6.53	124.68	128.60
1	AA	86	G	C5-C6-O6	-6.53	124.68	128.60
1	AA	92	U	O4'-C1'-N1	6.53	113.42	108.20
1	AA	141	G	O4'-C1'-N9	6.53	113.42	108.20
1	AA	412	A	C4-C5-C6	6.53	120.27	117.00
1	AA	947	G	O4'-C1'-N9	6.53	113.42	108.20
1	AA	1426	G	O4'-C1'-N9	6.53	113.42	108.20
3	AV	50	G	C5-C6-O6	-6.53	124.68	128.60
26	B7	119	A	O4'-C1'-N9	6.53	113.42	108.20
1	AA	283	U	O4'-C1'-N1	6.53	113.42	108.20
3	AV	33	A	O4'-C1'-N9	6.53	113.42	108.20
27	B8	2677	G	O4'-C1'-N9	6.53	113.42	108.20
3	AV	37	G	C5-C6-O6	-6.53	124.68	128.60
27	B8	35	G	O4'-C1'-N9	6.53	113.42	108.20
27	B8	458	G	O4'-C1'-N9	6.53	113.42	108.20
1	AA	512	U	O4'-C1'-N1	6.53	113.42	108.20
27	B8	93	G	C5-C6-O6	-6.53	124.69	128.60
27	B8	476	G	C5-C6-O6	-6.53	124.68	128.60
27	B8	888	C	O4'-C1'-N1	6.53	113.42	108.20
27	B8	1811	G	C5-C6-O6	-6.53	124.69	128.60
27	B8	2034	U	O4'-C1'-N1	6.53	113.42	108.20
1	AA	183	C	O4'-C1'-N1	6.52	113.42	108.20
1	AA	220	G	O4'-C1'-N9	6.52	113.42	108.20
1	AA	996	A	C5-C6-N6	-6.52	118.48	123.70
27	B8	2060	A	O4'-C1'-N9	6.52	113.42	108.20
27	B8	2779	U	O4'-C1'-N1	6.52	113.42	108.20
1	AA	654	G	C5-C6-O6	-6.52	124.69	128.60
27	B8	609	A	C4-C5-C6	6.52	120.26	117.00
1	AA	901	A	C5-C6-N6	-6.52	118.48	123.70
27	B8	2873	A	C4-C5-C6	6.52	120.26	117.00
1	AA	313	A	C4-C5-C6	6.52	120.26	117.00
1	AA	351	G	C5-C6-O6	-6.52	124.69	128.60
1	AA	1002	G	O4'-C1'-N9	6.52	113.42	108.20
26	B7	58	A	C4-C5-C6	6.52	120.26	117.00
27	B8	1408	G	C5-C6-O6	-6.52	124.69	128.60
27	B8	1876	A	N1-C6-N6	6.52	122.51	118.60
1	AA	583	A	O4'-C1'-N9	6.52	113.41	108.20
1	AA	592	G	O4'-C1'-N9	6.52	113.42	108.20
1	AA	1387	G	O4'-C1'-N9	6.52	113.41	108.20
26	B7	64	G	O4'-C1'-N9	6.52	113.41	108.20
27	B8	1668	A	P-O3'-C3'	6.52	127.52	119.70
27	B8	2766	A	C4-C5-C6	6.52	120.26	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	776	G	O4'-C1'-N9	6.52	113.41	108.20
27	B8	1577	C	N3-C4-N4	6.52	122.56	118.00
27	B8	544	C	C2-N1-C1'	6.51	125.97	118.80
27	B8	1002	G	O4'-C1'-N9	6.51	113.41	108.20
27	B8	1532	A	C5-C6-N6	-6.51	118.49	123.70
26	B7	76	G	C5-C6-O6	-6.51	124.69	128.60
27	B8	2627	G	C5-C6-O6	-6.51	124.69	128.60
1	AA	44	A	O4'-C1'-N9	6.51	113.41	108.20
1	AA	250	A	C4-C5-C6	6.51	120.25	117.00
1	AA	532	A	C4-C5-C6	6.51	120.26	117.00
1	AA	1222	G	O4'-C1'-N9	6.51	113.41	108.20
1	AA	1434	A	O4'-C1'-N9	6.51	113.41	108.20
27	B8	58	G	C5-C6-O6	-6.51	124.69	128.60
27	B8	708	G	O4'-C1'-N9	6.51	113.41	108.20
1	AA	782	A	O4'-C1'-N9	6.51	113.41	108.20
27	B8	213	A	C5-C6-N6	-6.51	118.49	123.70
27	B8	315	G	C5-C6-O6	-6.51	124.69	128.60
27	B8	855	G	C5-C6-O6	-6.51	124.69	128.60
27	B8	95	A	C5-C6-N6	-6.51	118.49	123.70
27	B8	424	G	O4'-C1'-N9	6.51	113.41	108.20
27	B8	515	A	C5-C6-N6	-6.51	118.49	123.70
27	B8	2524	G	O4'-C1'-N9	6.51	113.41	108.20
1	AA	12	U	O4'-C1'-N1	6.51	113.41	108.20
27	B8	1334	G	C5-C6-O6	-6.51	124.70	128.60
27	B8	1564	C	N3-C4-N4	6.51	122.56	118.00
27	B8	1756	G	C5-C6-O6	-6.51	124.70	128.60
1	AA	38	G	C5-C6-O6	-6.50	124.70	128.60
27	B8	391	A	C4-C5-C6	6.50	120.25	117.00
1	AA	1063	C	N3-C4-N4	6.50	122.55	118.00
1	AA	1219	A	C4-C5-C6	6.50	120.25	117.00
1	AA	1417	G	C5-C6-O6	-6.50	124.70	128.60
1	AA	259	G	O4'-C1'-N9	6.50	113.40	108.20
1	AA	731	G	O4'-C1'-N9	6.50	113.40	108.20
27	B8	1026	G	O4'-C1'-N9	6.50	113.40	108.20
27	B8	1531	C	N3-C4-N4	6.50	122.55	118.00
27	B8	2138	G	C5-C6-O6	-6.50	124.70	128.60
1	AA	712	A	O4'-C1'-N9	6.50	113.40	108.20
27	B8	400	G	N3-C2-N2	6.50	124.45	119.90
27	B8	2212	A	C4-C5-C6	6.50	120.25	117.00
27	B8	2508	G	O4'-C1'-N9	6.50	113.40	108.20
1	AA	256	U	O4'-C1'-N1	6.50	113.40	108.20
1	AA	1262	C	N3-C4-N4	6.50	122.55	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	871	U	O4'-C1'-N1	6.50	113.40	108.20
27	B8	1948	G	O4'-C1'-N9	6.50	113.40	108.20
1	AA	376	G	C5-C6-O6	-6.50	124.70	128.60
27	B8	230	G	O4'-C1'-N9	6.50	113.40	108.20
27	B8	1088	A	O4'-C1'-N9	6.50	113.40	108.20
27	B8	1702	G	O4'-C1'-N9	6.50	113.40	108.20
1	AA	472	U	O4'-C1'-N1	6.50	113.40	108.20
1	AA	1263	C	N3-C4-N4	6.50	122.55	118.00
27	B8	560	C	N3-C4-N4	6.50	122.55	118.00
27	B8	1700	A	C4-C5-C6	6.50	120.25	117.00
27	B8	2282	G	C5-C6-O6	-6.50	124.70	128.60
1	AA	82	G	C5-C6-O6	-6.49	124.70	128.60
1	AA	262	A	C5-C6-N6	-6.49	118.50	123.70
1	AA	305	G	C5-C6-O6	-6.49	124.70	128.60
1	AA	926	G	C5-C6-O6	-6.49	124.70	128.60
27	B8	689	A	C5-C6-N6	-6.49	118.50	123.70
27	B8	872	U	O4'-C1'-N1	6.49	113.39	108.20
27	B8	876	C	C5'-C4'-O4'	6.49	116.89	109.10
27	B8	1471	G	C5-C6-O6	-6.49	124.70	128.60
27	B8	2432	A	C4-C5-C6	6.49	120.25	117.00
27	B8	2611	C	N3-C4-N4	6.49	122.55	118.00
27	B8	412	A	C4-C5-C6	6.49	120.25	117.00
27	B8	1819	A	C4-C5-C6	6.49	120.25	117.00
1	AA	475	C	N3-C4-N4	6.49	122.54	118.00
1	AA	694	A	C4-C5-C6	6.49	120.25	117.00
1	AA	789	U	O4'-C1'-N1	6.49	113.39	108.20
27	B8	973	A	C4-C5-C6	6.49	120.25	117.00
27	B8	1237	A	C4-C5-C6	6.49	120.25	117.00
27	B8	1613	G	O4'-C1'-N9	6.49	113.39	108.20
27	B8	2051	A	C5-C6-N6	-6.49	118.51	123.70
27	B8	2537	U	O4'-C1'-N1	6.49	113.39	108.20
27	B8	2774	C	N3-C4-N4	6.49	122.54	118.00
27	B8	2821	A	C4-C5-C6	6.49	120.25	117.00
27	B8	2573	C	C6-N1-C1'	-6.49	113.01	120.80
1	AA	1079	G	C5-C6-O6	-6.49	124.71	128.60
27	B8	2127	G	C5-C6-O6	-6.49	124.71	128.60
27	B8	2816	G	C5-C6-O6	-6.49	124.71	128.60
27	B8	2863	C	N3-C4-N4	6.49	122.54	118.00
1	AA	597	G	O4'-C1'-N9	6.49	113.39	108.20
27	B8	305	C	N3-C4-N4	6.49	122.54	118.00
27	B8	1527	G	C5-C6-O6	-6.49	124.71	128.60
1	AA	410	G	O4'-C1'-N9	6.48	113.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1938	A	O4'-C1'-N9	6.48	113.39	108.20
1	AA	187	G	C5-C6-O6	-6.48	124.71	128.60
1	AA	208	U	O4'-C1'-N1	6.48	113.39	108.20
27	B8	532	A	C5-C6-N6	-6.48	118.51	123.70
27	B8	712	G	O4'-C1'-N9	6.48	113.39	108.20
27	B8	1524	G	C5-C6-O6	-6.48	124.71	128.60
27	B8	1580	A	C4-C5-C6	6.48	120.24	117.00
27	B8	2014	A	C4-C5-C6	6.48	120.24	117.00
27	B8	2665	A	C4-C5-C6	6.48	120.24	117.00
27	B8	2887	A	C4-C5-C6	6.48	120.24	117.00
1	AA	574	A	C4-C5-C6	6.48	120.24	117.00
1	AA	1123	U	O4'-C1'-N1	6.48	113.39	108.20
1	AA	1415	G	C5-C6-O6	-6.48	124.71	128.60
27	B8	1263	U	O4'-C1'-N1	6.48	113.38	108.20
27	B8	1371	G	O4'-C1'-N9	6.48	113.39	108.20
27	B8	2154	A	C4-C5-C6	6.48	120.24	117.00
1	AA	1111	A	C4-C5-C6	6.48	120.24	117.00
3	AV	9	A	C5-C6-N6	-6.48	118.52	123.70
26	B7	46	A	C5-C6-N1	-6.48	114.46	117.70
27	B8	889	C	C2-N1-C1'	6.48	125.93	118.80
1	AA	550	G	O4'-C1'-N9	6.48	113.38	108.20
1	AA	737	C	N3-C4-N4	6.48	122.53	118.00
27	B8	365	U	O4'-C1'-N1	6.48	113.38	108.20
27	B8	570	G	C5-C6-O6	-6.48	124.71	128.60
27	B8	1578	U	O4'-C1'-N1	6.48	113.38	108.20
27	B8	1648	U	O4'-C1'-N1	6.48	113.38	108.20
27	B8	2568	U	O4'-C1'-N1	6.48	113.38	108.20
27	B8	1066	U	O4'-C1'-N1	6.48	113.38	108.20
27	B8	1483	G	C5-C6-O6	-6.48	124.71	128.60
27	B8	1872	A	C4-C5-C6	6.48	120.24	117.00
1	AA	768	A	C4-C5-C6	6.47	120.24	117.00
1	AA	1541	U	P-O3'-C3'	6.47	127.47	119.70
27	B8	582	A	C5-C6-N6	-6.47	118.52	123.70
27	B8	1314	C	O4'-C1'-N1	6.47	113.38	108.20
27	B8	2256	G	O4'-C1'-N9	6.47	113.38	108.20
27	B8	2560	A	C5-C6-N1	-6.47	114.46	117.70
1	AA	133	U	O4'-C1'-N1	6.47	113.38	108.20
1	AA	159	G	C5-C6-O6	-6.47	124.72	128.60
27	B8	982	C	C2-N1-C1'	6.47	125.92	118.80
27	B8	1048	A	C4-C5-C6	6.47	120.24	117.00
27	B8	1392	A	C4-C5-C6	6.47	120.24	117.00
27	B8	2721	A	C4-C5-C6	6.47	120.24	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1306	A	C4-C5-C6	6.47	120.23	117.00
27	B8	1121	C	N3-C4-N4	6.47	122.53	118.00
27	B8	1166	G	C5-C6-O6	-6.47	124.72	128.60
1	AA	1434	A	C4-C5-C6	6.47	120.23	117.00
26	B7	74	U	O4'-C1'-N1	6.47	113.38	108.20
27	B8	882	G	C5-C6-O6	-6.47	124.72	128.60
27	B8	2662	A	C5-C6-N6	-6.47	118.52	123.70
1	AA	263	A	C4-C5-C6	6.47	120.23	117.00
1	AA	541	G	O4'-C1'-N9	6.47	113.38	108.20
1	AA	1324	A	C4-C5-C6	6.47	120.23	117.00
1	AA	1459	G	O4'-C1'-N9	6.47	113.37	108.20
27	B8	212	G	O4'-C1'-N9	6.47	113.37	108.20
27	B8	1667	G	C5-C6-O6	-6.47	124.72	128.60
1	AA	6	G	C5-C6-O6	-6.47	124.72	128.60
1	AA	139	A	O4'-C1'-N9	6.47	113.37	108.20
1	AA	886	G	C5-C6-O6	-6.47	124.72	128.60
1	AA	1488	G	C5-C6-O6	-6.47	124.72	128.60
27	B8	19	A	C5-C6-N6	-6.47	118.53	123.70
27	B8	2122	U	O4'-C1'-N1	6.47	113.37	108.20
1	AA	477	C	N3-C4-N4	6.46	122.53	118.00
27	B8	54	G	C5-C6-O6	-6.46	124.72	128.60
27	B8	207	A	O4'-C1'-N9	6.46	113.37	108.20
27	B8	752	A	C4-C5-C6	6.46	120.23	117.00
27	B8	1453	A	C4-C5-C6	6.46	120.23	117.00
27	B8	1700	A	C5-C6-N6	-6.46	118.53	123.70
27	B8	277	G	O4'-C1'-N9	6.46	113.37	108.20
27	B8	2735	G	C5-C6-O6	-6.46	124.72	128.60
1	AA	125	U	O4'-C1'-N1	6.46	113.37	108.20
1	AA	247	G	C5-C6-O6	-6.46	124.72	128.60
27	B8	600	G	C5-C6-O6	-6.46	124.72	128.60
27	B8	1020	A	O4'-C1'-N9	6.46	113.37	108.20
27	B8	2033	A	C4-C5-C6	6.46	120.23	117.00
27	B8	2271	G	O4'-C1'-N9	6.46	113.37	108.20
27	B8	2838	G	O4'-C1'-N9	6.46	113.37	108.20
1	AA	540	G	O4'-C1'-N9	6.46	113.37	108.20
1	AA	894	G	O4'-C1'-N9	6.46	113.37	108.20
3	AV	19	G	C5-C6-O6	-6.46	124.72	128.60
5	A0	166	TYR	CB-CG-CD2	-6.46	117.12	121.00
27	B8	503	A	C4-C5-C6	6.46	120.23	117.00
27	B8	1713	A	C4-C5-C6	6.46	120.23	117.00
27	B8	2499	C	N3-C4-N4	6.46	122.52	118.00
1	AA	138	G	O4'-C1'-N9	6.46	113.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	337	G	O4'-C1'-N9	6.46	113.37	108.20
1	AA	756	C	N3-C4-N4	6.46	122.52	118.00
27	B8	452	G	C5-C6-O6	-6.46	124.72	128.60
27	B8	1875	G	C5-C6-O6	-6.46	124.72	128.60
27	B8	2482	A	C4-C5-C6	6.46	120.23	117.00
27	B8	2595	G	C5-C6-O6	-6.46	124.72	128.60
1	AA	19	A	C4-C5-C6	6.46	120.23	117.00
1	AA	262	A	C5-C6-N1	-6.46	114.47	117.70
1	AA	818	G	C5-C6-O6	-6.46	124.73	128.60
1	AA	826	C	O4'-C1'-N1	6.46	113.37	108.20
27	B8	110	G	O4'-C1'-N9	6.46	113.36	108.20
27	B8	352	A	C4-C5-C6	6.46	120.23	117.00
27	B8	592	A	O4'-C1'-N9	6.46	113.36	108.20
27	B8	1189	A	C4-C5-C6	6.46	120.23	117.00
27	B8	1589	U	O4'-C1'-N1	6.46	113.37	108.20
27	B8	662	G	O4'-C1'-N9	6.46	113.36	108.20
1	AA	1248	A	O4'-C1'-N9	6.45	113.36	108.20
27	B8	2729	G	O4'-C1'-N9	6.45	113.36	108.20
1	AA	557	G	C5-C6-O6	-6.45	124.73	128.60
27	B8	167	A	C4-C5-C6	6.45	120.23	117.00
27	B8	1178	C	N3-C4-N4	6.45	122.52	118.00
1	AA	628	G	C5-C6-O6	-6.45	124.73	128.60
27	B8	1283	G	O4'-C1'-N9	6.45	113.36	108.20
27	B8	2190	G	C5-C6-O6	-6.45	124.73	128.60
1	AA	682	G	O4'-C1'-N9	6.45	113.36	108.20
1	AA	1438	G	O4'-C1'-N9	6.45	113.36	108.20
26	B7	119	A	C4-C5-C6	6.45	120.22	117.00
27	B8	104	A	C5-C6-N6	-6.45	118.54	123.70
27	B8	114	U	O4'-C1'-N1	6.45	113.36	108.20
27	B8	1535	A	C4-C5-C6	6.45	120.22	117.00
27	B8	1862	G	O4'-C1'-N9	6.45	113.36	108.20
27	B8	2811	G	O4'-C1'-N9	6.45	113.36	108.20
27	B8	2895	G	O4'-C1'-N9	6.45	113.36	108.20
1	AA	1441	A	O4'-C1'-N9	6.45	113.36	108.20
26	B7	35	C	C2-N1-C1'	6.45	125.89	118.80
27	B8	1235	G	C5-C6-O6	-6.45	124.73	128.60
27	B8	1315	C	N3-C4-N4	6.45	122.51	118.00
27	B8	2544	G	O4'-C1'-N9	6.45	113.36	108.20
27	B8	713	G	C5-C6-O6	-6.44	124.73	128.60
27	B8	866	A	C4-C5-C6	6.44	120.22	117.00
27	B8	1930	G	C5-C6-O6	-6.44	124.73	128.60
1	AA	419	C	N3-C4-N4	6.44	122.51	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1127	G	C5-C6-O6	-6.44	124.73	128.60
27	B8	196	A	C4-C5-C6	6.44	120.22	117.00
27	B8	801	G	C5-C6-O6	-6.44	124.73	128.60
27	B8	2464	G	O4'-C1'-N9	6.44	113.35	108.20
1	AA	128	G	C5-C6-O6	-6.44	124.74	128.60
1	AA	498	A	C4-C5-C6	6.44	120.22	117.00
1	AA	915	A	C5-C6-N6	-6.44	118.55	123.70
1	AA	1039	G	O4'-C1'-N9	6.44	113.35	108.20
1	AA	1173	U	O4'-C1'-N1	6.44	113.35	108.20
27	B8	782	A	C4-C5-C6	6.44	120.22	117.00
27	B8	1703	G	O4'-C1'-N9	6.44	113.35	108.20
27	B8	2706	A	C4-C5-C6	6.44	120.22	117.00
1	AA	1062	U	O4'-C1'-N1	6.44	113.35	108.20
27	B8	264	C	O4'-C1'-N1	6.44	113.35	108.20
27	B8	406	G	O4'-C1'-N9	6.44	113.35	108.20
27	B8	2130	U	O4'-C1'-N1	6.44	113.35	108.20
1	AA	459	A	C4-C5-C6	6.44	120.22	117.00
1	AA	865	A	O4'-C1'-N9	6.44	113.35	108.20
1	AA	1406	U	O4'-C1'-N1	6.44	113.35	108.20
27	B8	37	C	N3-C4-N4	6.43	122.50	118.00
27	B8	522	A	O4'-C1'-N9	6.43	113.35	108.20
27	B8	716	A	C4-C5-C6	6.43	120.22	117.00
27	B8	2546	U	O4'-C1'-N1	6.43	113.35	108.20
1	AA	536	C	O4'-C1'-N1	6.43	113.35	108.20
27	B8	330	A	C4-C5-C6	6.43	120.22	117.00
27	B8	1730	C	C2-N1-C1'	6.43	125.88	118.80
27	B8	2150	C	N3-C4-N4	6.43	122.50	118.00
27	B8	2269	G	C5-C6-O6	-6.43	124.74	128.60
1	AA	355	C	N3-C4-N4	6.43	122.50	118.00
27	B8	1170	C	N3-C4-N4	6.43	122.50	118.00
27	B8	1773	A	C5-C6-N6	-6.43	118.56	123.70
1	AA	371	A	C5-C6-N6	-6.43	118.56	123.70
1	AA	376	G	O4'-C1'-N9	6.43	113.34	108.20
1	AA	974	A	C4-C5-C6	6.43	120.22	117.00
1	AA	1324	A	O4'-C1'-N9	6.43	113.34	108.20
27	B8	975	A	O4'-C1'-N9	6.43	113.34	108.20
27	B8	1436	G	C5-C6-O6	-6.43	124.74	128.60
27	B8	1922	G	O4'-C1'-N9	6.43	113.34	108.20
27	B8	2035	G	C5-C6-O6	-6.43	124.74	128.60
27	B8	2309	A	C4-C5-C6	6.43	120.22	117.00
27	B8	2444	G	C5-C6-O6	-6.43	124.74	128.60
1	AA	1172	C	N3-C4-N4	6.43	122.50	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AV	46	G	C5-C6-O6	-6.43	124.74	128.60
1	AA	1	A	C4-C5-C6	6.43	120.21	117.00
1	AA	692	U	O4'-C1'-N1	6.43	113.34	108.20
27	B8	581	C	N3-C4-N4	6.43	122.50	118.00
27	B8	1565	C	O4'-C1'-N1	6.43	113.34	108.20
27	B8	1755	A	O4'-C1'-N9	6.43	113.34	108.20
27	B8	2793	C	O4'-C1'-N1	6.43	113.34	108.20
1	AA	695	A	C4-C5-C6	6.42	120.21	117.00
1	AA	1018	G	C5-C6-O6	-6.42	124.75	128.60
1	AA	1403	C	O4'-C1'-N1	6.42	113.34	108.20
27	B8	107	G	O4'-C1'-N9	6.42	113.34	108.20
27	B8	1275	A	C4-C5-C6	6.42	120.21	117.00
27	B8	2365	G	C5-C6-O6	-6.42	124.75	128.60
1	AA	581	G	O4'-C1'-N9	6.42	113.34	108.20
1	AA	389	A	C4-C5-C6	6.42	120.21	117.00
1	AA	581	G	C5-C6-O6	-6.42	124.75	128.60
27	B8	276	U	C2-N1-C1'	6.42	125.41	117.70
27	B8	1211	C	C2-N1-C1'	6.42	125.86	118.80
27	B8	1300	G	C5-C6-O6	-6.42	124.75	128.60
27	B8	1898	U	O4'-C1'-N1	6.42	113.34	108.20
1	AA	309	A	O4'-C1'-N9	6.42	113.34	108.20
3	AV	64	U	O4'-C1'-N1	6.42	113.34	108.20
27	B8	189	G	O4'-C1'-N9	6.42	113.34	108.20
27	B8	324	A	O4'-C1'-N9	6.42	113.34	108.20
27	B8	1717	A	C4-C5-C6	6.42	120.21	117.00
27	B8	2899	A	O4'-C1'-N9	6.42	113.34	108.20
1	AA	2	A	C4-C5-C6	6.42	120.21	117.00
1	AA	219	U	O4'-C1'-N1	6.42	113.33	108.20
1	AA	433	G	C5-C6-O6	-6.42	124.75	128.60
27	B8	105	C	N3-C4-N4	6.42	122.49	118.00
27	B8	685	A	C5-C6-N6	-6.42	118.56	123.70
27	B8	802	A	C4-C5-C6	6.42	120.21	117.00
27	B8	1787	A	C5-C6-N6	-6.42	118.56	123.70
1	AA	447	G	C5-C6-O6	-6.42	124.75	128.60
1	AA	448	A	O4'-C1'-N9	6.42	113.33	108.20
3	AV	22	A	C4-C5-C6	6.42	120.21	117.00
27	B8	300	A	C4-C5-C6	6.42	120.21	117.00
1	AA	1266	G	C5-C6-O6	-6.42	124.75	128.60
3	AV	56	U	O4'-C1'-N1	6.42	113.33	108.20
27	B8	28	A	C5-C6-N6	-6.42	118.57	123.70
27	B8	349	U	O4'-C1'-N1	6.42	113.33	108.20
27	B8	1086	A	C5-C6-N1	-6.42	114.49	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	38	G	O4'-C1'-N9	6.41	113.33	108.20
27	B8	1599	U	O4'-C1'-N1	6.41	113.33	108.20
27	B8	1770	G	C5-C6-O6	-6.41	124.75	128.60
27	B8	2265	U	O4'-C1'-N1	6.41	113.33	108.20
27	B8	2505	G	O4'-C1'-N9	6.41	113.33	108.20
1	AA	1179	A	C4-C5-C6	6.41	120.21	117.00
27	B8	10	A	C4-C5-C6	6.41	120.21	117.00
27	B8	1260	A	C5-C6-N6	-6.41	118.57	123.70
1	AA	192	A	C5-C6-N6	-6.41	118.57	123.70
27	B8	1916	A	O4'-C1'-N9	6.41	113.33	108.20
26	B7	2	G	O4'-C1'-N9	6.41	113.33	108.20
27	B8	755	U	O4'-C1'-N1	6.41	113.33	108.20
27	B8	899	A	C5-C6-N6	-6.41	118.57	123.70
27	B8	1000	A	C4-C5-C6	6.41	120.20	117.00
27	B8	2045	C	N3-C4-N4	6.41	122.49	118.00
27	B8	2791	G	C5-C6-O6	-6.41	124.75	128.60
3	AV	27	A	C4-C5-C6	6.41	120.20	117.00
27	B8	356	G	O4'-C1'-N9	6.41	113.33	108.20
27	B8	1476	U	O4'-C1'-N1	6.41	113.33	108.20
1	AA	1191	A	C4-C5-C6	6.41	120.20	117.00
27	B8	1639	C	N3-C4-N4	6.41	122.48	118.00
27	B8	1757	A	C4-C5-C6	6.41	120.20	117.00
27	B8	1259	G	O4'-C1'-N9	6.40	113.32	108.20
27	B8	1808	A	C4-C5-C6	6.40	120.20	117.00
27	B8	2170	A	C4-C5-C6	6.40	120.20	117.00
1	AA	21	G	C5-C6-O6	-6.40	124.76	128.60
1	AA	399	G	O4'-C1'-N9	6.40	113.32	108.20
27	B8	299	A	C4-C5-C6	6.40	120.20	117.00
27	B8	2284	A	C5-C6-N6	-6.40	118.58	123.70
1	AA	482	A	C5-C6-N6	-6.40	118.58	123.70
1	AA	1138	G	O4'-C1'-N9	6.40	113.32	108.20
1	AA	1268	G	C5-C6-O6	-6.40	124.76	128.60
26	B7	42	C	O4'-C1'-N1	6.40	113.32	108.20
27	B8	1642	G	O4'-C1'-N9	6.40	113.32	108.20
27	B8	1713	A	C5-C6-N6	-6.40	118.58	123.70
27	B8	1929	G	C5-C6-O6	-6.40	124.76	128.60
27	B8	2013	A	C4-C5-C6	6.40	120.20	117.00
27	B8	707	G	O4'-C1'-N9	6.40	113.32	108.20
27	B8	711	G	O4'-C1'-N9	6.40	113.32	108.20
27	B8	1874	C	N3-C4-N4	6.40	122.48	118.00
1	AA	228	A	C4-C5-C6	6.40	120.20	117.00
1	AA	421	U	C2-N1-C1'	6.40	125.38	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	556	C	N3-C4-N4	6.40	122.48	118.00
1	AA	893	C	N3-C4-N4	6.40	122.48	118.00
1	AA	1399	C	O4'-C1'-N1	6.40	113.32	108.20
3	AV	77	A	C4-C5-C6	6.40	120.20	117.00
27	B8	55	G	C5-C6-O6	-6.40	124.76	128.60
27	B8	1285	A	C4-C5-C6	6.40	120.20	117.00
27	B8	1787	A	C4-C5-C6	6.40	120.20	117.00
27	B8	2175	C	P-O3'-C3'	6.40	127.38	119.70
1	AA	608	A	O4'-C1'-N9	6.40	113.32	108.20
27	B8	1103	A	C4-C5-C6	6.40	120.20	117.00
1	AA	1011	C	O4'-C1'-N1	6.39	113.31	108.20
1	AA	1331	G	C5-C6-O6	-6.39	124.76	128.60
27	B8	28	A	O4'-C1'-N9	6.39	113.32	108.20
27	B8	317	G	C5-C6-O6	-6.39	124.76	128.60
27	B8	1027	A	C5-C6-N6	-6.39	118.58	123.70
27	B8	1132	U	O4'-C1'-N1	6.39	113.32	108.20
27	B8	1781	U	O4'-C1'-N1	6.39	113.31	108.20
27	B8	2655	G	C5-C6-O6	-6.39	124.76	128.60
1	AA	378	G	C5-C6-O6	-6.39	124.76	128.60
1	AA	1491	G	C5-C6-O6	-6.39	124.76	128.60
27	B8	1309	G	O4'-C1'-N9	6.39	113.31	108.20
27	B8	2446	G	C5-C6-O6	-6.39	124.76	128.60
27	B8	1953	A	C4-C5-C6	6.39	120.19	117.00
27	B8	2793	C	N3-C4-N4	6.39	122.47	118.00
1	AA	52	C	N3-C4-N4	6.39	122.47	118.00
1	AA	343	U	O4'-C1'-N1	6.39	113.31	108.20
1	AA	990	C	O4'-C1'-N1	6.39	113.31	108.20
26	B7	112	G	O4'-C1'-N9	6.39	113.31	108.20
27	B8	418	C	N3-C4-N4	6.39	122.47	118.00
27	B8	449	A	C4-C5-C6	6.39	120.19	117.00
27	B8	748	G	C5-C6-O6	-6.39	124.77	128.60
27	B8	1346	G	O4'-C1'-N9	6.39	113.31	108.20
27	B8	2800	A	O4'-C1'-N9	6.39	113.31	108.20
1	AA	1507	A	C4-C5-C6	6.39	120.19	117.00
1	AA	1493	A	C4-C5-C6	6.39	120.19	117.00
27	B8	1341	G	C5-C6-O6	-6.39	124.77	128.60
27	B8	1980	G	C5-C6-O6	-6.39	124.77	128.60
1	AA	147	G	O4'-C1'-N9	6.38	113.31	108.20
27	B8	595	C	N3-C4-N4	6.38	122.47	118.00
27	B8	1712	U	O4'-C1'-N1	6.38	113.31	108.20
27	B8	2901	C	N3-C4-N4	6.38	122.47	118.00
1	AA	202	G	C5-C6-O6	-6.38	124.77	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	629	A	C4-C5-C6	6.38	120.19	117.00
1	AA	1499	A	C4-C5-C6	6.38	120.19	117.00
27	B8	2776	A	C4-C5-C6	6.38	120.19	117.00
1	AA	109	A	C4-C5-C6	6.38	120.19	117.00
1	AA	495	A	C5-C6-N1	-6.38	114.51	117.70
1	AA	1423	G	O4'-C1'-N9	6.38	113.31	108.20
27	B8	64	A	C5-C6-N1	-6.38	114.51	117.70
27	B8	655	A	O4'-C1'-N9	6.38	113.31	108.20
27	B8	1122	G	C5-C6-O6	-6.38	124.77	128.60
27	B8	1359	A	O4'-C1'-N9	6.38	113.31	108.20
27	B8	2062	A	C4-C5-C6	6.38	120.19	117.00
27	B8	2258	C	O4'-C1'-N1	6.38	113.31	108.20
27	B8	2686	G	O4'-C1'-N9	6.38	113.31	108.20
1	AA	987	G	O4'-C1'-N9	6.38	113.30	108.20
1	AA	1110	A	C4-C5-C6	6.38	120.19	117.00
27	B8	260	G	O4'-C1'-N9	6.38	113.30	108.20
1	AA	1112	C	O4'-C1'-N1	6.38	113.30	108.20
3	AV	30	G	O4'-C1'-N9	6.38	113.30	108.20
1	AA	77	A	C5-C6-N6	-6.38	118.60	123.70
1	AA	270	A	C5-C6-N6	-6.38	118.60	123.70
27	B8	219	A	C4-C5-C6	6.38	120.19	117.00
27	B8	329	G	C5-C6-O6	-6.38	124.77	128.60
27	B8	2602	A	C4-C5-C6	6.38	120.19	117.00
27	B8	2606	C	N3-C4-N4	6.38	122.46	118.00
27	B8	2900	A	C5-C6-N6	-6.38	118.60	123.70
1	AA	28	A	O4'-C1'-N9	6.38	113.30	108.20
27	B8	2406	A	C4-C5-C6	6.38	120.19	117.00
1	AA	53	A	O4'-C1'-N9	6.37	113.30	108.20
1	AA	776	G	O4'-C1'-N9	6.37	113.30	108.20
1	AA	1095	U	O4'-C1'-N1	6.37	113.30	108.20
27	B8	243	U	O4'-C1'-N1	6.37	113.30	108.20
27	B8	1664	A	C5-C6-N6	-6.37	118.60	123.70
27	B8	2632	A	C5-C6-N6	-6.37	118.60	123.70
1	AA	176	C	N3-C4-N4	6.37	122.46	118.00
1	AA	742	G	C5-C6-O6	-6.37	124.78	128.60
27	B8	571	U	O4'-C1'-N1	6.37	113.30	108.20
27	B8	1921	G	O4'-C1'-N9	6.37	113.30	108.20
27	B8	2297	A	C5-C6-N1	-6.37	114.51	117.70
41	BM	43	ALA	N-CA-CB	6.37	119.02	110.10
1	AA	386	C	O4'-C1'-N1	6.37	113.30	108.20
1	AA	455	G	O4'-C1'-N9	6.37	113.30	108.20
1	AA	941	G	O4'-C1'-N9	6.37	113.29	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1244	G	O4'-C1'-N9	6.37	113.30	108.20
1	AA	1534	A	C4-C5-C6	6.37	120.18	117.00
27	B8	13	A	C5-C6-N6	-6.37	118.61	123.70
27	B8	2442	C	N3-C4-N4	6.37	122.46	118.00
27	B8	2451	A	O4'-C1'-N9	6.37	113.30	108.20
27	B8	2113	U	O4'-C1'-N1	6.37	113.29	108.20
26	B7	101	A	C5-C6-N6	-6.37	118.61	123.70
27	B8	1098	A	C4-C5-C6	6.37	120.18	117.00
27	B8	1692	U	O4'-C1'-N1	6.37	113.29	108.20
27	B8	1745	A	C4-C5-C6	6.37	120.18	117.00
27	B8	2079	U	O4'-C1'-N1	6.37	113.29	108.20
1	AA	1496	C	N3-C4-N4	6.36	122.45	118.00
27	B8	420	C	N3-C4-N4	6.36	122.45	118.00
27	B8	1861	G	O4'-C1'-N9	6.36	113.29	108.20
27	B8	1880	U	O4'-C1'-N1	6.36	113.29	108.20
27	B8	2434	A	C4-C5-C6	6.36	120.18	117.00
27	B8	881	G	C5-C6-O6	-6.36	124.78	128.60
27	B8	1823	G	C5-C6-O6	-6.36	124.78	128.60
27	B8	2030	A	C4-C5-C6	6.36	120.18	117.00
27	B8	2358	A	C4-C5-C6	6.36	120.18	117.00
1	AA	1105	A	O4'-C1'-N9	6.36	113.29	108.20
1	AA	1480	A	O4'-C1'-N9	6.36	113.29	108.20
27	B8	284	U	O4'-C1'-N1	6.36	113.29	108.20
27	B8	403	U	O4'-C1'-N1	6.36	113.29	108.20
27	B8	1061	U	C6-N1-C1'	-6.36	112.30	121.20
27	B8	1317	G	O4'-C1'-N9	6.36	113.29	108.20
27	B8	1689	A	C4-C5-C6	6.36	120.18	117.00
1	AA	312	C	N3-C4-N4	6.36	122.45	118.00
1	AA	1332	A	O4'-C1'-N9	6.36	113.29	108.20
1	AA	1338	G	C5-C6-O6	-6.36	124.78	128.60
1	AA	1456	A	C4-C5-C6	6.36	120.18	117.00
26	B7	39	A	C5-C6-N6	-6.36	118.61	123.70
27	B8	16	C	N3-C4-N4	6.36	122.45	118.00
27	B8	45	G	O4'-C1'-N9	6.36	113.29	108.20
27	B8	428	A	C4-C5-C6	6.36	120.18	117.00
27	B8	547	A	C4-C5-C6	6.36	120.18	117.00
27	B8	2732	G	O4'-C1'-N9	6.36	113.29	108.20
1	AA	1072	G	O4'-C1'-N9	6.36	113.28	108.20
3	AV	12	G	C5-C6-O6	-6.36	124.79	128.60
27	B8	1347	A	C5-C6-N1	-6.36	114.52	117.70
27	B8	2076	U	C2-N1-C1'	6.36	125.33	117.70
1	AA	1074	G	C5-C6-O6	-6.35	124.79	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1207	C	N3-C4-N4	6.35	122.45	118.00
27	B8	2850	A	C4-C5-C6	6.35	120.18	117.00
1	AA	595	A	C4-C5-C6	6.35	120.18	117.00
1	AA	777	A	C4-C5-C6	6.35	120.18	117.00
1	AA	989	U	O4'-C1'-N1	6.35	113.28	108.20
27	B8	255	A	C4-C5-C6	6.35	120.18	117.00
27	B8	390	U	O4'-C1'-N1	6.35	113.28	108.20
27	B8	999	U	O4'-C1'-N1	6.35	113.28	108.20
27	B8	2517	C	N3-C4-N4	6.35	122.45	118.00
1	AA	517	G	C5-C6-O6	-6.35	124.79	128.60
27	B8	101	A	C4-C5-C6	6.35	120.18	117.00
27	B8	1187	G	C5-C6-O6	-6.35	124.79	128.60
27	B8	1203	U	O4'-C1'-N1	6.35	113.28	108.20
1	AA	676	A	C5-C6-N1	-6.35	114.53	117.70
1	AA	866	C	N3-C4-N4	6.35	122.44	118.00
1	AA	1206	G	O4'-C1'-N9	6.35	113.28	108.20
27	B8	575	A	C5-C6-N1	-6.35	114.53	117.70
27	B8	607	U	O4'-C1'-N1	6.35	113.28	108.20
27	B8	863	A	C4-C5-C6	6.35	120.17	117.00
27	B8	1163	G	O4'-C1'-N9	6.35	113.28	108.20
27	B8	2006	C	N3-C4-N4	6.35	122.44	118.00
1	AA	128	G	O4'-C1'-N9	6.35	113.28	108.20
1	AA	318	G	O4'-C1'-N9	6.35	113.28	108.20
1	AA	367	U	O4'-C1'-N1	6.35	113.28	108.20
27	B8	217	A	C4-C5-C6	6.35	120.17	117.00
27	B8	242	G	C5-C6-O6	-6.35	124.79	128.60
27	B8	2173	A	C4-C5-C6	6.35	120.17	117.00
1	AA	146	G	O4'-C1'-N9	6.35	113.28	108.20
1	AA	1219	A	C5-C6-N6	-6.35	118.62	123.70
27	B8	417	C	N3-C4-N4	6.35	122.44	118.00
27	B8	752	A	O4'-C1'-N9	6.35	113.28	108.20
27	B8	1288	G	C5-C6-O6	-6.35	124.79	128.60
27	B8	2261	C	N3-C4-N4	6.35	122.44	118.00
27	B8	2425	A	C4-C5-C6	6.35	120.17	117.00
1	AA	155	A	O4'-C1'-N9	6.34	113.28	108.20
1	AA	162	A	C5-C6-N1	-6.34	114.53	117.70
1	AA	1475	G	C5-C6-O6	-6.34	124.79	128.60
27	B8	227	A	C4-C5-C6	6.34	120.17	117.00
27	B8	1669	A	C5-C6-N1	-6.34	114.53	117.70
27	B8	1802	A	C5-C6-N1	-6.34	114.53	117.70
27	B8	268	C	O4'-C1'-N1	6.34	113.27	108.20
27	B8	1197	G	C5-C6-O6	-6.34	124.79	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1754	A	C4-C5-C6	6.34	120.17	117.00
27	B8	2127	G	O4'-C1'-N9	6.34	113.27	108.20
32	BD	31	ALA	N-CA-CB	6.34	118.98	110.10
1	AA	1530	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	635	C	N3-C4-N4	6.34	122.44	118.00
27	B8	938	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	1368	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	1886	U	O4'-C1'-N1	6.34	113.27	108.20
27	B8	1962	C	N3-C4-N4	6.34	122.44	118.00
27	B8	492	A	C4-C5-C6	6.34	120.17	117.00
27	B8	1465	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	1548	A	O4'-C1'-N9	6.34	113.27	108.20
27	B8	2015	A	O4'-C1'-N9	6.34	113.27	108.20
27	B8	2072	C	N3-C4-N4	6.34	122.44	118.00
27	B8	857	G	C5-C6-O6	-6.34	124.80	128.60
27	B8	1573	G	C5-C6-O6	-6.34	124.80	128.60
27	B8	2262	U	O4'-C1'-N1	6.34	113.27	108.20
1	AA	47	C	N3-C4-N4	6.34	122.44	118.00
1	AA	74	A	O4'-C1'-N9	6.34	113.27	108.20
1	AA	1180	A	C4-C5-C6	6.34	120.17	117.00
1	AA	1199	U	O4'-C1'-N1	6.34	113.27	108.20
27	B8	142	A	O4'-C1'-N9	6.34	113.27	108.20
27	B8	186	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	728	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	1498	C	N3-C4-N4	6.34	122.44	118.00
27	B8	1860	G	O4'-C1'-N9	6.34	113.27	108.20
27	B8	1918	A	C5-C6-N6	-6.34	118.63	123.70
27	B8	1996	C	N3-C4-N4	6.33	122.43	118.00
27	B8	2575	C	N3-C4-N4	6.33	122.43	118.00
3	AV	71	C	N3-C4-N4	6.33	122.43	118.00
27	B8	1613	G	C5-C6-O6	-6.33	124.80	128.60
27	B8	2352	A	C5-C6-N1	-6.33	114.53	117.70
1	AA	408	A	C4-C5-C6	6.33	120.17	117.00
1	AA	1030	U	C2-N1-C1'	6.33	125.30	117.70
27	B8	138	U	O4'-C1'-N1	6.33	113.27	108.20
27	B8	237	C	N3-C4-N4	6.33	122.43	118.00
27	B8	2165	C	O4'-C1'-N1	6.33	113.27	108.20
27	B8	2168	G	O4'-C1'-N9	6.33	113.27	108.20
27	B8	2322	A	C4-C5-C6	6.33	120.17	117.00
27	B8	91	A	C4-C5-C6	6.33	120.17	117.00
27	B8	529	A	C4-C5-C6	6.33	120.17	117.00
27	B8	1780	A	O4'-C1'-N9	6.33	113.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2666	C	C6-N1-C1'	-6.33	113.20	120.80
1	AA	869	G	C5-C6-O6	-6.33	124.80	128.60
27	B8	54	G	O4'-C1'-N9	6.33	113.26	108.20
27	B8	185	G	O4'-C1'-N9	6.33	113.26	108.20
27	B8	216	A	O4'-C1'-N9	6.33	113.26	108.20
27	B8	1557	C	O4'-C1'-N1	6.33	113.26	108.20
27	B8	1724	G	O4'-C1'-N9	6.33	113.26	108.20
27	B8	2787	C	N3-C4-N4	6.33	122.43	118.00
1	AA	284	C	N3-C4-N4	6.33	122.43	118.00
1	AA	586	C	N3-C4-N4	6.33	122.43	118.00
1	AA	727	G	C5-C6-O6	-6.33	124.80	128.60
1	AA	1189	U	O4'-C1'-N1	6.33	113.26	108.20
27	B8	699	A	C4-C5-C6	6.33	120.16	117.00
1	AA	461	A	C4-C5-C6	6.33	120.16	117.00
1	AA	814	A	C4-C5-C6	6.33	120.16	117.00
1	AA	1360	A	C5-C6-N6	-6.33	118.64	123.70
26	B7	75	G	O4'-C1'-N9	6.33	113.26	108.20
27	B8	619	G	O4'-C1'-N9	6.33	113.26	108.20
1	AA	204	G	O4'-C1'-N9	6.32	113.26	108.20
27	B8	87	U	O4'-C1'-N1	6.32	113.26	108.20
27	B8	909	A	O4'-C1'-N9	6.32	113.26	108.20
27	B8	1264	A	C5-C6-N6	-6.32	118.64	123.70
27	B8	2065	C	N3-C4-N4	6.32	122.43	118.00
1	AA	830	G	O4'-C1'-N9	6.32	113.26	108.20
27	B8	750	A	C4-C5-C6	6.32	120.16	117.00
27	B8	644	A	C4-C5-C6	6.32	120.16	117.00
1	AA	70	U	O4'-C1'-N1	6.32	113.25	108.20
27	B8	577	G	O4'-C1'-N9	6.32	113.25	108.20
1	AA	738	C	N3-C4-N4	6.32	122.42	118.00
1	AA	1513	A	C5-C6-N6	-6.32	118.65	123.70
27	B8	732	C	N3-C4-N4	6.32	122.42	118.00
27	B8	1496	A	C5-C6-N6	-6.32	118.65	123.70
27	B8	2101	A	O4'-C1'-N9	6.32	113.25	108.20
27	B8	2134	A	C4-C5-C6	6.32	120.16	117.00
1	AA	892	A	O4'-C1'-N9	6.32	113.25	108.20
1	AA	1501	C	O4'-C1'-N1	6.32	113.25	108.20
27	B8	479	A	C4-C5-C6	6.32	120.16	117.00
27	B8	1509	A	C4-C5-C6	6.32	120.16	117.00
27	B8	1738	G	C5-C6-O6	-6.32	124.81	128.60
27	B8	2733	A	C4-C5-C6	6.31	120.16	117.00
1	AA	177	G	N1-C6-O6	6.31	123.69	119.90
1	AA	803	G	O4'-C1'-N9	6.31	113.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1119	C	N3-C4-N4	6.31	122.42	118.00
1	AA	1489	G	O4'-C1'-N9	6.31	113.25	108.20
27	B8	726	G	C5-C6-O6	-6.31	124.81	128.60
27	B8	1227	G	C5-C6-O6	-6.31	124.81	128.60
27	B8	1345	C	N3-C4-N4	6.31	122.42	118.00
27	B8	2033	A	O4'-C1'-N9	6.31	113.25	108.20
27	B8	656	G	O4'-C1'-N9	6.31	113.25	108.20
27	B8	1635	A	C4-C5-C6	6.31	120.16	117.00
27	B8	2215	C	N3-C4-N4	6.31	122.42	118.00
27	B8	2709	G	O4'-C1'-N9	6.31	113.25	108.20
1	AA	573	A	C4-C5-C6	6.31	120.16	117.00
1	AA	614	C	N3-C4-N4	6.31	122.42	118.00
1	AA	1455	G	O4'-C1'-N9	6.31	113.25	108.20
1	AA	1498	U	O4'-C1'-N1	6.31	113.25	108.20
3	AV	34	U	O4'-C1'-N1	6.31	113.25	108.20
27	B8	881	G	O4'-C1'-N9	6.31	113.25	108.20
27	B8	1737	G	C5-C6-O6	-6.31	124.81	128.60
1	AA	245	U	O4'-C1'-N1	6.31	113.25	108.20
27	B8	684	G	C5-C6-O6	-6.31	124.81	128.60
27	B8	797	G	O4'-C1'-N9	6.31	113.25	108.20
26	B7	53	A	O4'-C1'-N9	6.31	113.25	108.20
27	B8	1269	A	C4-C5-C6	6.31	120.15	117.00
1	AA	101	A	C4-C5-C6	6.30	120.15	117.00
1	AA	247	G	O4'-C1'-N9	6.30	113.24	108.20
1	AA	868	C	N3-C4-N4	6.30	122.41	118.00
27	B8	294	A	C5-C6-N6	-6.30	118.66	123.70
27	B8	2331	G	C5-C6-O6	-6.30	124.82	128.60
27	B8	2788	C	N3-C4-N4	6.30	122.41	118.00
1	AA	468	A	C5-C6-N1	-6.30	114.55	117.70
26	B7	94	A	O4'-C1'-N9	6.30	113.24	108.20
27	B8	109	C	N3-C4-N4	6.30	122.41	118.00
27	B8	2154	A	C5-C6-N6	-6.30	118.66	123.70
27	B8	2899	A	C4-C5-C6	6.30	120.15	117.00
1	AA	739	C	N3-C4-N4	6.30	122.41	118.00
1	AA	859	G	O4'-C1'-N9	6.30	113.24	108.20
1	AA	895	G	C5-C6-O6	-6.30	124.82	128.60
1	AA	1291	U	O4'-C1'-N1	6.30	113.24	108.20
3	AV	74	A	O4'-C1'-N9	6.30	113.24	108.20
27	B8	2089	C	N3-C4-N4	6.30	122.41	118.00
27	B8	2551	C	N3-C4-N4	6.30	122.41	118.00
27	B8	2667	C	N3-C4-N4	6.30	122.41	118.00
27	B8	2682	A	C4-C5-C6	6.30	120.15	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2904	U	O4'-C1'-N1	6.30	113.24	108.20
1	AA	1345	U	O4'-C1'-N1	6.30	113.24	108.20
27	B8	1041	G	O4'-C1'-N9	6.30	113.24	108.20
27	B8	2675	A	C5-C6-N1	-6.30	114.55	117.70
1	AA	205	A	C4-C5-C6	6.30	120.15	117.00
27	B8	132	G	O4'-C1'-N9	6.30	113.24	108.20
1	AA	1447	A	C5-C6-N1	-6.30	114.55	117.70
27	B8	111	A	C4-C5-C6	6.30	120.15	117.00
27	B8	535	G	O4'-C1'-N9	6.30	113.24	108.20
27	B8	1287	A	O4'-C1'-N9	6.30	113.24	108.20
27	B8	1972	G	C5-C6-O6	-6.30	124.82	128.60
1	AA	106	C	N3-C4-N4	6.29	122.41	118.00
1	AA	675	A	C4-C5-C6	6.29	120.15	117.00
27	B8	936	A	C4-C5-C6	6.29	120.15	117.00
27	B8	2151	U	O4'-C1'-N1	6.29	113.24	108.20
27	B8	2591	C	N3-C4-N4	6.29	122.41	118.00
1	AA	81	A	C4-C5-C6	6.29	120.15	117.00
1	AA	432	A	C4-C5-C6	6.29	120.15	117.00
1	AA	937	A	C4-C5-C6	6.29	120.15	117.00
27	B8	1469	A	O4'-C1'-N9	6.29	113.23	108.20
27	B8	2216	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	397	A	C4-C5-C6	6.29	120.15	117.00
1	AA	509	A	C4-C5-C6	6.29	120.15	117.00
1	AA	932	C	N3-C4-N4	6.29	122.40	118.00
26	B7	8	C	N3-C4-N4	6.29	122.40	118.00
27	B8	711	G	C5-C6-O6	-6.29	124.83	128.60
27	B8	1847	A	C4-C5-C6	6.29	120.15	117.00
1	AA	299	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	320	A	C5-C6-N6	-6.29	118.67	123.70
1	AA	1437	A	C5-C6-N6	-6.29	118.67	123.70
27	B8	1698	A	C4-C5-C6	6.29	120.14	117.00
27	B8	2430	A	C5-C6-N6	-6.29	118.67	123.70
1	AA	1000	A	C5-C6-N6	-6.29	118.67	123.70
1	AA	1028	C	N3-C4-N4	6.29	122.40	118.00
3	AV	76	C	N3-C4-N4	6.29	122.40	118.00
27	B8	298	G	N3-C2-N2	6.29	124.30	119.90
27	B8	438	G	O4'-C1'-N9	6.29	113.23	108.20
27	B8	641	U	O4'-C1'-N1	6.29	113.23	108.20
27	B8	1117	C	N3-C4-N4	6.29	122.40	118.00
27	B8	1214	A	O4'-C1'-N9	6.29	113.23	108.20
27	B8	1279	G	O4'-C1'-N9	6.29	113.23	108.20
27	B8	2042	A	C4-C5-C6	6.29	120.14	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2353	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	645	G	O4'-C1'-N9	6.29	113.23	108.20
27	B8	2218	G	O4'-C1'-N9	6.29	113.23	108.20
27	B8	2266	A	C4-C5-C6	6.29	120.14	117.00
1	AA	199	A	C5-C6-N6	-6.29	118.67	123.70
1	AA	255	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	765	G	C5-C6-O6	-6.29	124.83	128.60
1	AA	886	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	934	C	N3-C4-C5	-6.29	119.39	121.90
1	AA	1397	C	N3-C4-N4	6.29	122.40	118.00
27	B8	25	U	O4'-C1'-N1	6.29	113.23	108.20
27	B8	484	C	N3-C4-N4	6.29	122.40	118.00
27	B8	675	A	C4-C5-C6	6.29	120.14	117.00
27	B8	681	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	161	A	C4-C5-C6	6.28	120.14	117.00
1	AA	1102	A	C4-C5-C6	6.28	120.14	117.00
1	AA	1488	G	O4'-C1'-N9	6.28	113.23	108.20
27	B8	886	A	C4-C5-C6	6.28	120.14	117.00
27	B8	982	C	O4'-C1'-N1	6.28	113.23	108.20
27	B8	1244	A	O4'-C1'-N9	6.28	113.23	108.20
27	B8	1593	A	C4-C5-C6	6.28	120.14	117.00
27	B8	2050	C	O4'-C1'-N1	6.28	113.23	108.20
27	B8	2827	C	N3-C4-N4	6.28	122.40	118.00
27	B8	125	A	C4-C5-C6	6.28	120.14	117.00
27	B8	1928	A	C4-C5-C6	6.28	120.14	117.00
27	B8	2205	A	O4'-C1'-N9	6.28	113.23	108.20
27	B8	2738	A	C5-C6-N1	-6.28	114.56	117.70
27	B8	379	G	O4'-C1'-N9	6.28	113.22	108.20
27	B8	482	A	C4-C5-C6	6.28	120.14	117.00
27	B8	505	A	C4-C5-C6	6.28	120.14	117.00
27	B8	572	A	C4-C5-C6	6.28	120.14	117.00
27	B8	1104	C	N3-C4-C5	-6.28	119.39	121.90
27	B8	2407	A	C4-C5-C6	6.28	120.14	117.00
27	B8	2612	C	N3-C4-N4	6.28	122.40	118.00
27	B8	2008	C	N3-C4-N4	6.28	122.39	118.00
1	AA	214	C	N3-C4-N4	6.28	122.39	118.00
1	AA	1398	A	C4-C5-C6	6.28	120.14	117.00
27	B8	1695	G	C5-C6-O6	-6.28	124.83	128.60
27	B8	2351	G	N3-C2-N2	6.28	124.30	119.90
27	B8	2745	C	N3-C4-N4	6.28	122.39	118.00
27	B8	2748	A	O4'-C1'-N9	6.28	113.22	108.20
1	AA	1415	G	O4'-C1'-N9	6.28	113.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	6	A	C4-C5-C6	6.28	120.14	117.00
27	B8	188	G	O4'-C1'-N9	6.28	113.22	108.20
27	B8	251	A	C5-C6-N1	-6.28	114.56	117.70
27	B8	1246	A	O4'-C1'-N9	6.28	113.22	108.20
27	B8	1579	A	C5-C6-N6	-6.28	118.68	123.70
27	B8	1596	A	O4'-C1'-N9	6.28	113.22	108.20
27	B8	1668	A	C4-C5-C6	6.28	120.14	117.00
27	B8	1864	U	O4'-C1'-N1	6.28	113.22	108.20
3	AV	68	G	O4'-C1'-N9	6.27	113.22	108.20
26	B7	50	A	O4'-C1'-N9	6.27	113.22	108.20
27	B8	1124	G	O4'-C1'-N9	6.27	113.22	108.20
27	B8	1353	A	O4'-C1'-N9	6.27	113.22	108.20
27	B8	1813	G	O4'-C1'-N9	6.27	113.22	108.20
27	B8	1988	G	O4'-C1'-N9	6.27	113.22	108.20
27	B8	2745	C	O4'-C1'-N1	6.27	113.22	108.20
1	AA	179	A	C4-C5-C6	6.27	120.14	117.00
1	AA	670	G	O4'-C1'-N9	6.27	113.22	108.20
1	AA	1525	G	C5-C6-O6	-6.27	124.84	128.60
2	AX	22	A	C4-C5-C6	6.27	120.14	117.00
27	B8	671	C	N3-C4-N4	6.27	122.39	118.00
27	B8	2518	A	C5-C6-N6	-6.27	118.68	123.70
27	B8	2558	C	N3-C4-N4	6.27	122.39	118.00
1	AA	334	C	N3-C4-N4	6.27	122.39	118.00
1	AA	990	C	N3-C4-N4	6.27	122.39	118.00
1	AA	1066	C	N3-C4-N4	6.27	122.39	118.00
27	B8	136	G	O4'-C1'-N9	6.27	113.22	108.20
27	B8	707	G	C5-C6-O6	-6.27	124.84	128.60
1	AA	40	C	N3-C4-N4	6.27	122.39	118.00
1	AA	958	A	C4-C5-C6	6.27	120.14	117.00
1	AA	1361	G	C5-C6-O6	-6.27	124.84	128.60
27	B8	892	A	C4-C5-C6	6.27	120.14	117.00
27	B8	1582	C	N3-C4-N4	6.27	122.39	118.00
27	B8	2335	A	O4'-C1'-N9	6.27	113.22	108.20
27	B8	2391	G	C5-C6-O6	-6.27	124.84	128.60
27	B8	2855	C	N3-C4-N4	6.27	122.39	118.00
1	AA	1145	A	C5-C6-N1	-6.27	114.57	117.70
27	B8	1127	A	C5-C6-N6	-6.27	118.69	123.70
27	B8	1673	G	C5-C6-O6	-6.27	124.84	128.60
27	B8	2715	C	N3-C4-N4	6.27	122.39	118.00
1	AA	357	G	C5-C6-O6	-6.27	124.84	128.60
27	B8	1085	A	C5-C6-N6	-6.27	118.69	123.70
27	B8	1433	A	O4'-C1'-N9	6.27	113.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2579	C	N3-C4-N4	6.27	122.39	118.00
1	AA	130	A	C4-C5-C6	6.26	120.13	117.00
1	AA	1357	A	C4-C5-C6	6.26	120.13	117.00
26	B7	20	G	O4'-C1'-N9	6.26	113.21	108.20
27	B8	583	G	O4'-C1'-N9	6.26	113.21	108.20
27	B8	861	A	C5-C6-N6	-6.26	118.69	123.70
27	B8	1927	A	C5-C6-N1	-6.26	114.57	117.70
27	B8	1969	A	C4-C5-C6	6.26	120.13	117.00
27	B8	2274	A	C5-C6-N6	-6.26	118.69	123.70
27	B8	2516	A	O4'-C1'-N9	6.26	113.21	108.20
1	AA	313	A	O4'-C1'-N9	6.26	113.21	108.20
1	AA	1422	G	O4'-C1'-N9	6.26	113.21	108.20
27	B8	1705	A	C5-C6-N6	-6.26	118.69	123.70
1	AA	266	G	C5-C6-O6	-6.26	124.84	128.60
1	AA	838	G	O4'-C1'-N9	6.26	113.21	108.20
1	AA	962	C	N3-C4-N4	6.26	122.38	118.00
1	AA	1363	A	C4-C5-C6	6.26	120.13	117.00
27	B8	651	G	O4'-C1'-N9	6.26	113.21	108.20
27	B8	1957	C	N3-C4-N4	6.26	122.38	118.00
27	B8	2771	C	N3-C4-N4	6.26	122.38	118.00
1	AA	576	C	O4'-C1'-N1	6.26	113.21	108.20
27	B8	38	A	C4-C5-C6	6.26	120.13	117.00
27	B8	177	G	C5-C6-O6	-6.26	124.84	128.60
27	B8	2736	A	C4-C5-C6	6.26	120.13	117.00
1	AA	300	A	C5-C6-N6	-6.26	118.69	123.70
27	B8	1434	A	C5-C6-N6	-6.26	118.69	123.70
27	B8	2513	A	C5-C6-N1	-6.26	114.57	117.70
1	AA	338	A	C4-C5-C6	6.26	120.13	117.00
1	AA	746	A	C4-C5-C6	6.26	120.13	117.00
1	AA	1014	A	C4-C5-C6	6.26	120.13	117.00
1	AA	1420	U	O4'-C1'-N1	6.26	113.20	108.20
26	B7	115	A	C5-C6-N6	-6.26	118.69	123.70
27	B8	1143	A	C5-C6-N6	-6.26	118.69	123.70
27	B8	2253	G	O4'-C1'-N9	6.26	113.20	108.20
27	B8	2274	A	C4-C5-C6	6.26	120.13	117.00
1	AA	1129	C	N3-C4-N4	6.25	122.38	118.00
27	B8	2631	G	O4'-C1'-N9	6.25	113.20	108.20
27	B8	2778	A	C4-C5-C6	6.25	120.13	117.00
1	AA	758	C	N3-C4-N4	6.25	122.38	118.00
27	B8	1187	G	O4'-C1'-N9	6.25	113.20	108.20
27	B8	1228	G	O4'-C1'-N9	6.25	113.20	108.20
1	AA	23	C	N3-C4-N4	6.25	122.38	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	98	A	C4-C5-C6	6.25	120.13	117.00
27	B8	1088	A	C4-C5-C6	6.25	120.13	117.00
27	B8	1901	A	C4-C5-C6	6.25	120.13	117.00
27	B8	2222	C	N3-C4-N4	6.25	122.38	118.00
27	B8	2843	G	O4'-C1'-N9	6.25	113.20	108.20
27	B8	1900	A	C5-C6-N1	-6.25	114.58	117.70
1	AA	988	G	O4'-C1'-N9	6.25	113.20	108.20
1	AA	1038	C	N3-C4-N4	6.25	122.38	118.00
26	B7	27	C	N3-C4-N4	6.25	122.37	118.00
27	B8	182	A	C4-C5-C6	6.25	120.12	117.00
27	B8	246	C	N3-C4-N4	6.25	122.37	118.00
27	B8	966	G	O4'-C1'-N9	6.25	113.20	108.20
27	B8	1867	G	O4'-C1'-N9	6.25	113.20	108.20
27	B8	2043	C	N3-C4-N4	6.25	122.37	118.00
28	BA	314	GLN	CB-CA-C	6.25	122.89	110.40
1	AA	51	A	C4-C5-C6	6.25	120.12	117.00
1	AA	848	C	N3-C4-N4	6.25	122.37	118.00
1	AA	1269	A	C5-C6-N6	-6.25	118.70	123.70
27	B8	1367	A	O4'-C1'-N9	6.25	113.20	108.20
27	B8	2316	G	O4'-C1'-N9	6.25	113.20	108.20
28	BA	401	PHE	N-CA-CB	6.25	121.84	110.60
1	AA	1022	A	C5-C6-N1	-6.25	114.58	117.70
27	B8	33	C	N3-C4-N4	6.25	122.37	118.00
27	B8	2105	U	O4'-C1'-N1	6.25	113.20	108.20
27	B8	2439	A	C4-C5-C6	6.25	120.12	117.00
1	AA	9	G	O4'-C1'-N9	6.24	113.19	108.20
1	AA	607	A	C4-C5-C6	6.24	120.12	117.00
1	AA	858	G	C5-C6-O6	-6.24	124.85	128.60
1	AA	1053	G	C5-C6-O6	-6.24	124.85	128.60
26	B7	84	G	O4'-C1'-N9	6.24	113.19	108.20
27	B8	378	C	N3-C4-N4	6.24	122.37	118.00
27	B8	402	A	O4'-C1'-N9	6.24	113.19	108.20
27	B8	509	C	N3-C4-C5	-6.24	119.40	121.90
27	B8	1482	G	O4'-C1'-N9	6.24	113.19	108.20
27	B8	2613	U	O4'-C1'-N1	6.24	113.19	108.20
27	B8	2646	C	N3-C4-N4	6.24	122.37	118.00
1	AA	864	A	C4-C5-C6	6.24	120.12	117.00
27	B8	1557	C	N3-C4-N4	6.24	122.37	118.00
27	B8	1871	A	C4-C5-C6	6.24	120.12	117.00
1	AA	1445	U	O4'-C1'-N1	6.24	113.19	108.20
27	B8	42	A	O4'-C1'-N9	6.24	113.19	108.20
27	B8	670	A	C4-C5-C6	6.24	120.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	759	G	O4'-C1'-N9	6.24	113.19	108.20
27	B8	1240	U	O4'-C1'-N1	6.24	113.19	108.20
27	B8	1620	G	O4'-C1'-N9	6.24	113.19	108.20
27	B8	1659	G	O4'-C1'-N9	6.24	113.19	108.20
1	AA	1048	G	O4'-C1'-N9	6.24	113.19	108.20
1	AA	1231	G	C5-C6-O6	-6.24	124.86	128.60
27	B8	984	A	C4-C5-C6	6.24	120.12	117.00
27	B8	1510	G	O4'-C1'-N9	6.24	113.19	108.20
27	B8	1687	G	C5-C6-O6	-6.24	124.86	128.60
27	B8	2726	A	C4-C5-C6	6.24	120.12	117.00
1	AA	624	C	N3-C4-N4	6.24	122.37	118.00
1	AA	675	A	O4'-C1'-N9	6.24	113.19	108.20
1	AA	845	A	C4-C5-C6	6.24	120.12	117.00
27	B8	195	A	C5-C6-N6	-6.24	118.71	123.70
27	B8	986	C	N3-C4-N4	6.24	122.37	118.00
27	B8	1638	C	N3-C4-N4	6.24	122.37	118.00
27	B8	1885	A	C4-C5-C6	6.24	120.12	117.00
27	B8	2719	G	C5-C6-O6	-6.24	124.86	128.60
1	AA	415	A	C4-C5-C6	6.24	120.12	117.00
1	AA	1288	A	C4-C5-C6	6.24	120.12	117.00
1	AA	1385	G	O4'-C1'-N9	6.24	113.19	108.20
26	B7	53	A	C4-C5-C6	6.24	120.12	117.00
27	B8	415	A	C5-C6-N6	-6.24	118.71	123.70
27	B8	1356	G	C5-C6-O6	-6.24	124.86	128.60
26	B7	3	C	N3-C4-N4	6.23	122.36	118.00
27	B8	123	G	O4'-C1'-N9	6.23	113.19	108.20
27	B8	705	A	C5-C6-N6	-6.23	118.71	123.70
27	B8	1131	G	C5-C6-O6	-6.23	124.86	128.60
27	B8	1275	A	C5-C6-N6	-6.23	118.71	123.70
27	B8	1490	A	C4-C5-C6	6.23	120.12	117.00
27	B8	1793	C	N3-C4-N4	6.23	122.36	118.00
1	AA	887	G	O4'-C1'-N9	6.23	113.19	108.20
1	AA	1080	A	C5-C6-N6	-6.23	118.71	123.70
27	B8	210	C	N3-C4-N4	6.23	122.36	118.00
27	B8	696	G	C5-C6-O6	-6.23	124.86	128.60
27	B8	1144	A	C4-C5-C6	6.23	120.12	117.00
27	B8	1726	C	N3-C4-N4	6.23	122.36	118.00
27	B8	2088	A	O4'-C1'-N9	6.23	113.19	108.20
27	B8	2178	C	P-O3'-C3'	6.23	127.18	119.70
27	B8	2463	C	N3-C4-N4	6.23	122.36	118.00
27	B8	2495	G	O4'-C1'-N9	6.23	113.19	108.20
1	AA	27	G	O4'-C1'-N9	6.23	113.19	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	316	C	N3-C4-N4	6.23	122.36	118.00
1	AA	435	A	C4-C5-C6	6.23	120.11	117.00
1	AA	626	G	O4'-C1'-N9	6.23	113.18	108.20
3	AV	27	A	C5-C6-N6	-6.23	118.72	123.70
27	B8	77	G	O4'-C1'-N9	6.23	113.18	108.20
27	B8	429	A	C4-C5-C6	6.23	120.11	117.00
27	B8	718	A	C4-C5-C6	6.23	120.11	117.00
27	B8	2660	A	C4-C5-C6	6.23	120.11	117.00
1	AA	139	A	C5-C6-N6	-6.23	118.72	123.70
27	B8	126	A	C4-C5-C6	6.23	120.11	117.00
27	B8	565	C	N3-C4-N4	6.23	122.36	118.00
27	B8	2886	A	O4'-C1'-N9	6.23	113.18	108.20
1	AA	171	A	C4-C5-C6	6.23	120.11	117.00
1	AA	852	G	C5-C6-O6	-6.23	124.86	128.60
1	AA	1482	G	C5-C6-O6	-6.23	124.86	128.60
1	AA	1502	A	C4-C5-C6	6.23	120.11	117.00
27	B8	2795	C	N3-C4-N4	6.23	122.36	118.00
28	BA	249	ALA	N-CA-CB	6.23	118.82	110.10
27	B8	152	A	C5-C6-N6	-6.23	118.72	123.70
27	B8	2018	G	O4'-C1'-N9	6.23	113.18	108.20
1	AA	77	A	C4-C5-C6	6.22	120.11	117.00
1	AA	474	G	O4'-C1'-N9	6.22	113.18	108.20
27	B8	52	A	C5-C6-N1	-6.22	114.59	117.70
27	B8	621	A	O4'-C1'-N9	6.22	113.18	108.20
27	B8	1317	G	C5-C6-O6	-6.22	124.86	128.60
27	B8	1387	A	C5-C6-N6	-6.22	118.72	123.70
27	B8	1618	A	C4-C5-C6	6.22	120.11	117.00
27	B8	2632	A	C4-C5-C6	6.22	120.11	117.00
1	AA	98	A	C5-C6-N6	-6.22	118.72	123.70
1	AA	1281	C	O4'-C1'-N1	6.22	113.18	108.20
27	B8	111	A	O4'-C1'-N9	6.22	113.18	108.20
27	B8	822	G	O4'-C1'-N9	6.22	113.18	108.20
27	B8	831	G	C5-C6-O6	-6.22	124.87	128.60
27	B8	878	A	C4-C5-C6	6.22	120.11	117.00
27	B8	2225	A	C5-C6-N1	-6.22	114.59	117.70
1	AA	32	A	C4-C5-C6	6.22	120.11	117.00
1	AA	33	A	C4-C5-C6	6.22	120.11	117.00
1	AA	623	C	N3-C4-N4	6.22	122.36	118.00
27	B8	377	G	O4'-C1'-N9	6.22	113.18	108.20
27	B8	1084	A	C4-C5-C6	6.22	120.11	117.00
27	B8	1464	G	O4'-C1'-N9	6.22	113.18	108.20
27	B8	2003	A	C4-C5-C6	6.22	120.11	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	15	G	O4'-C1'-N9	6.22	113.17	108.20
1	AA	326	G	C5-C6-O6	-6.22	124.87	128.60
1	AA	1158	C	C2-N1-C1'	6.22	125.64	118.80
5	A0	166	TYR	CB-CG-CD1	6.22	124.73	121.00
27	B8	347	A	C5-C6-N6	-6.22	118.72	123.70
27	B8	1331	G	C5-C6-O6	-6.22	124.87	128.60
27	B8	1696	G	O4'-C1'-N9	6.22	113.18	108.20
27	B8	1934	C	N3-C4-N4	6.22	122.35	118.00
27	B8	2392	A	C4-C5-C6	6.22	120.11	117.00
27	B8	2577	A	C4-C5-C6	6.22	120.11	117.00
27	B8	2753	A	C4-C5-C6	6.22	120.11	117.00
27	B8	2816	G	O4'-C1'-N9	6.22	113.18	108.20
1	AA	144	G	O4'-C1'-N9	6.22	113.17	108.20
1	AA	1274	A	O4'-C1'-N9	6.22	113.17	108.20
1	AA	1276	G	O4'-C1'-N9	6.22	113.17	108.20
27	B8	629	G	O4'-C1'-N9	6.22	113.17	108.20
27	B8	1762	A	C4-C5-C6	6.22	120.11	117.00
27	B8	2704	C	N3-C4-N4	6.22	122.35	118.00
1	AA	192	A	C4-C5-C6	6.22	120.11	117.00
1	AA	713	G	O4'-C1'-N9	6.22	113.17	108.20
1	AA	732	C	N3-C4-N4	6.22	122.35	118.00
1	AA	1046	A	C5-C6-N6	-6.22	118.73	123.70
1	AA	1526	G	O4'-C1'-N9	6.22	113.17	108.20
27	B8	386	G	C5-C6-O6	-6.22	124.87	128.60
27	B8	1205	A	C4-C5-C6	6.22	120.11	117.00
1	AA	10	A	C4-C5-C6	6.21	120.11	117.00
1	AA	16	A	C4-C5-C6	6.21	120.11	117.00
1	AA	463	U	O4'-C1'-N1	6.21	113.17	108.20
1	AA	1224	U	O4'-C1'-N1	6.21	113.17	108.20
27	B8	267	C	N3-C4-N4	6.21	122.35	118.00
27	B8	323	C	C6-N1-C1'	-6.21	113.34	120.80
27	B8	454	A	C4-C5-C6	6.21	120.11	117.00
27	B8	1722	A	C5-C6-N1	-6.21	114.59	117.70
27	B8	1892	C	N3-C4-N4	6.21	122.35	118.00
27	B8	1966	A	C4-C5-C6	6.21	120.11	117.00
1	AA	621	A	C4-C5-C6	6.21	120.11	117.00
2	AX	21	A	C4-C5-C6	6.21	120.11	117.00
27	B8	1244	A	C5-C6-N6	-6.21	118.73	123.70
1	AA	681	A	C5-C6-N1	-6.21	114.59	117.70
1	AA	745	G	O4'-C1'-N9	6.21	113.17	108.20
1	AA	964	A	C4-C5-C6	6.21	120.11	117.00
27	B8	680	C	N3-C4-N4	6.21	122.35	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	925	A	C5-C6-N1	-6.21	114.59	117.70
27	B8	1054	A	C4-C5-C6	6.21	120.11	117.00
27	B8	1321	A	C4-C5-C6	6.21	120.11	117.00
27	B8	2126	A	C4-C5-C6	6.21	120.11	117.00
27	B8	2738	A	C4-C5-C6	6.21	120.11	117.00
27	B8	2792	A	C4-C5-C6	6.21	120.11	117.00
27	B8	360	U	O4'-C1'-N1	6.21	113.17	108.20
27	B8	1713	A	C5-C6-N1	-6.21	114.60	117.70
27	B8	2879	A	C4-C5-C6	6.21	120.11	117.00
1	AA	227	G	O4'-C1'-N9	6.21	113.17	108.20
1	AA	359	G	O4'-C1'-N9	6.21	113.17	108.20
1	AA	1057	G	C5-C6-O6	-6.21	124.88	128.60
1	AA	1092	A	C4-C5-C6	6.21	120.10	117.00
27	B8	563	A	C4-C5-C6	6.21	120.10	117.00
27	B8	1969	A	O4'-C1'-N9	6.21	113.17	108.20
27	B8	2071	A	C4-C5-C6	6.21	120.10	117.00
27	B8	2114	A	C4-C5-C6	6.21	120.10	117.00
27	B8	2223	G	O4'-C1'-N9	6.21	113.17	108.20
27	B8	2649	C	N3-C4-N4	6.21	122.34	118.00
1	AA	599	C	N3-C4-N4	6.21	122.34	118.00
1	AA	855	U	O4'-C1'-N1	6.21	113.16	108.20
27	B8	117	G	O4'-C1'-N9	6.21	113.16	108.20
27	B8	119	A	O4'-C1'-N9	6.21	113.16	108.20
27	B8	840	C	N3-C4-N4	6.21	122.34	118.00
27	B8	1052	C	N3-C4-N4	6.21	122.34	118.00
1	AA	285	C	N3-C4-N4	6.20	122.34	118.00
1	AA	349	A	C5-C6-N1	-6.20	114.60	117.70
1	AA	524	G	O4'-C1'-N9	6.20	113.16	108.20
27	B8	1301	A	C4-C5-C6	6.20	120.10	117.00
27	B8	1316	U	O4'-C1'-N1	6.20	113.16	108.20
27	B8	2038	G	C5-C6-O6	-6.20	124.88	128.60
27	B8	2273	A	C4-C5-C6	6.20	120.10	117.00
1	AA	363	A	C4-C5-C6	6.20	120.10	117.00
27	B8	384	A	C4-C5-C6	6.20	120.10	117.00
27	B8	2764	A	C4-C5-C6	6.20	120.10	117.00
1	AA	112	G	C5-C6-O6	-6.20	124.88	128.60
27	B8	1586	A	C4-C5-C6	6.20	120.10	117.00
27	B8	1916	A	C4-C5-C6	6.20	120.10	117.00
27	B8	2491	U	O4'-C1'-N1	6.20	113.16	108.20
1	AA	186	C	N3-C4-N4	6.20	122.34	118.00
1	AA	494	G	C5-C6-O6	-6.20	124.88	128.60
1	AA	895	G	O4'-C1'-N9	6.20	113.16	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	964	A	C5-C6-N6	-6.20	118.74	123.70
1	AA	1236	A	C5-C6-N6	-6.20	118.74	123.70
27	B8	326	G	O4'-C1'-N9	6.20	113.16	108.20
1	AA	1256	A	C4-C5-C6	6.20	120.10	117.00
1	AA	1357	A	C5-C6-N6	-6.20	118.74	123.70
27	B8	1253	A	C4-C5-C6	6.20	120.10	117.00
1	AA	1421	G	C5-C6-O6	-6.20	124.88	128.60
1	AA	1457	G	O4'-C1'-N9	6.20	113.16	108.20
27	B8	26	G	C5-C6-O6	-6.20	124.88	128.60
27	B8	2614	A	C4-C5-C6	6.20	120.10	117.00
27	B8	2706	A	O4'-C1'-N9	6.20	113.16	108.20
1	AA	538	G	O4'-C1'-N9	6.19	113.16	108.20
1	AA	741	G	C5-C6-O6	-6.19	124.88	128.60
27	B8	21	A	C4-C5-C6	6.19	120.10	117.00
27	B8	1022	G	O4'-C1'-N9	6.19	113.16	108.20
1	AA	129	A	O4'-C1'-N9	6.19	113.16	108.20
1	AA	1122	U	O4'-C1'-N1	6.19	113.15	108.20
27	B8	160	A	C4-C5-C6	6.19	120.10	117.00
27	B8	461	C	N3-C4-N4	6.19	122.33	118.00
27	B8	1737	G	P-O3'-C3'	6.19	127.13	119.70
27	B8	2168	G	N3-C2-N2	6.19	124.23	119.90
27	B8	2354	C	N3-C4-N4	6.19	122.33	118.00
27	B8	2557	G	O4'-C1'-N9	6.19	113.15	108.20
1	AA	622	A	O4'-C1'-N9	6.19	113.15	108.20
1	AA	777	A	O4'-C1'-N9	6.19	113.15	108.20
1	AA	940	C	N3-C4-N4	6.19	122.33	118.00
26	B7	49	C	N3-C4-N4	6.19	122.33	118.00
27	B8	730	A	C4-C5-C6	6.19	120.09	117.00
27	B8	1704	C	N3-C4-N4	6.19	122.33	118.00
1	AA	86	G	O4'-C1'-N9	6.19	113.15	108.20
1	AA	577	G	O4'-C1'-N9	6.19	113.15	108.20
27	B8	661	A	C4-C5-C6	6.19	120.09	117.00
27	B8	1095	A	C5-C6-N6	-6.19	118.75	123.70
27	B8	2080	A	C4-C5-C6	6.19	120.09	117.00
27	B8	2184	A	C5-C6-N6	-6.19	118.75	123.70
1	AA	865	A	C5-C6-N6	-6.19	118.75	123.70
27	B8	1042	G	O4'-C1'-N9	6.19	113.15	108.20
27	B8	2741	A	C4-C5-C6	6.19	120.09	117.00
1	AA	460	A	C5-C6-N1	-6.19	114.61	117.70
27	B8	1413	A	C5-C6-N6	-6.19	118.75	123.70
27	B8	1422	G	O4'-C1'-N9	6.19	113.15	108.20
27	B8	1544	A	C4-C5-C6	6.19	120.09	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1644	C	N3-C4-N4	6.19	122.33	118.00
27	B8	2453	A	C5-C6-N6	-6.19	118.75	123.70
1	AA	66	A	C4-C5-C6	6.18	120.09	117.00
26	B7	29	A	C5-C6-N6	-6.18	118.75	123.70
27	B8	68	G	O4'-C1'-N9	6.18	113.15	108.20
27	B8	168	G	O4'-C1'-N9	6.18	113.15	108.20
27	B8	491	G	C5'-C4'-O4'	6.18	116.52	109.10
27	B8	1818	U	O4'-C1'-N1	6.18	113.15	108.20
27	B8	1900	A	C4-C5-C6	6.18	120.09	117.00
1	AA	35	G	O4'-C1'-N9	6.18	113.15	108.20
1	AA	373	A	C4-C5-C6	6.18	120.09	117.00
1	AA	1418	A	C5-C6-N6	-6.18	118.75	123.70
27	B8	415	A	C4-C5-C6	6.18	120.09	117.00
27	B8	465	G	C5-C6-O6	-6.18	124.89	128.60
27	B8	1144	A	C5-C6-N6	-6.18	118.75	123.70
27	B8	165	A	C4-C5-C6	6.18	120.09	117.00
27	B8	1504	A	C4-C5-C6	6.18	120.09	117.00
27	B8	2025	C	N3-C4-C5	-6.18	119.43	121.90
1	AA	431	A	O4'-C1'-N9	6.18	113.14	108.20
1	AA	1153	G	O4'-C1'-N9	6.18	113.14	108.20
27	B8	71	A	C4-C5-C6	6.18	120.09	117.00
27	B8	1008	A	C4-C5-C6	6.18	120.09	117.00
1	AA	1344	C	N3-C4-N4	6.18	122.32	118.00
27	B8	2	G	O4'-C1'-N9	6.18	113.14	108.20
27	B8	293	U	O4'-C1'-N1	6.18	113.14	108.20
27	B8	2330	G	O4'-C1'-N9	6.18	113.14	108.20
27	B8	2746	U	O4'-C1'-N1	6.18	113.14	108.20
1	AA	181	A	O4'-C1'-N9	6.18	113.14	108.20
1	AA	466	A	C4-C5-C6	6.18	120.09	117.00
27	B8	33	C	O4'-C1'-N1	6.18	113.14	108.20
27	B8	197	A	C4-C5-C6	6.18	120.09	117.00
27	B8	655	A	C5-C6-N6	-6.18	118.76	123.70
27	B8	816	C	N3-C4-N4	6.18	122.32	118.00
27	B8	1069	A	C4-C5-C6	6.18	120.09	117.00
27	B8	1810	A	C4-C5-C6	6.18	120.09	117.00
27	B8	2488	G	O4'-C1'-N9	6.18	113.14	108.20
1	AA	236	A	C4-C5-C6	6.17	120.09	117.00
1	AA	1044	A	C4-C5-C6	6.17	120.09	117.00
1	AA	1309	G	O4'-C1'-N9	6.17	113.14	108.20
27	B8	172	A	O4'-C1'-N9	6.17	113.14	108.20
27	B8	368	A	C4-C5-C6	6.17	120.09	117.00
27	B8	620	G	O4'-C1'-N9	6.17	113.14	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1543	G	O4'-C1'-N9	6.17	113.14	108.20
27	B8	2375	G	C5-C6-O6	-6.17	124.89	128.60
27	B8	2461	A	C4-C5-C6	6.17	120.09	117.00
27	B8	2512	C	N3-C4-N4	6.17	122.32	118.00
27	B8	2810	A	C4-C5-C6	6.17	120.09	117.00
1	AA	872	A	C4-C5-C6	6.17	120.09	117.00
1	AA	879	C	N3-C4-N4	6.17	122.32	118.00
1	AA	1093	A	C4-C5-C6	6.17	120.09	117.00
1	AA	1099	G	C5-C6-O6	-6.17	124.90	128.60
27	B8	389	G	O4'-C1'-N9	6.17	113.14	108.20
27	B8	947	A	C4-C5-C6	6.17	120.09	117.00
27	B8	2047	C	N3-C4-N4	6.17	122.32	118.00
1	AA	294	U	O4'-C1'-N1	6.17	113.14	108.20
1	AA	1449	C	N3-C4-N4	6.17	122.32	118.00
27	B8	282	A	C5-C6-N1	-6.17	114.61	117.70
27	B8	689	A	C4-C5-C6	6.17	120.09	117.00
27	B8	815	C	N3-C4-N4	6.17	122.32	118.00
27	B8	876	C	N3-C4-N4	6.17	122.32	118.00
27	B8	1755	A	C5-C6-N6	-6.17	118.76	123.70
27	B8	2428	G	O4'-C1'-N9	6.17	113.14	108.20
1	AA	749	A	O4'-C1'-N9	6.17	113.14	108.20
27	B8	730	A	C5-C6-N6	-6.17	118.76	123.70
1	AA	265	G	O4'-C1'-N9	6.17	113.13	108.20
1	AA	650	G	C5-C6-O6	-6.17	124.90	128.60
1	AA	664	G	C5-C6-O6	-6.17	124.90	128.60
1	AA	1359	C	N3-C4-N4	6.17	122.32	118.00
27	B8	1039	A	C4-C5-C6	6.17	120.08	117.00
27	B8	1425	G	O4'-C1'-N9	6.17	113.14	108.20
27	B8	2402	U	O4'-C1'-N1	6.17	113.13	108.20
1	AA	328	C	O4'-C1'-N1	6.17	113.13	108.20
1	AA	456	A	C5-C6-N1	-6.17	114.62	117.70
1	AA	630	A	C4-C5-C6	6.17	120.08	117.00
11	AG	161	PHE	CB-CG-CD2	-6.17	116.48	120.80
26	B7	11	C	O4'-C1'-N1	6.17	113.13	108.20
27	B8	606	U	O4'-C1'-N1	6.17	113.13	108.20
27	B8	614	A	C4-C5-C6	6.17	120.08	117.00
27	B8	2386	A	C5-C6-N6	-6.17	118.77	123.70
27	B8	2403	C	N3-C4-N4	6.17	122.32	118.00
27	B8	2765	A	C4-C5-C6	6.17	120.08	117.00
1	AA	442	G	O4'-C1'-N9	6.17	113.13	108.20
18	AN	52	ARG	NE-CZ-NH1	6.17	123.38	120.30
27	B8	492	A	O4'-C1'-N9	6.17	113.13	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2420	C	N3-C4-N4	6.17	122.31	118.00
26	B7	85	G	O4'-C1'-N9	6.16	113.13	108.20
26	B7	104	A	C5-C6-N6	-6.16	118.77	123.70
27	B8	690	G	C5-C6-O6	-6.16	124.90	128.60
27	B8	1022	G	C5-C6-O6	-6.16	124.90	128.60
27	B8	1885	A	O4'-C1'-N9	6.16	113.13	108.20
27	B8	2152	G	C5-C6-O6	-6.16	124.90	128.60
27	B8	2581	G	C5-C6-O6	-6.16	124.90	128.60
1	AA	1377	A	C4-C5-C6	6.16	120.08	117.00
1	AA	36	C	N3-C4-N4	6.16	122.31	118.00
1	AA	754	C	C2-N1-C1'	6.16	125.58	118.80
1	AA	981	U	O4'-C1'-N1	6.16	113.13	108.20
1	AA	1297	G	O4'-C1'-N9	6.16	113.13	108.20
27	B8	833	A	C4-C5-C6	6.16	120.08	117.00
27	B8	1062	G	O4'-C1'-N9	6.16	113.13	108.20
27	B8	2147	A	C4-C5-C6	6.16	120.08	117.00
1	AA	142	G	O4'-C1'-N9	6.16	113.13	108.20
1	AA	306	A	C4-C5-C6	6.16	120.08	117.00
1	AA	313	A	C5-C6-N6	-6.16	118.77	123.70
1	AA	832	G	O4'-C1'-N9	6.16	113.13	108.20
1	AA	937	A	O4'-C1'-N9	6.16	113.13	108.20
1	AA	956	U	O4'-C1'-N1	6.16	113.13	108.20
1	AA	1022	A	C4-C5-C6	6.16	120.08	117.00
27	B8	663	G	O4'-C1'-N9	6.16	113.13	108.20
27	B8	2166	U	O4'-C1'-N1	6.16	113.13	108.20
27	B8	2882	A	C5-C6-N1	-6.16	114.62	117.70
1	AA	1251	A	O4'-C1'-N9	6.16	113.13	108.20
27	B8	988	A	C4-C5-C6	6.16	120.08	117.00
27	B8	1133	A	C4-C5-C6	6.16	120.08	117.00
27	B8	1251	C	N3-C4-N4	6.16	122.31	118.00
1	AA	33	A	C5-C6-N6	-6.16	118.78	123.70
1	AA	410	G	N3-C2-N2	6.16	124.21	119.90
1	AA	1096	C	N3-C4-N4	6.16	122.31	118.00
1	AA	1339	A	C5-C6-N1	-6.16	114.62	117.70
27	B8	1918	A	C4-C5-C6	6.16	120.08	117.00
27	B8	2267	A	C5-C6-N6	-6.16	118.78	123.70
1	AA	862	C	N3-C4-N4	6.15	122.31	118.00
27	B8	644	A	C5-C6-N6	-6.15	118.78	123.70
27	B8	789	A	C4-C5-C6	6.15	120.08	117.00
1	AA	764	C	N3-C4-N4	6.15	122.31	118.00
1	AA	1098	C	N3-C4-N4	6.15	122.31	118.00
1	AA	1242	G	O4'-C1'-N9	6.15	113.12	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1434	A	C5-C6-N6	-6.15	118.78	123.70
27	B8	1608	A	C5-C6-N1	-6.15	114.62	117.70
27	B8	2531	A	C5-C6-N1	-6.15	114.62	117.70
1	AA	908	A	O4'-C1'-N9	6.15	113.12	108.20
1	AA	1128	C	N3-C4-C5	-6.15	119.44	121.90
26	B7	34	A	O4'-C1'-N9	6.15	113.12	108.20
27	B8	342	A	C4-C5-C6	6.15	120.08	117.00
27	B8	472	A	C4-C5-C6	6.15	120.08	117.00
27	B8	927	A	C4-C5-C6	6.15	120.08	117.00
27	B8	1307	A	O4'-C1'-N9	6.15	113.12	108.20
27	B8	1417	C	N3-C4-N4	6.15	122.31	118.00
27	B8	1897	G	O4'-C1'-N9	6.15	113.12	108.20
27	B8	2037	A	O4'-C1'-N9	6.15	113.12	108.20
27	B8	2388	A	C4-C5-C6	6.15	120.08	117.00
27	B8	2481	G	C5-C6-O6	-6.15	124.91	128.60
1	AA	1061	G	O4'-C1'-N9	6.15	113.12	108.20
27	B8	792	A	C4-C5-C6	6.15	120.07	117.00
27	B8	953	G	O4'-C1'-N9	6.15	113.12	108.20
27	B8	1805	A	O4'-C1'-N9	6.15	113.12	108.20
27	B8	2717	C	N3-C4-N4	6.15	122.30	118.00
1	AA	311	C	N3-C4-N4	6.15	122.30	118.00
26	B7	91	C	N3-C4-N4	6.15	122.30	118.00
27	B8	1204	A	C4-C5-C6	6.15	120.07	117.00
27	B8	1950	G	C5-C6-O6	-6.15	124.91	128.60
27	B8	2228	G	O4'-C1'-N9	6.15	113.12	108.20
27	B8	2873	A	C5-C6-N6	-6.15	118.78	123.70
1	AA	80	A	C4-C5-C6	6.15	120.07	117.00
27	B8	122	G	O4'-C1'-N9	6.15	113.12	108.20
1	AA	211	G	C5-C6-O6	-6.14	124.91	128.60
1	AA	898	G	C5-C6-O6	-6.14	124.91	128.60
27	B8	146	A	O4'-C1'-N9	6.14	113.12	108.20
27	B8	258	G	O4'-C1'-N9	6.14	113.11	108.20
27	B8	325	G	O4'-C1'-N9	6.14	113.11	108.20
27	B8	1063	G	O4'-C1'-N9	6.14	113.11	108.20
27	B8	1603	A	C4-C5-C6	6.14	120.07	117.00
27	B8	2411	A	C4-C5-C6	6.14	120.07	117.00
1	AA	321	A	O4'-C1'-N9	6.14	113.11	108.20
1	AA	779	C	N3-C4-N4	6.14	122.30	118.00
1	AA	1156	G	N3-C2-N2	6.14	124.20	119.90
1	AA	1435	G	O4'-C1'-N9	6.14	113.11	108.20
27	B8	218	A	C4-C5-C6	6.14	120.07	117.00
27	B8	367	G	O4'-C1'-N9	6.14	113.11	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	160	A	C4-C5-C6	6.14	120.07	117.00
1	AA	743	A	C4-C5-C6	6.14	120.07	117.00
1	AA	790	A	C4-C5-C6	6.14	120.07	117.00
1	AA	1374	A	C5-C6-N6	-6.14	118.79	123.70
26	B7	27	C	P-O5'-C5'	6.14	130.72	120.90
27	B8	309	A	C4-C5-C6	6.14	120.07	117.00
27	B8	354	A	C5-C6-N1	-6.14	114.63	117.70
27	B8	910	A	C4-C5-C6	6.14	120.07	117.00
1	AA	297	G	O4'-C1'-N9	6.14	113.11	108.20
27	B8	73	A	O4'-C1'-N9	6.14	113.11	108.20
27	B8	144	A	C4-C5-C6	6.14	120.07	117.00
27	B8	226	A	C5-C6-N6	-6.14	118.79	123.70
27	B8	920	A	O4'-C1'-N9	6.14	113.11	108.20
27	B8	1561	C	N3-C4-N4	6.14	122.30	118.00
27	B8	1924	C	N3-C4-N4	6.14	122.30	118.00
1	AA	393	A	C4-C5-C6	6.13	120.07	117.00
1	AA	873	A	C5-C6-N1	-6.13	114.63	117.70
26	B7	86	G	O4'-C1'-N9	6.13	113.11	108.20
26	B7	87	U	O4'-C1'-N1	6.13	113.11	108.20
27	B8	585	G	N3-C2-N2	6.13	124.19	119.90
27	B8	1287	A	C4-C5-C6	6.13	120.07	117.00
27	B8	1358	G	O4'-C1'-N9	6.13	113.11	108.20
27	B8	1495	A	C4-C5-C6	6.13	120.07	117.00
1	AA	572	A	C4-C5-C6	6.13	120.07	117.00
1	AA	675	A	C5-C6-N6	-6.13	118.79	123.70
27	B8	152	A	C4-C5-C6	6.13	120.07	117.00
27	B8	1877	A	C4-C5-C6	6.13	120.07	117.00
1	AA	189	A	C4-C5-C6	6.13	120.07	117.00
1	AA	471	U	O4'-C1'-N1	6.13	113.11	108.20
1	AA	763	G	O4'-C1'-N9	6.13	113.11	108.20
1	AA	817	C	N3-C4-C5	-6.13	119.45	121.90
1	AA	1088	G	O4'-C1'-N9	6.13	113.11	108.20
27	B8	353	C	N3-C4-N4	6.13	122.29	118.00
27	B8	592	A	C5-C6-N1	-6.13	114.63	117.70
27	B8	1134	A	C4-C5-C6	6.13	120.06	117.00
27	B8	1253	A	C5-C6-N1	-6.13	114.63	117.70
27	B8	1431	A	C4-C5-C6	6.13	120.07	117.00
27	B8	1994	C	N3-C4-N4	6.13	122.29	118.00
27	B8	896	A	C4-C5-C6	6.13	120.06	117.00
1	AA	560	A	C4-C5-C6	6.13	120.06	117.00
3	AV	58	A	C4-C5-C6	6.13	120.06	117.00
26	B7	92	C	N3-C4-N4	6.13	122.29	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	510	C	N3-C4-N4	6.13	122.29	118.00
27	B8	915	C	N3-C4-N4	6.13	122.29	118.00
27	B8	1752	C	N3-C4-C5	-6.13	119.45	121.90
27	B8	2688	G	C5-C6-O6	-6.13	124.92	128.60
1	AA	724	G	O4'-C1'-N9	6.13	113.10	108.20
1	AA	968	A	C4-C5-C6	6.13	120.06	117.00
1	AA	1318	A	C4-C5-C6	6.13	120.06	117.00
27	B8	743	A	C5-C6-N6	-6.13	118.80	123.70
27	B8	1574	C	N3-C4-N4	6.13	122.29	118.00
27	B8	1654	A	C4-C5-C6	6.13	120.06	117.00
27	B8	1673	G	O4'-C1'-N9	6.13	113.10	108.20
27	B8	2470	G	O4'-C1'-N9	6.13	113.10	108.20
27	B8	30	G	O4'-C1'-N9	6.12	113.10	108.20
27	B8	409	G	O4'-C1'-N9	6.12	113.10	108.20
27	B8	2405	G	N3-C2-N2	6.12	124.19	119.90
1	AA	206	C	N3-C4-N4	6.12	122.29	118.00
1	AA	536	C	N3-C4-N4	6.12	122.29	118.00
1	AA	629	A	O4'-C1'-N9	6.12	113.10	108.20
1	AA	742	G	O4'-C1'-N9	6.12	113.10	108.20
1	AA	1319	A	C4-C5-C6	6.12	120.06	117.00
1	AA	1408	A	O4'-C1'-N9	6.12	113.10	108.20
1	AA	1479	C	N3-C4-C5	-6.12	119.45	121.90
27	B8	584	C	N3-C4-N4	6.12	122.29	118.00
27	B8	858	G	C5-C6-O6	-6.12	124.92	128.60
27	B8	911	A	C4-C5-C6	6.12	120.06	117.00
27	B8	1039	A	O4'-C1'-N9	6.12	113.10	108.20
1	AA	1275	A	C4-C5-C6	6.12	120.06	117.00
1	AA	1441	A	C4-C5-C6	6.12	120.06	117.00
3	AV	70	G	O4'-C1'-N9	6.12	113.10	108.20
27	B8	93	G	O4'-C1'-N9	6.12	113.10	108.20
27	B8	795	C	N3-C4-N4	6.12	122.28	118.00
27	B8	1262	A	C4-C5-C6	6.12	120.06	117.00
27	B8	1529	G	C5-C6-O6	-6.12	124.93	128.60
27	B8	1876	A	O4'-C1'-N9	6.12	113.10	108.20
27	B8	2095	A	C4-C5-C6	6.12	120.06	117.00
1	AA	909	A	O4'-C1'-N9	6.12	113.10	108.20
27	B8	666	A	C5-C6-N6	-6.12	118.80	123.70
1	AA	173	U	O4'-C1'-N1	6.12	113.09	108.20
1	AA	201	G	C5-C6-O6	-6.12	124.93	128.60
1	AA	416	G	O4'-C1'-N9	6.12	113.09	108.20
1	AA	1019	A	C4-C5-C6	6.12	120.06	117.00
27	B8	94	A	O4'-C1'-N9	6.12	113.09	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1186	G	C5-C6-O6	-6.12	124.93	128.60
27	B8	1288	G	O4'-C1'-N9	6.12	113.09	108.20
27	B8	1393	A	C4-C5-C6	6.12	120.06	117.00
27	B8	1517	G	O4'-C1'-N9	6.12	113.09	108.20
27	B8	1579	A	C4-C5-C6	6.12	120.06	117.00
1	AA	131	A	C4-C5-C6	6.12	120.06	117.00
27	B8	65	U	O4'-C1'-N1	6.12	113.09	108.20
27	B8	1299	G	O4'-C1'-N9	6.12	113.09	108.20
27	B8	1991	U	O4'-C1'-N1	6.12	113.09	108.20
1	AA	238	A	C4-C5-C6	6.12	120.06	117.00
1	AA	295	C	N3-C4-N4	6.12	122.28	118.00
1	AA	309	A	C5-C6-N6	-6.12	118.81	123.70
1	AA	579	A	C4-C5-C6	6.12	120.06	117.00
1	AA	784	A	C4-C5-C6	6.12	120.06	117.00
27	B8	1072	C	N3-C4-N4	6.12	122.28	118.00
27	B8	1354	A	C5-C6-N6	-6.12	118.81	123.70
27	B8	2773	C	N3-C4-N4	6.12	122.28	118.00
1	AA	119	A	C5-C6-N1	-6.11	114.64	117.70
1	AA	942	G	C5-C6-O6	-6.11	124.93	128.60
1	AA	1167	A	C5-C6-N6	-6.11	118.81	123.70
1	AA	1254	A	C5-C6-N1	-6.11	114.64	117.70
27	B8	73	A	C4-C5-C6	6.11	120.06	117.00
27	B8	1366	A	C4-C5-C6	6.11	120.06	117.00
27	B8	2227	A	C4-C5-C6	6.11	120.06	117.00
27	B8	2711	A	C5-C6-N6	-6.11	118.81	123.70
1	AA	545	C	N3-C4-N4	6.11	122.28	118.00
1	AA	953	G	O4'-C1'-N9	6.11	113.09	108.20
27	B8	1215	G	O4'-C1'-N9	6.11	113.09	108.20
27	B8	1590	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	2333	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	2700	A	C5-C6-N6	-6.11	118.81	123.70
1	AA	404	G	O4'-C1'-N9	6.11	113.09	108.20
1	AA	1131	G	C5-C6-O6	-6.11	124.93	128.60
1	AA	1150	A	C4-C5-C6	6.11	120.06	117.00
1	AA	1451	U	O4'-C1'-N1	6.11	113.09	108.20
27	B8	19	A	O4'-C1'-N9	6.11	113.09	108.20
27	B8	127	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	200	U	O4'-C1'-N1	6.11	113.09	108.20
27	B8	502	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	1505	A	C4-C5-C6	6.11	120.06	117.00
27	B8	2361	G	C5-C6-O6	-6.11	124.93	128.60
27	B8	996	A	C4-C5-C6	6.11	120.06	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1168	G	O4'-C1'-N9	6.11	113.09	108.20
27	B8	1179	G	O4'-C1'-N9	6.11	113.09	108.20
27	B8	1359	A	C4-C5-C6	6.11	120.05	117.00
26	B7	62	C	N3-C4-N4	6.11	122.28	118.00
27	B8	151	C	N3-C4-C5	-6.11	119.46	121.90
27	B8	155	A	C5-C6-N1	-6.11	114.65	117.70
27	B8	1718	G	C5-C6-O6	-6.11	124.94	128.60
27	B8	1739	A	O4'-C1'-N9	6.11	113.09	108.20
27	B8	2037	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	2237	G	N3-C2-N2	6.11	124.17	119.90
27	B8	2336	A	C4-C5-C6	6.11	120.05	117.00
27	B8	2622	U	O4'-C1'-N1	6.11	113.09	108.20
27	B8	2799	A	C4-C5-C6	6.11	120.05	117.00
1	AA	8	A	C4-C5-C6	6.11	120.05	117.00
1	AA	8	A	O4'-C1'-N9	6.11	113.08	108.20
1	AA	42	G	O4'-C1'-N9	6.11	113.08	108.20
1	AA	1052	U	O4'-C1'-N1	6.11	113.08	108.20
1	AA	1487	G	C5-C6-O6	-6.11	124.94	128.60
26	B7	78	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	575	A	C4-C5-C6	6.11	120.05	117.00
27	B8	616	A	C4-C5-C6	6.11	120.05	117.00
27	B8	845	A	C4-C5-C6	6.11	120.05	117.00
27	B8	1365	A	C4-C5-C6	6.11	120.05	117.00
27	B8	2042	A	C5-C6-N6	-6.11	118.81	123.70
27	B8	2576	G	C5-C6-O6	-6.11	124.94	128.60
1	AA	1074	G	O4'-C1'-N9	6.10	113.08	108.20
27	B8	1433	A	C4-C5-C6	6.10	120.05	117.00
27	B8	2864	G	O4'-C1'-N9	6.10	113.08	108.20
1	AA	238	A	C5-C6-N6	-6.10	118.82	123.70
27	B8	372	G	O4'-C1'-N9	6.10	113.08	108.20
27	B8	613	A	C4-C5-C6	6.10	120.05	117.00
27	B8	637	A	C4-C5-C6	6.10	120.05	117.00
27	B8	793	A	C4-C5-C6	6.10	120.05	117.00
27	B8	885	C	N3-C4-N4	6.10	122.27	118.00
27	B8	960	A	C4-C5-C6	6.10	120.05	117.00
27	B8	1192	G	O4'-C1'-N9	6.10	113.08	108.20
27	B8	1318	U	O4'-C1'-N1	6.10	113.08	108.20
27	B8	1583	A	O4'-C1'-N9	6.10	113.08	108.20
27	B8	2598	A	C5-C6-N6	-6.10	118.82	123.70
26	B7	58	A	C5-C6-N6	-6.10	118.82	123.70
27	B8	1550	C	N3-C4-N4	6.10	122.27	118.00
27	B8	1868	C	N3-C4-N4	6.10	122.27	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	252	U	O4'-C1'-N1	6.10	113.08	108.20
1	AA	722	G	C5-C6-O6	-6.10	124.94	128.60
1	AA	918	A	C4-C5-C6	6.10	120.05	117.00
26	B7	101	A	O4'-C1'-N9	6.10	113.08	108.20
27	B8	474	G	O4'-C1'-N9	6.10	113.08	108.20
27	B8	859	G	N3-C2-N2	6.10	124.17	119.90
27	B8	988	A	O4'-C1'-N9	6.10	113.08	108.20
1	AA	202	G	O4'-C1'-N9	6.10	113.08	108.20
1	AA	840	C	O4'-C1'-N1	6.10	113.08	108.20
27	B8	342	A	C5-C6-N6	-6.10	118.82	123.70
27	B8	825	A	O4'-C1'-N9	6.10	113.08	108.20
27	B8	861	A	O4'-C1'-N9	6.10	113.08	108.20
27	B8	1640	A	C5-C6-N6	-6.10	118.82	123.70
27	B8	1932	A	O4'-C1'-N9	6.10	113.08	108.20
27	B8	2885	G	O4'-C1'-N9	6.10	113.08	108.20
1	AA	18	C	N3-C4-N4	6.10	122.27	118.00
1	AA	718	A	C4-C5-C6	6.10	120.05	117.00
1	AA	726	C	N3-C4-N4	6.10	122.27	118.00
27	B8	630	G	O4'-C1'-N9	6.10	113.08	108.20
1	AA	360	G	O4'-C1'-N9	6.09	113.08	108.20
1	AA	975	A	C4-C5-C6	6.09	120.05	117.00
1	AA	975	A	O4'-C1'-N9	6.09	113.08	108.20
1	AA	1514	G	O4'-C1'-N9	6.09	113.08	108.20
27	B8	883	G	C5-C6-O6	-6.09	124.94	128.60
27	B8	1373	A	O4'-C1'-N9	6.09	113.08	108.20
27	B8	1512	C	N3-C4-N4	6.09	122.27	118.00
27	B8	1973	G	O4'-C1'-N9	6.09	113.08	108.20
27	B8	2589	A	C4-C5-C6	6.09	120.05	117.00
27	B8	2896	C	N3-C4-N4	6.09	122.27	118.00
27	B8	2252	G	C5-C6-O6	-6.09	124.94	128.60
1	AA	761	G	O4'-C1'-N9	6.09	113.07	108.20
1	AA	919	A	C5-C6-N1	-6.09	114.66	117.70
1	AA	1476	A	C5-C6-N1	-6.09	114.65	117.70
27	B8	626	A	C4-C5-C6	6.09	120.05	117.00
27	B8	818	G	C5-C6-O6	-6.09	124.95	128.60
27	B8	2186	G	O4'-C1'-N9	6.09	113.07	108.20
27	B8	2727	A	C4-C5-C6	6.09	120.05	117.00
1	AA	427	U	O4'-C1'-N1	6.09	113.07	108.20
1	AA	1195	C	N3-C4-N4	6.09	122.26	118.00
27	B8	964	C	N3-C4-N4	6.09	122.26	118.00
27	B8	1512	C	O4'-C1'-N1	6.09	113.07	108.20
27	B8	1525	A	C4-C5-C6	6.09	120.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2117	A	C4-C5-C6	6.09	120.05	117.00
27	B8	2283	C	N3-C4-N4	6.09	122.26	118.00
27	B8	2288	A	C4-C5-C6	6.09	120.05	117.00
45	BQ	23	TYR	CB-CG-CD1	-6.09	117.35	121.00
1	AA	596	A	C4-C5-C6	6.09	120.04	117.00
1	AA	831	A	O4'-C1'-N9	6.09	113.07	108.20
1	AA	1437	A	C4-C5-C6	6.09	120.04	117.00
1	AA	1458	G	O4'-C1'-N9	6.09	113.07	108.20
26	B7	113	C	N3-C4-N4	6.09	122.26	118.00
27	B8	337	C	N3-C4-N4	6.09	122.26	118.00
27	B8	722	A	C4-C5-C6	6.09	120.04	117.00
27	B8	1014	A	O4'-C1'-N9	6.09	113.07	108.20
27	B8	2207	C	N3-C4-N4	6.09	122.26	118.00
1	AA	649	A	O4'-C1'-N9	6.09	113.07	108.20
27	B8	761	A	C5-C6-N6	-6.09	118.83	123.70
27	B8	1061	U	O4'-C1'-N1	6.09	113.07	108.20
27	B8	1080	A	O4'-C1'-N9	6.09	113.07	108.20
27	B8	2345	G	C5-C6-O6	-6.09	124.95	128.60
1	AA	1185	G	O4'-C1'-N9	6.08	113.07	108.20
27	B8	2670	A	C4-C5-C6	6.08	120.04	117.00
1	AA	527	G	O4'-C1'-N9	6.08	113.07	108.20
1	AA	1508	A	O4'-C1'-N9	6.08	113.07	108.20
27	B8	435	C	O4'-C1'-N1	6.08	113.07	108.20
27	B8	790	U	O4'-C1'-N1	6.08	113.07	108.20
27	B8	918	A	C5-C6-N1	-6.08	114.66	117.70
27	B8	1156	A	C4-C5-C6	6.08	120.04	117.00
27	B8	2566	A	C5-C6-N1	-6.08	114.66	117.70
27	B8	2658	C	N3-C4-N4	6.08	122.26	118.00
1	AA	53	A	C5-C6-N6	-6.08	118.84	123.70
1	AA	221	C	N3-C4-N4	6.08	122.26	118.00
1	AA	403	C	N3-C4-N4	6.08	122.26	118.00
1	AA	483	C	N3-C4-N4	6.08	122.26	118.00
1	AA	539	A	C4-C5-C6	6.08	120.04	117.00
1	AA	1229	A	C4-C5-C6	6.08	120.04	117.00
27	B8	362	A	C4-C5-C6	6.08	120.04	117.00
27	B8	858	G	O4'-C1'-N9	6.08	113.06	108.20
27	B8	1626	A	C4-C5-C6	6.08	120.04	117.00
27	B8	1630	A	O4'-C1'-N9	6.08	113.07	108.20
1	AA	151	A	C5-C6-N1	-6.08	114.66	117.70
27	B8	925	A	C4-C5-C6	6.08	120.04	117.00
27	B8	1566	A	C4-C5-C6	6.08	120.04	117.00
27	B8	2627	G	O4'-C1'-N9	6.08	113.06	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	155	A	C4-C5-C6	6.08	120.04	117.00
1	AA	695	A	C5-C6-N6	-6.08	118.84	123.70
1	AA	1245	C	N3-C4-N4	6.08	122.25	118.00
1	AA	1285	A	C4-C5-C6	6.08	120.04	117.00
27	B8	477	A	C4-C5-C6	6.08	120.04	117.00
27	B8	985	C	N3-C4-N4	6.08	122.25	118.00
27	B8	1151	A	C4-C5-C6	6.08	120.04	117.00
27	B8	1268	A	C4-C5-C6	6.08	120.04	117.00
27	B8	1846	G	O4'-C1'-N9	6.08	113.06	108.20
27	B8	2300	C	N3-C4-N4	6.08	122.25	118.00
27	B8	2494	G	O4'-C1'-N9	6.08	113.06	108.20
27	B8	2792	A	P-O3'-C3'	6.08	127.00	119.70
27	B8	1020	A	C4-C5-C6	6.08	120.04	117.00
27	B8	1735	A	C4-C5-C6	6.08	120.04	117.00
27	B8	2156	G	O4'-C1'-N9	6.08	113.06	108.20
27	B8	2826	A	C4-C5-C6	6.08	120.04	117.00
1	AA	1146	A	C4-C5-C6	6.08	120.04	117.00
1	AA	1226	C	O4'-C1'-N1	6.08	113.06	108.20
1	AA	1314	C	N3-C4-N4	6.08	122.25	118.00
11	AG	161	PHE	CB-CG-CD1	6.08	125.05	120.80
27	B8	1298	C	N3-C4-N4	6.08	122.25	118.00
27	B8	1424	G	O4'-C1'-N9	6.08	113.06	108.20
27	B8	1551	A	C5-C6-N1	-6.08	114.66	117.70
27	B8	2433	A	C4-C5-C6	6.08	120.04	117.00
27	B8	2560	A	C4-C5-C6	6.08	120.04	117.00
1	AA	683	G	C5-C6-O6	-6.07	124.95	128.60
1	AA	1151	A	C4-C5-C6	6.07	120.04	117.00
1	AA	1503	A	C4-C5-C6	6.07	120.04	117.00
26	B7	45	A	O4'-C1'-N9	6.07	113.06	108.20
27	B8	262	A	C4-C5-C6	6.07	120.04	117.00
27	B8	450	G	C5-C6-O6	-6.07	124.96	128.60
27	B8	2323	G	O4'-C1'-N9	6.07	113.06	108.20
1	AA	445	G	O4'-C1'-N9	6.07	113.06	108.20
27	B8	676	A	O4'-C1'-N9	6.07	113.06	108.20
27	B8	2572	A	C4-C5-C6	6.07	120.04	117.00
1	AA	1102	A	C5-C6-N1	-6.07	114.67	117.70
1	AA	1287	A	C4-C5-C6	6.07	120.03	117.00
1	AA	1299	A	C4-C5-C6	6.07	120.03	117.00
1	AA	1372	U	O4'-C1'-N1	6.07	113.06	108.20
1	AA	1407	C	N3-C4-N4	6.07	122.25	118.00
27	B8	513	A	C5-C6-N6	-6.07	118.84	123.70
27	B8	829	A	P-O3'-C3'	6.07	126.98	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1206	G	O4'-C1'-N9	6.07	113.06	108.20
27	B8	2513	A	C4-C5-C6	6.07	120.03	117.00
1	AA	1	A	O4'-C1'-N9	6.07	113.06	108.20
1	AA	116	A	O4'-C1'-N9	6.07	113.06	108.20
1	AA	531	U	O4'-C1'-N1	6.07	113.06	108.20
27	B8	255	A	C5-C6-N6	-6.07	118.84	123.70
27	B8	263	G	O4'-C1'-N9	6.07	113.06	108.20
27	B8	2370	G	O4'-C1'-N9	6.07	113.06	108.20
1	AA	182	A	C4-C5-C6	6.07	120.03	117.00
1	AA	514	C	N3-C4-N4	6.07	122.25	118.00
1	AA	1201	A	C4-C5-C6	6.07	120.03	117.00
26	B7	29	A	C4-C5-C6	6.07	120.03	117.00
27	B8	737	C	N3-C4-N4	6.07	122.25	118.00
27	B8	1470	A	C5-C6-N6	-6.07	118.85	123.70
27	B8	1829	A	C5-C6-N6	-6.07	118.85	123.70
27	B8	2238	G	C5-C6-O6	-6.07	124.96	128.60
27	B8	2287	A	C4-C5-C6	6.07	120.03	117.00
1	AA	473	U	O4'-C1'-N1	6.07	113.05	108.20
1	AA	501	C	N3-C4-N4	6.07	122.25	118.00
1	AA	1188	A	C4-C5-C6	6.07	120.03	117.00
27	B8	168	G	C5-C6-O6	-6.07	124.96	128.60
27	B8	182	A	C5-C6-N1	-6.07	114.67	117.70
27	B8	1640	A	C4-C5-C6	6.07	120.03	117.00
27	B8	1672	A	C4-C5-C6	6.07	120.03	117.00
27	B8	2376	A	C4-C5-C6	6.07	120.03	117.00
1	AA	28	A	C4-C5-C6	6.06	120.03	117.00
1	AA	181	A	C4-C5-C6	6.06	120.03	117.00
1	AA	1487	G	O4'-C1'-N9	6.06	113.05	108.20
27	B8	725	G	O4'-C1'-N9	6.06	113.05	108.20
27	B8	1641	A	C5-C6-N1	-6.06	114.67	117.70
27	B8	2084	C	N3-C4-N4	6.06	122.25	118.00
27	B8	2158	A	C4-C5-C6	6.06	120.03	117.00
1	AA	253	A	C5-C6-N6	-6.06	118.85	123.70
27	B8	381	G	O4'-C1'-N9	6.06	113.05	108.20
27	B8	788	A	C4-C5-C6	6.06	120.03	117.00
27	B8	2380	C	N3-C4-N4	6.06	122.24	118.00
27	B8	2503	A	C4-C5-C6	6.06	120.03	117.00
27	B8	2742	G	O4'-C1'-N9	6.06	113.05	108.20
1	AA	1468	A	C5-C6-N1	-6.06	114.67	117.70
27	B8	631	A	C4-C5-C6	6.06	120.03	117.00
27	B8	2399	G	O4'-C1'-N9	6.06	113.05	108.20
1	AA	1397	C	C6-N1-C1'	-6.06	113.53	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	451	U	O4'-C1'-N1	6.06	113.05	108.20
27	B8	1229	C	N3-C4-N4	6.06	122.24	118.00
27	B8	1285	A	C5-C6-N6	-6.06	118.85	123.70
27	B8	2230	G	O4'-C1'-N9	6.06	113.05	108.20
27	B8	2346	A	C4-C5-C6	6.06	120.03	117.00
27	B8	2437	G	O4'-C1'-N9	6.06	113.05	108.20
27	B8	2565	A	C4-C5-C6	6.06	120.03	117.00
1	AA	235	C	N3-C4-N4	6.06	122.24	118.00
1	AA	470	C	N3-C4-N4	6.06	122.24	118.00
1	AA	831	A	C4-C5-C6	6.06	120.03	117.00
26	B7	60	C	N3-C4-N4	6.06	122.24	118.00
27	B8	461	C	O4'-C1'-N1	6.06	113.05	108.20
27	B8	1095	A	C4-C5-C6	6.06	120.03	117.00
27	B8	1755	A	C4-C5-C6	6.06	120.03	117.00
1	AA	385	C	N3-C4-N4	6.06	122.24	118.00
1	AA	782	A	C4-C5-C6	6.06	120.03	117.00
27	B8	1560	G	O4'-C1'-N9	6.06	113.05	108.20
27	B8	2629	U	O4'-C1'-N1	6.06	113.05	108.20
27	B8	2760	C	N3-C4-N4	6.06	122.24	118.00
1	AA	502	A	C4-C5-C6	6.05	120.03	117.00
1	AA	1164	G	O4'-C1'-N9	6.05	113.04	108.20
1	AA	1207	G	O4'-C1'-N9	6.05	113.04	108.20
3	AV	60	A	O4'-C1'-N9	6.05	113.04	108.20
27	B8	248	G	O4'-C1'-N9	6.05	113.04	108.20
27	B8	1508	A	C4-C5-C6	6.05	120.03	117.00
27	B8	1597	A	C4-C5-C6	6.05	120.03	117.00
27	B8	1849	G	O4'-C1'-N9	6.05	113.04	108.20
27	B8	2562	U	O4'-C1'-N1	6.05	113.04	108.20
1	AA	816	A	C4-C5-C6	6.05	120.03	117.00
26	B7	39	A	C4-C5-C6	6.05	120.03	117.00
27	B8	28	A	C4-C5-C6	6.05	120.03	117.00
27	B8	818	G	N3-C2-N2	6.05	124.14	119.90
1	AA	1152	A	C4-C5-C6	6.05	120.03	117.00
1	AA	1257	A	C4-C5-C6	6.05	120.03	117.00
26	B7	59	A	C4-C5-C6	6.05	120.03	117.00
26	B7	63	C	N3-C4-C5	-6.05	119.48	121.90
27	B8	216	A	C5-C6-N1	-6.05	114.67	117.70
27	B8	734	A	C4-C5-C6	6.05	120.03	117.00
27	B8	1067	A	C4-C5-C6	6.05	120.03	117.00
27	B8	1268	A	O4'-C1'-N9	6.05	113.04	108.20
27	B8	2144	G	O4'-C1'-N9	6.05	113.04	108.20
1	AA	679	C	N3-C4-C5	-6.05	119.48	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	996	A	C4-C5-C6	6.05	120.03	117.00
27	B8	149	A	C5-C6-N6	-6.05	118.86	123.70
27	B8	1918	A	O4'-C1'-N9	6.05	113.04	108.20
27	B8	2730	C	N3-C4-N4	6.05	122.23	118.00
1	AA	883	C	N3-C4-N4	6.05	122.23	118.00
1	AA	1465	A	C4-C5-C6	6.05	120.02	117.00
27	B8	1983	G	C5-C6-O6	-6.05	124.97	128.60
27	B8	2070	A	O4'-C1'-N9	6.05	113.04	108.20
27	B8	2692	G	O4'-C1'-N9	6.05	113.04	108.20
1	AA	977	A	C4-C5-C6	6.05	120.02	117.00
27	B8	1077	A	C4-C5-C6	6.05	120.02	117.00
27	B8	1336	A	C4-C5-C6	6.05	120.02	117.00
27	B8	1811	G	O4'-C1'-N9	6.05	113.04	108.20
27	B8	1942	C	O4'-C1'-N1	6.05	113.04	108.20
27	B8	2197	U	O4'-C1'-N1	6.05	113.04	108.20
1	AA	515	G	O4'-C1'-N9	6.04	113.04	108.20
1	AA	1004	A	C4-C5-C6	6.04	120.02	117.00
27	B8	184	C	N3-C4-N4	6.04	122.23	118.00
27	B8	781	A	C4-C5-C6	6.04	120.02	117.00
1	AA	30	U	O4'-C1'-N1	6.04	113.03	108.20
27	B8	13	A	C4-C5-C6	6.04	120.02	117.00
27	B8	751	A	C4-C5-C6	6.04	120.02	117.00
27	B8	1385	A	C5-C6-N1	-6.04	114.68	117.70
27	B8	1677	A	C5-C6-N6	-6.04	118.87	123.70
27	B8	1803	A	C4-C5-C6	6.04	120.02	117.00
1	AA	440	C	N3-C4-N4	6.04	122.23	118.00
1	AA	794	A	O4'-C1'-N9	6.04	113.03	108.20
27	B8	56	A	C4-C5-C6	6.04	120.02	117.00
27	B8	167	A	C5-C6-N6	-6.04	118.87	123.70
27	B8	508	A	C4-C5-C6	6.04	120.02	117.00
27	B8	987	C	N3-C4-N4	6.04	122.23	118.00
27	B8	1038	G	O4'-C1'-N9	6.04	113.03	108.20
27	B8	1304	A	O4'-C1'-N9	6.04	113.03	108.20
27	B8	1855	U	O4'-C1'-N1	6.04	113.03	108.20
27	B8	2184	A	C4-C5-C6	6.04	120.02	117.00
27	B8	2270	A	C4-C5-C6	6.04	120.02	117.00
27	B8	2505	G	C5-C6-O6	-6.04	124.97	128.60
1	AA	10	A	C5-C6-N6	-6.04	118.87	123.70
1	AA	97	G	C5-C6-O6	-6.04	124.98	128.60
1	AA	663	A	C5-C6-N1	-6.04	114.68	117.70
1	AA	718	A	O4'-C1'-N9	6.04	113.03	108.20
27	B8	324	A	C4-C5-C6	6.04	120.02	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	34	C	N3-C4-N4	6.04	122.23	118.00
1	AA	1091	U	O4'-C1'-N1	6.04	113.03	108.20
1	AA	1316	G	P-O3'-C3'	6.04	126.95	119.70
2	AX	18	C	N3-C4-N4	6.04	122.23	118.00
27	B8	344	A	O4'-C1'-N9	6.04	113.03	108.20
27	B8	1526	C	N3-C4-N4	6.04	122.23	118.00
27	B8	2171	A	C4-C5-C6	6.04	120.02	117.00
27	B8	2183	A	C4-C5-C6	6.04	120.02	117.00
27	B8	2263	C	N3-C4-N4	6.04	122.23	118.00
27	B8	2385	C	N3-C4-N4	6.04	122.23	118.00
1	AA	315	A	C5-C6-N1	-6.04	114.68	117.70
27	B8	957	C	N3-C4-N4	6.04	122.23	118.00
27	B8	1055	G	O4'-C1'-N9	6.04	113.03	108.20
27	B8	1204	A	C5-C6-N6	-6.04	118.87	123.70
1	AA	53	A	C4-C5-C6	6.04	120.02	117.00
1	AA	365	U	O4'-C1'-N1	6.04	113.03	108.20
1	AA	459	A	C5-C6-N1	-6.04	114.68	117.70
27	B8	439	A	C5-C6-N1	-6.04	114.68	117.70
27	B8	1236	G	C5-C6-O6	-6.04	124.98	128.60
27	B8	1344	U	O4'-C1'-N1	6.04	113.03	108.20
27	B8	1383	A	C4-C5-C6	6.04	120.02	117.00
27	B8	2048	G	O4'-C1'-N9	6.04	113.03	108.20
27	B8	2281	A	C5-C6-N6	-6.04	118.87	123.70
27	B8	2507	C	N3-C4-N4	6.04	122.22	118.00
27	B8	2634	A	C4-C5-C6	6.04	120.02	117.00
28	BA	383	PHE	CB-CG-CD2	6.04	125.02	120.80
1	AA	223	A	C4-C5-C6	6.03	120.02	117.00
1	AA	383	A	C5-C6-N1	-6.03	114.68	117.70
1	AA	435	A	O4'-C1'-N9	6.03	113.03	108.20
1	AA	755	G	O4'-C1'-N9	6.03	113.03	108.20
1	AA	1167	A	O4'-C1'-N9	6.03	113.03	108.20
1	AA	1404	C	N3-C4-N4	6.03	122.22	118.00
1	AA	1473	G	O4'-C1'-N9	6.03	113.03	108.20
27	B8	187	G	O4'-C1'-N9	6.03	113.03	108.20
27	B8	291	G	O4'-C1'-N9	6.03	113.03	108.20
27	B8	432	A	C4-C5-C6	6.03	120.02	117.00
27	B8	945	A	C4-C5-C6	6.03	120.02	117.00
27	B8	1190	G	O4'-C1'-N9	6.03	113.03	108.20
27	B8	1532	A	C4-C5-C6	6.03	120.02	117.00
27	B8	1894	C	N3-C4-N4	6.03	122.22	118.00
27	B8	2279	G	O4'-C1'-N9	6.03	113.03	108.20
27	B8	2471	A	C5-C6-N6	-6.03	118.87	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2900	A	C4-C5-C6	6.03	120.02	117.00
1	AA	228	A	C5-C6-N6	-6.03	118.87	123.70
27	B8	1233	C	N3-C4-N4	6.03	122.22	118.00
27	B8	2117	A	O4'-C1'-N9	6.03	113.03	108.20
1	AA	493	A	C5-C6-N6	-6.03	118.88	123.70
1	AA	979	C	N3-C4-N4	6.03	122.22	118.00
27	B8	320	A	C4-C5-C6	6.03	120.02	117.00
27	B8	453	A	C4-C5-C6	6.03	120.02	117.00
27	B8	541	A	C4-C5-C6	6.03	120.02	117.00
1	AA	1114	C	N3-C4-N4	6.03	122.22	118.00
1	AA	1140	C	N3-C4-C5	-6.03	119.49	121.90
27	B8	1314	C	N3-C4-N4	6.03	122.22	118.00
27	B8	1524	G	O4'-C1'-N9	6.03	113.02	108.20
27	B8	2369	A	C5-C6-N6	-6.03	118.88	123.70
1	AA	16	A	C5-C6-N1	-6.03	114.69	117.70
1	AA	706	A	C4-C5-C6	6.03	120.01	117.00
1	AA	1209	C	N3-C4-N4	6.03	122.22	118.00
27	B8	572	A	C5-C6-N6	-6.03	118.88	123.70
27	B8	991	C	N3-C4-C5	-6.03	119.49	121.90
27	B8	1591	A	O4'-C1'-N9	6.03	113.02	108.20
27	B8	1735	A	O4'-C1'-N9	6.03	113.02	108.20
27	B8	1791	A	C4-C5-C6	6.03	120.01	117.00
27	B8	2031	A	C4-C5-C6	6.03	120.01	117.00
27	B8	2534	A	C4-C5-C6	6.03	120.01	117.00
27	B8	2541	A	C5-C6-N6	-6.03	118.88	123.70
3	AV	75	C	N3-C4-C5	-6.03	119.49	121.90
27	B8	94	A	C4-C5-C6	6.03	120.01	117.00
27	B8	222	A	C4-C5-C6	6.03	120.01	117.00
27	B8	522	A	C4-C5-C6	6.03	120.01	117.00
27	B8	678	C	N3-C4-N4	6.03	122.22	118.00
27	B8	937	C	N3-C4-N4	6.03	122.22	118.00
27	B8	1084	A	C5-C6-N1	-6.03	114.69	117.70
27	B8	1261	C	N3-C4-N4	6.03	122.22	118.00
27	B8	2138	G	O4'-C1'-N9	6.03	113.02	108.20
1	AA	179	A	C5-C6-N1	-6.02	114.69	117.70
1	AA	499	A	C4-C5-C6	6.02	120.01	117.00
1	AA	519	C	N3-C4-C5	-6.02	119.49	121.90
27	B8	68	G	C5-C6-O6	-6.02	124.99	128.60
1	AA	336	A	C5-C6-N1	-6.02	114.69	117.70
1	AA	493	A	C4-C5-C6	6.02	120.01	117.00
1	AA	892	A	C4-C5-C6	6.02	120.01	117.00
1	AA	1443	C	N3-C4-N4	6.02	122.22	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	736	C	N3-C4-N4	6.02	122.22	118.00
27	B8	892	A	C5-C6-N6	-6.02	118.88	123.70
27	B8	2371	G	O4'-C1'-N9	6.02	113.02	108.20
1	AA	984	C	N3-C4-N4	6.02	122.22	118.00
27	B8	786	C	N3-C4-N4	6.02	122.22	118.00
27	B8	1676	A	C5-C6-N6	-6.02	118.88	123.70
1	AA	59	A	C4-C5-C6	6.02	120.01	117.00
1	AA	320	A	O4'-C1'-N9	6.02	113.02	108.20
1	AA	1542	A	O4'-C1'-N9	6.02	113.02	108.20
3	AV	33	A	C4-C5-C6	6.02	120.01	117.00
26	B7	38	C	N3-C4-N4	6.02	122.21	118.00
27	B8	172	A	C4-C5-C6	6.02	120.01	117.00
27	B8	322	A	C5-C6-N1	-6.02	114.69	117.70
27	B8	1084	A	C5-C6-N6	-6.02	118.89	123.70
27	B8	2054	A	C4-C5-C6	6.02	120.01	117.00
27	B8	2679	A	O4'-C1'-N9	6.02	113.02	108.20
1	AA	547	A	C4-C5-C6	6.02	120.01	117.00
1	AA	1246	A	O4'-C1'-N9	6.02	113.01	108.20
27	B8	173	A	O4'-C1'-N9	6.02	113.01	108.20
27	B8	468	G	O4'-C1'-N9	6.02	113.01	108.20
27	B8	743	A	O4'-C1'-N9	6.02	113.01	108.20
27	B8	1571	A	O4'-C1'-N9	6.02	113.02	108.20
27	B8	2516	A	C5-C6-N6	-6.02	118.89	123.70
1	AA	329	A	C4-C5-C6	6.02	120.01	117.00
3	AV	16	C	O4'-C1'-N1	6.02	113.01	108.20
27	B8	231	A	C4-C5-C6	6.02	120.01	117.00
27	B8	726	G	O4'-C1'-N9	6.02	113.01	108.20
27	B8	2178	C	C6-N1-C1'	-6.02	113.58	120.80
1	AA	356	A	C5-C6-N6	-6.01	118.89	123.70
1	AA	1130	A	C5-C6-N6	-6.01	118.89	123.70
3	AV	4	C	N3-C4-N4	6.01	122.21	118.00
27	B8	20	C	N3-C4-N4	6.01	122.21	118.00
27	B8	148	U	O4'-C1'-N1	6.01	113.01	108.20
27	B8	231	A	C5-C6-N1	-6.01	114.69	117.70
27	B8	341	C	N3-C4-N4	6.01	122.21	118.00
27	B8	506	G	O4'-C1'-N9	6.01	113.01	108.20
27	B8	1029	A	C5-C6-N1	-6.01	114.69	117.70
27	B8	1336	A	C5-C6-N6	-6.01	118.89	123.70
27	B8	1632	A	C4-C5-C6	6.01	120.01	117.00
27	B8	1913	A	C4-C5-C6	6.01	120.01	117.00
27	B8	2224	G	C5-C6-O6	-6.01	124.99	128.60
3	AV	50	G	O4'-C1'-N9	6.01	113.01	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	760	G	O4'-C1'-N9	6.01	113.01	108.20
27	B8	1384	A	C5-C6-N6	-6.01	118.89	123.70
27	B8	2531	A	C4-C5-C6	6.01	120.01	117.00
1	AA	400	C	N3-C4-N4	6.01	122.21	118.00
1	AA	969	A	O4'-C1'-N9	6.01	113.01	108.20
27	B8	262	A	C5-C6-N1	-6.01	114.69	117.70
27	B8	979	A	C4-C5-C6	6.01	120.01	117.00
27	B8	1302	A	C5-C6-N1	-6.01	114.69	117.70
27	B8	1541	C	N3-C4-N4	6.01	122.21	118.00
27	B8	1665	A	C4-C5-C6	6.01	120.01	117.00
27	B8	1998	A	C4-C5-C6	6.01	120.00	117.00
27	B8	2327	A	C4-C5-C6	6.01	120.01	117.00
27	B8	2377	A	C4-C5-C6	6.01	120.01	117.00
27	B8	2453	A	C4-C5-C6	6.01	120.01	117.00
1	AA	82	G	O4'-C1'-N9	6.01	113.01	108.20
1	AA	120	A	C4-C5-C6	6.01	120.00	117.00
1	AA	237	G	O4'-C1'-N9	6.01	113.01	108.20
27	B8	599	A	C5-C6-N6	-6.01	118.89	123.70
27	B8	975	A	C5-C6-N1	-6.01	114.69	117.70
27	B8	2278	A	C5-C6-N6	-6.01	118.89	123.70
27	B8	2475	C	N3-C4-C5	-6.01	119.50	121.90
27	B8	2653	U	O4'-C1'-N1	6.01	113.01	108.20
27	B8	742	A	C5-C6-N6	-6.01	118.89	123.70
27	B8	1086	A	O4'-C1'-N9	6.01	113.01	108.20
27	B8	1678	A	C4-C5-C6	6.01	120.00	117.00
27	B8	2349	G	O4'-C1'-N9	6.01	113.01	108.20
27	B8	2678	C	N3-C4-N4	6.01	122.21	118.00
27	B8	2831	G	O4'-C1'-N9	6.01	113.01	108.20
1	AA	1200	C	O4'-C1'-N1	6.01	113.01	108.20
1	AA	1521	C	N3-C4-N4	6.01	122.20	118.00
27	B8	259	G	O4'-C1'-N9	6.01	113.01	108.20
27	B8	1297	C	N3-C4-N4	6.01	122.20	118.00
27	B8	1821	A	O4'-C1'-N9	6.01	113.00	108.20
28	BA	383	PHE	CB-CG-CD1	-6.01	116.59	120.80
1	AA	174	A	C4-C5-C6	6.00	120.00	117.00
27	B8	921	C	N3-C4-N4	6.00	122.20	118.00
27	B8	1822	C	N3-C4-N4	6.00	122.20	118.00
27	B8	1958	C	N3-C4-N4	6.00	122.20	118.00
27	B8	2635	A	C4-C5-C6	6.00	120.00	117.00
1	AA	704	A	C4-C5-C6	6.00	120.00	117.00
27	B8	236	C	N3-C4-N4	6.00	122.20	118.00
27	B8	311	A	C4-C5-C6	6.00	120.00	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	698	C	N3-C4-N4	6.00	122.20	118.00
27	B8	991	C	N3-C4-N4	6.00	122.20	118.00
27	B8	1174	U	O4'-C1'-N1	6.00	113.00	108.20
27	B8	2381	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	2679	A	C5-C6-N6	-6.00	118.90	123.70
1	AA	143	A	C4-C5-C6	6.00	120.00	117.00
1	AA	418	C	N3-C4-N4	6.00	122.20	118.00
1	AA	502	A	O4'-C1'-N9	6.00	113.00	108.20
1	AA	602	A	O4'-C1'-N9	6.00	113.00	108.20
1	AA	1502	A	O4'-C1'-N9	6.00	113.00	108.20
27	B8	83	A	C4-C5-C6	6.00	120.00	117.00
27	B8	213	A	C4-C5-C6	6.00	120.00	117.00
27	B8	492	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	504	A	C4-C5-C6	6.00	120.00	117.00
27	B8	820	A	O4'-C1'-N9	6.00	113.00	108.20
27	B8	995	C	C2-N1-C1'	6.00	125.40	118.80
27	B8	2094	A	C4-C5-C6	6.00	120.00	117.00
1	AA	831	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	2142	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	2301	C	N3-C4-N4	6.00	122.20	118.00
27	B8	2486	C	N3-C4-N4	6.00	122.20	118.00
1	AA	374	A	C4-C5-C6	6.00	120.00	117.00
26	B7	35	C	C6-N1-C1'	-6.00	113.60	120.80
27	B8	289	G	O4'-C1'-N9	6.00	113.00	108.20
27	B8	423	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	677	A	O4'-C1'-N9	6.00	113.00	108.20
27	B8	808	G	O4'-C1'-N9	6.00	113.00	108.20
27	B8	2211	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	2485	G	O4'-C1'-N9	6.00	113.00	108.20
27	B8	2814	A	C4-C5-C6	6.00	120.00	117.00
1	AA	286	C	N3-C4-N4	6.00	122.20	118.00
1	AA	364	A	C4-C5-C6	6.00	120.00	117.00
1	AA	422	C	O4'-C1'-N1	6.00	113.00	108.20
1	AA	715	A	C4-C5-C6	6.00	120.00	117.00
1	AA	1394	A	C4-C5-C6	6.00	120.00	117.00
27	B8	447	A	C4-C5-C6	6.00	120.00	117.00
27	B8	602	A	C5-C6-N6	-6.00	118.90	123.70
27	B8	623	C	N3-C4-N4	6.00	122.20	118.00
27	B8	1342	A	C4-C5-C6	6.00	120.00	117.00
27	B8	1795	C	N3-C4-C5	-6.00	119.50	121.90
27	B8	2497	A	C4-C5-C6	6.00	120.00	117.00
1	AA	465	A	C5-C6-N6	-6.00	118.90	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	208	C	N3-C4-N4	6.00	122.20	118.00
27	B8	743	A	C4-C5-C6	6.00	120.00	117.00
27	B8	1593	A	C5-C6-N6	-6.00	118.90	123.70
1	AA	673	A	O4'-C1'-N9	5.99	113.00	108.20
3	AV	36	G	O4'-C1'-N9	5.99	113.00	108.20
27	B8	44	A	C4-C5-C6	5.99	120.00	117.00
27	B8	693	A	C5-C6-N6	-5.99	118.91	123.70
27	B8	896	A	O4'-C1'-N9	5.99	113.00	108.20
27	B8	1779	U	O4'-C1'-N1	5.99	113.00	108.20
27	B8	2564	A	C4-C5-C6	5.99	120.00	117.00
27	B8	2853	C	N3-C4-N4	5.99	122.20	118.00
1	AA	327	A	C5-C6-N1	-5.99	114.70	117.70
27	B8	347	A	C4-C5-C6	5.99	120.00	117.00
27	B8	1350	C	N3-C4-N4	5.99	122.19	118.00
27	B8	1932	A	C4-C5-C6	5.99	120.00	117.00
27	B8	2643	G	O4'-C1'-N9	5.99	112.99	108.20
1	AA	328	C	N3-C4-N4	5.99	122.19	118.00
1	AA	356	A	O4'-C1'-N9	5.99	112.99	108.20
1	AA	817	C	N3-C4-N4	5.99	122.19	118.00
2	AX	16	C	N3-C4-N4	5.99	122.19	118.00
27	B8	183	C	N3-C4-N4	5.99	122.19	118.00
27	B8	1193	G	O4'-C1'-N9	5.99	112.99	108.20
27	B8	1361	G	O4'-C1'-N9	5.99	112.99	108.20
27	B8	2381	A	C4-C5-C6	5.99	120.00	117.00
27	B8	2461	A	O4'-C1'-N9	5.99	112.99	108.20
1	AA	374	A	O4'-C1'-N9	5.99	112.99	108.20
1	AA	641	U	O4'-C1'-N1	5.99	112.99	108.20
1	AA	1035	A	C4-C5-C6	5.99	119.99	117.00
1	AA	1369	C	N3-C4-N4	5.99	122.19	118.00
27	B8	643	A	C4-C5-C6	5.99	119.99	117.00
27	B8	912	C	N3-C4-N4	5.99	122.19	118.00
27	B8	1166	G	O4'-C1'-N9	5.99	112.99	108.20
27	B8	1801	A	C4-C5-C6	5.99	120.00	117.00
27	B8	1836	C	N3-C4-N4	5.99	122.19	118.00
27	B8	1890	A	C4-C5-C6	5.99	119.99	117.00
27	B8	2024	G	O4'-C1'-N9	5.99	112.99	108.20
27	B8	2363	G	O4'-C1'-N9	5.99	112.99	108.20
27	B8	2461	A	C5-C6-N6	-5.99	118.91	123.70
27	B8	2616	C	N3-C4-N4	5.99	122.19	118.00
27	B8	2752	C	N3-C4-N4	5.99	122.19	118.00
27	B8	2755	C	N3-C4-N4	5.99	122.19	118.00
26	B7	116	G	O4'-C1'-N9	5.99	112.99	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	292	G	O4'-C1'-N9	5.99	112.99	108.20
1	AA	1147	C	N3-C4-N4	5.99	122.19	118.00
27	B8	1403	A	C4-C5-C6	5.99	119.99	117.00
27	B8	1433	A	C5-C6-N1	-5.99	114.71	117.70
27	B8	1448	G	O4'-C1'-N9	5.99	112.99	108.20
27	B8	2101	A	C4-C5-C6	5.99	119.99	117.00
1	AA	766	A	C4-C5-C6	5.98	119.99	117.00
26	B7	82	U	O4'-C1'-N1	5.98	112.99	108.20
27	B8	439	A	C4-C5-C6	5.98	119.99	117.00
27	B8	1064	C	N3-C4-N4	5.98	122.19	118.00
27	B8	1290	C	N3-C4-N4	5.98	122.19	118.00
27	B8	1844	C	N3-C4-N4	5.98	122.19	118.00
1	AA	1105	A	C5-C6-N6	-5.98	118.91	123.70
27	B8	190	A	C5-C6-N6	-5.98	118.92	123.70
27	B8	1783	A	C4-C5-C6	5.98	119.99	117.00
27	B8	2198	A	C5-C6-N6	-5.98	118.91	123.70
27	B8	2530	A	C1'-O4'-C4'	-5.98	105.11	109.90
45	BQ	23	TYR	CB-CG-CD2	5.98	124.59	121.00
1	AA	120	A	C5-C6-N6	-5.98	118.92	123.70
1	AA	232	G	C5-C6-O6	-5.98	125.01	128.60
1	AA	878	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1287	A	C5-C6-N6	-5.98	118.92	123.70
27	B8	501	A	C4-C5-C6	5.98	119.99	117.00
27	B8	1404	C	N3-C4-N4	5.98	122.19	118.00
27	B8	2027	G	O4'-C1'-N9	5.98	112.98	108.20
27	B8	47	C	N3-C4-N4	5.98	122.19	118.00
27	B8	589	U	O4'-C1'-N1	5.98	112.98	108.20
27	B8	2503	A	C5-C6-N6	-5.98	118.92	123.70
1	AA	182	A	O4'-C1'-N9	5.98	112.98	108.20
1	AA	303	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1032	G	O4'-C1'-N9	5.98	112.98	108.20
1	AA	1103	C	N3-C4-N4	5.98	122.18	118.00
27	B8	538	A	O4'-C1'-N9	5.98	112.98	108.20
27	B8	1152	C	N3-C4-N4	5.98	122.18	118.00
27	B8	1278	C	N3-C4-N4	5.98	122.18	118.00
27	B8	1938	A	C4-C5-C6	5.98	119.99	117.00
1	AA	366	A	C4-C5-C6	5.97	119.99	117.00
1	AA	451	A	C4-C5-C6	5.97	119.99	117.00
1	AA	686	U	O4'-C1'-N1	5.97	112.98	108.20
1	AA	1155	A	O4'-C1'-N9	5.97	112.98	108.20
26	B7	99	A	C5-C6-N1	-5.97	114.71	117.70
1	AA	288	A	C4-C5-C6	5.97	119.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	609	A	C4-C5-C6	5.97	119.99	117.00
1	AA	743	A	C5-C6-N6	-5.97	118.92	123.70
1	AA	1104	G	O4'-C1'-N9	5.97	112.98	108.20
1	AA	1371	G	C5-C6-O6	-5.97	125.02	128.60
27	B8	481	G	C5-C6-O6	-5.97	125.02	128.60
27	B8	540	C	N3-C4-N4	5.97	122.18	118.00
27	B8	550	C	N3-C4-C5	-5.97	119.51	121.90
27	B8	777	G	O4'-C1'-N9	5.97	112.98	108.20
27	B8	802	A	C5-C6-N1	-5.97	114.71	117.70
27	B8	1091	G	C5-C6-O6	-5.97	125.02	128.60
27	B8	1430	G	O4'-C1'-N9	5.97	112.98	108.20
27	B8	2135	A	C4-C5-C6	5.97	119.99	117.00
27	B8	2221	G	O4'-C1'-N9	5.97	112.98	108.20
27	B8	2758	A	C5-C6-N6	-5.97	118.92	123.70
1	AA	391	G	O4'-C1'-N9	5.97	112.98	108.20
27	B8	1413	A	C4-C5-C6	5.97	119.98	117.00
27	B8	1587	G	C5-C6-O6	-5.97	125.02	128.60
27	B8	2846	G	O4'-C1'-N9	5.97	112.98	108.20
1	AA	716	A	C5-C6-N1	-5.97	114.72	117.70
1	AA	877	G	O4'-C1'-N9	5.97	112.98	108.20
1	AA	1181	G	C5-C6-O6	-5.97	125.02	128.60
1	AA	1428	A	C4-C5-C6	5.97	119.98	117.00
27	B8	241	A	C4-C5-C6	5.97	119.98	117.00
27	B8	1165	A	C5-C6-N1	-5.97	114.72	117.70
27	B8	1854	A	O4'-C1'-N9	5.97	112.98	108.20
27	B8	2099	U	O4'-C1'-N1	5.97	112.97	108.20
27	B8	2172	U	O4'-C1'-N1	5.97	112.97	108.20
27	B8	2211	A	C4-C5-C6	5.97	119.98	117.00
27	B8	2241	A	C4-C5-C6	5.97	119.98	117.00
27	B8	2350	C	N3-C4-N4	5.97	122.18	118.00
27	B8	130	C	N3-C4-N4	5.97	122.18	118.00
27	B8	270	A	C4-C5-C6	5.97	119.98	117.00
27	B8	892	A	O4'-C1'-N9	5.97	112.97	108.20
27	B8	2588	G	O4'-C1'-N9	5.97	112.97	108.20
1	AA	184	G	O4'-C1'-N9	5.97	112.97	108.20
1	AA	1170	A	C5-C6-N6	-5.97	118.93	123.70
1	AA	1196	A	C4-C5-C6	5.97	119.98	117.00
27	B8	1070	A	C4-C5-C6	5.97	119.98	117.00
27	B8	2176	A	O4'-C1'-N9	5.97	112.97	108.20
27	B8	2723	C	N3-C4-N4	5.97	122.18	118.00
1	AA	1059	C	N3-C4-N4	5.96	122.18	118.00
1	AA	1325	C	N3-C4-N4	5.96	122.17	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	A	C4-C5-C6	5.96	119.98	117.00
27	B8	586	A	C4-C5-C6	5.96	119.98	117.00
27	B8	1367	A	C5-C6-N6	-5.96	118.93	123.70
27	B8	2196	C	N3-C4-N4	5.96	122.18	118.00
27	B8	2382	G	O4'-C1'-N9	5.96	112.97	108.20
27	B8	2888	C	N3-C4-N4	5.96	122.17	118.00
1	AA	1284	C	N3-C4-N4	5.96	122.17	118.00
27	B8	1247	A	C4-C5-C6	5.96	119.98	117.00
1	AA	702	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1081	A	C5-C6-N6	-5.96	118.93	123.70
1	AA	1108	G	O4'-C1'-N9	5.96	112.97	108.20
1	AA	1251	A	C4-C5-C6	5.96	119.98	117.00
27	B8	103	A	O4'-C1'-N9	5.96	112.97	108.20
27	B8	281	C	N3-C4-N4	5.96	122.17	118.00
27	B8	528	A	C4-C5-C6	5.96	119.98	117.00
27	B8	603	A	C4-C5-C6	5.96	119.98	117.00
27	B8	804	A	C4-C5-C6	5.96	119.98	117.00
27	B8	878	A	C5-C6-N6	-5.96	118.93	123.70
27	B8	1919	A	C4-C5-C6	5.96	119.98	117.00
27	B8	2094	A	C5-C6-N6	-5.96	118.93	123.70
46	BR	3	ALA	N-CA-CB	5.96	118.45	110.10
1	AA	793	U	O4'-C1'-N1	5.96	112.97	108.20
27	B8	452	G	O4'-C1'-N9	5.96	112.97	108.20
27	B8	1471	G	O4'-C1'-N9	5.96	112.97	108.20
1	AA	225	C	N3-C4-N4	5.96	122.17	118.00
1	AA	1169	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1239	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1519	A	C4-C5-C6	5.96	119.98	117.00
27	B8	750	A	C5-C6-N6	-5.96	118.93	123.70
27	B8	1118	C	N3-C4-N4	5.96	122.17	118.00
27	B8	1634	A	C5-C6-N1	-5.96	114.72	117.70
27	B8	1650	A	C5-C6-N6	-5.96	118.93	123.70
27	B8	2037	A	C4-C5-C6	5.96	119.98	117.00
27	B8	2143	C	N3-C4-N4	5.96	122.17	118.00
27	B8	2426	A	C4-C5-C6	5.96	119.98	117.00
1	AA	496	A	C4-C5-C6	5.96	119.98	117.00
1	AA	899	C	N3-C4-C5	-5.96	119.52	121.90
1	AA	1082	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1163	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1500	A	C4-C5-C6	5.96	119.98	117.00
27	B8	297	G	O4'-C1'-N9	5.96	112.97	108.20
27	B8	391	A	C5-C6-N6	-5.96	118.94	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	936	A	C5-C6-N6	-5.96	118.94	123.70
27	B8	1754	A	C5-C6-N6	-5.96	118.94	123.70
27	B8	1778	U	O4'-C1'-N1	5.96	112.97	108.20
27	B8	1829	A	C4-C5-C6	5.96	119.98	117.00
27	B8	2590	A	C4-C5-C6	5.96	119.98	117.00
27	B8	2796	U	O4'-C1'-N1	5.96	112.97	108.20
1	AA	241	G	O4'-C1'-N9	5.96	112.96	108.20
1	AA	456	A	O4'-C1'-N9	5.96	112.96	108.20
1	AA	469	C	N3-C4-N4	5.96	122.17	118.00
1	AA	1502	A	C5-C6-N1	-5.96	114.72	117.70
27	B8	108	G	O4'-C1'-N9	5.96	112.96	108.20
27	B8	282	A	O4'-C1'-N9	5.96	112.96	108.20
27	B8	346	A	C5-C6-N1	-5.96	114.72	117.70
27	B8	653	U	C2-N1-C1'	5.96	124.85	117.70
27	B8	1286	A	C5-C6-N1	-5.96	114.72	117.70
27	B8	2278	A	C4-C5-C6	5.96	119.98	117.00
1	AA	80	A	C5-C6-N1	-5.95	114.72	117.70
1	AA	681	A	C4-C5-C6	5.95	119.98	117.00
27	B8	89	A	C4-C5-C6	5.95	119.98	117.00
27	B8	361	G	O4'-C1'-N9	5.95	112.96	108.20
27	B8	1826	G	O4'-C1'-N9	5.95	112.96	108.20
1	AA	243	A	C4-C5-C6	5.95	119.98	117.00
27	B8	905	A	C4-C5-C6	5.95	119.98	117.00
27	B8	1866	A	C5-C6-N6	-5.95	118.94	123.70
1	AA	129	A	C4-C5-C6	5.95	119.98	117.00
1	AA	600	A	O4'-C1'-N9	5.95	112.96	108.20
1	AA	767	A	C4-C5-C6	5.95	119.98	117.00
1	AA	1163	A	O4'-C1'-N9	5.95	112.96	108.20
27	B8	147	C	N3-C4-N4	5.95	122.17	118.00
27	B8	156	A	C4-C5-C6	5.95	119.97	117.00
27	B8	179	C	N3-C4-N4	5.95	122.17	118.00
27	B8	456	C	N3-C4-C5	-5.95	119.52	121.90
27	B8	980	A	C4-C5-C6	5.95	119.97	117.00
27	B8	1065	U	O4'-C1'-N1	5.95	112.96	108.20
27	B8	1637	A	C5-C6-N1	-5.95	114.72	117.70
27	B8	2175	C	N3-C4-N4	5.95	122.17	118.00
27	B8	2448	A	C4-C5-C6	5.95	119.97	117.00
1	AA	613	C	N3-C4-N4	5.95	122.17	118.00
1	AA	1520	C	N3-C4-N4	5.95	122.16	118.00
27	B8	102	U	O4'-C1'-N1	5.95	112.96	108.20
27	B8	254	G	O4'-C1'-N9	5.95	112.96	108.20
27	B8	637	A	C5-C6-N6	-5.95	118.94	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	806	C	N3-C4-N4	5.95	122.16	118.00
27	B8	2854	G	O4'-C1'-N9	5.95	112.96	108.20
1	AA	28	A	C5-C6-N6	-5.95	118.94	123.70
1	AA	282	A	C4-C5-C6	5.95	119.97	117.00
26	B7	21	G	O4'-C1'-N9	5.95	112.96	108.20
27	B8	611	C	N3-C4-N4	5.95	122.16	118.00
1	AA	156	C	N3-C4-N4	5.95	122.16	118.00
1	AA	363	A	O4'-C1'-N9	5.95	112.96	108.20
1	AA	546	A	C4-C5-C6	5.95	119.97	117.00
27	B8	60	G	O4'-C1'-N9	5.95	112.96	108.20
27	B8	564	C	N3-C4-N4	5.95	122.16	118.00
27	B8	706	A	C4-C5-C6	5.95	119.97	117.00
27	B8	1856	U	O4'-C1'-N1	5.95	112.96	108.20
27	B8	2679	A	C4-C5-C6	5.95	119.97	117.00
1	AA	271	C	N3-C4-N4	5.94	122.16	118.00
1	AA	314	C	N3-C4-N4	5.94	122.16	118.00
1	AA	826	C	N3-C4-C5	-5.94	119.52	121.90
1	AA	912	C	N3-C4-N4	5.94	122.16	118.00
27	B8	1676	A	C4-C5-C6	5.94	119.97	117.00
27	B8	2294	G	O4'-C1'-N9	5.94	112.95	108.20
1	AA	320	A	C4-C5-C6	5.94	119.97	117.00
22	AR	4	PHE	CB-CG-CD1	5.94	124.96	120.80
27	B8	923	G	O4'-C1'-N9	5.94	112.95	108.20
27	B8	1270	C	N3-C4-N4	5.94	122.16	118.00
27	B8	1272	A	C4-C5-C6	5.94	119.97	117.00
27	B8	1845	G	O4'-C1'-N9	5.94	112.95	108.20
27	B8	2374	C	N3-C4-N4	5.94	122.16	118.00
27	B8	2770	G	O4'-C1'-N9	5.94	112.95	108.20
1	AA	73	C	N3-C4-N4	5.94	122.16	118.00
1	AA	874	G	O4'-C1'-N9	5.94	112.95	108.20
26	B7	28	C	N3-C4-N4	5.94	122.16	118.00
27	B8	401	A	C4-C5-C6	5.94	119.97	117.00
27	B8	1042	G	C5-C6-O6	-5.94	125.03	128.60
27	B8	1817	G	C5-C6-O6	-5.94	125.04	128.60
27	B8	2053	G	O4'-C1'-N9	5.94	112.95	108.20
27	B8	2171	A	O4'-C1'-N9	5.94	112.95	108.20
27	B8	841	G	O4'-C1'-N9	5.94	112.95	108.20
27	B8	2129	C	C2-N1-C1'	5.94	125.33	118.80
1	AA	130	A	P-O3'-C3'	5.94	126.83	119.70
1	AA	637	C	N3-C4-N4	5.94	122.16	118.00
1	AA	900	A	C4-C5-C6	5.94	119.97	117.00
1	AA	1340	A	O4'-C1'-N9	5.94	112.95	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	706	A	O4'-C1'-N9	5.94	112.95	108.20
27	B8	1080	A	C4-C5-C6	5.94	119.97	117.00
27	B8	1082	U	O4'-C1'-N1	5.94	112.95	108.20
27	B8	1507	C	N3-C4-N4	5.94	122.16	118.00
27	B8	1730	C	C6-N1-C1'	-5.94	113.67	120.80
27	B8	1810	A	C5-C6-N6	-5.94	118.95	123.70
1	AA	269	C	N3-C4-N4	5.93	122.15	118.00
1	AA	478	A	C5-C6-N6	-5.93	118.95	123.70
1	AA	559	A	C4-C5-C6	5.93	119.97	117.00
1	AA	832	G	C5-C6-O6	-5.93	125.04	128.60
1	AA	893	C	N3-C4-C5	-5.93	119.53	121.90
1	AA	922	G	C5-C6-O6	-5.93	125.04	128.60
1	AA	1230	C	N3-C4-N4	5.93	122.15	118.00
1	AA	1269	A	O4'-C1'-N9	5.93	112.95	108.20
1	AA	1501	C	N3-C4-N4	5.93	122.15	118.00
3	AV	60	A	C4-C5-C6	5.93	119.97	117.00
27	B8	14	A	C4-C5-C6	5.93	119.97	117.00
27	B8	346	A	C4-C5-C6	5.93	119.97	117.00
27	B8	538	A	C4-C5-C6	5.93	119.97	117.00
27	B8	582	A	C4-C5-C6	5.93	119.97	117.00
27	B8	690	G	O4'-C1'-N9	5.93	112.95	108.20
27	B8	1158	C	N3-C4-N4	5.93	122.15	118.00
27	B8	1216	G	O4'-C1'-N9	5.93	112.95	108.20
27	B8	2880	C	N3-C4-N4	5.93	122.15	118.00
1	AA	78	A	O4'-C1'-N9	5.93	112.95	108.20
1	AA	816	A	O4'-C1'-N9	5.93	112.95	108.20
1	AA	1160	G	O4'-C1'-N9	5.93	112.95	108.20
27	B8	89	A	C5-C6-N1	-5.93	114.73	117.70
27	B8	400	G	O4'-C1'-N9	5.93	112.95	108.20
27	B8	1000	A	O4'-C1'-N9	5.93	112.94	108.20
27	B8	1150	C	N3-C4-N4	5.93	122.15	118.00
27	B8	2284	A	O4'-C1'-N9	5.93	112.95	108.20
27	B8	2574	G	O4'-C1'-N9	5.93	112.95	108.20
1	AA	574	A	C5-C6-N6	-5.93	118.95	123.70
1	AA	1272	G	O4'-C1'-N9	5.93	112.94	108.20
1	AA	1333	A	C4-C5-C6	5.93	119.97	117.00
27	B8	104	A	C4-C5-C6	5.93	119.97	117.00
27	B8	287	G	O4'-C1'-N9	5.93	112.94	108.20
27	B8	2281	A	C4-C5-C6	5.93	119.97	117.00
27	B8	2600	A	O4'-C1'-N9	5.93	112.94	108.20
1	AA	596	A	C5-C6-N6	-5.93	118.96	123.70
27	B8	340	A	O4'-C1'-N9	5.93	112.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	844	A	C4-C5-C6	5.93	119.96	117.00
27	B8	1392	A	O4'-C1'-N9	5.93	112.94	108.20
27	B8	1572	A	C5-C6-N6	-5.93	118.96	123.70
27	B8	2826	A	O4'-C1'-N9	5.93	112.94	108.20
27	B8	2837	A	C4-C5-C6	5.93	119.97	117.00
1	AA	915	A	C4-C5-C6	5.93	119.96	117.00
1	AA	948	C	N3-C4-N4	5.93	122.15	118.00
27	B8	483	A	C4-C5-C6	5.93	119.96	117.00
27	B8	2397	G	C5-C6-O6	-5.93	125.04	128.60
27	B8	2753	A	C5-C6-N6	-5.93	118.96	123.70
27	B8	2902	C	N3-C4-N4	5.93	122.15	118.00
1	AA	554	A	O4'-C1'-N9	5.93	112.94	108.20
1	AA	735	C	N3-C4-N4	5.93	122.15	118.00
1	AA	768	A	C5-C6-N6	-5.93	118.96	123.70
1	AA	829	G	O4'-C1'-N9	5.93	112.94	108.20
27	B8	84	A	C4-C5-C6	5.93	119.96	117.00
27	B8	862	G	O4'-C1'-N9	5.93	112.94	108.20
27	B8	1127	A	C5-C6-N1	-5.93	114.74	117.70
27	B8	1224	U	O4'-C1'-N1	5.93	112.94	108.20
27	B8	2019	A	C4-C5-C6	5.93	119.96	117.00
1	AA	1110	A	C5-C6-N6	-5.92	118.96	123.70
1	AA	1223	C	N3-C4-N4	5.92	122.15	118.00
1	AA	1234	C	N3-C4-N4	5.92	122.15	118.00
1	AA	1306	A	C5-C6-N6	-5.92	118.96	123.70
3	AV	22	A	C5-C6-N6	-5.92	118.96	123.70
27	B8	83	A	C5-C6-N6	-5.92	118.96	123.70
27	B8	357	C	N3-C4-N4	5.92	122.15	118.00
27	B8	1128	G	O4'-C1'-N9	5.92	112.94	108.20
1	AA	532	A	O4'-C1'-N9	5.92	112.94	108.20
1	AA	1137	C	C2-N1-C1'	5.92	125.32	118.80
27	B8	632	A	C4-C5-C6	5.92	119.96	117.00
27	B8	2031	A	C5-C6-N6	-5.92	118.96	123.70
1	AA	655	A	C4-C5-C6	5.92	119.96	117.00
1	AA	1151	A	C5-C6-N6	-5.92	118.96	123.70
1	AA	1175	G	O4'-C1'-N9	5.92	112.94	108.20
1	AA	1450	U	O4'-C1'-N1	5.92	112.94	108.20
27	B8	152	A	O4'-C1'-N9	5.92	112.94	108.20
27	B8	322	A	C4-C5-C6	5.92	119.96	117.00
27	B8	739	A	C4-C5-C6	5.92	119.96	117.00
27	B8	981	A	C4-C5-C6	5.92	119.96	117.00
27	B8	1200	C	N3-C4-N4	5.92	122.14	118.00
27	B8	1264	A	C4-C5-C6	5.92	119.96	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1265	A	C4-C5-C6	5.92	119.96	117.00
27	B8	1356	G	O4'-C1'-N9	5.92	112.94	108.20
27	B8	1399	C	N3-C4-N4	5.92	122.14	118.00
27	B8	1740	G	O4'-C1'-N9	5.92	112.94	108.20
27	B8	1905	C	N3-C4-N4	5.92	122.14	118.00
27	B8	1927	A	C4-C5-C6	5.92	119.96	117.00
27	B8	1999	C	N3-C4-N4	5.92	122.14	118.00
27	B8	2466	C	N3-C4-N4	5.92	122.14	118.00
1	AA	842	U	C2-N1-C1'	5.92	124.80	117.70
27	B8	274	C	N3-C4-N4	5.92	122.14	118.00
27	B8	323	C	N3-C4-N4	5.92	122.14	118.00
27	B8	902	C	N3-C4-N4	5.92	122.14	118.00
27	B8	2600	A	C5-C6-N6	-5.92	118.96	123.70
27	B8	513	A	O4'-C1'-N9	5.92	112.93	108.20
27	B8	756	A	C4-C5-C6	5.92	119.96	117.00
27	B8	954	G	O4'-C1'-N9	5.92	112.94	108.20
27	B8	1129	A	O4'-C1'-N9	5.92	112.94	108.20
27	B8	1889	A	C4-C5-C6	5.92	119.96	117.00
27	B8	1941	C	N3-C4-N4	5.92	122.14	118.00
27	B8	1953	A	C5-C6-N1	-5.92	114.74	117.70
27	B8	1998	A	O4'-C1'-N9	5.92	112.94	108.20
27	B8	2859	G	C5-C6-O6	-5.92	125.05	128.60
1	AA	59	A	C5-C6-N6	-5.92	118.97	123.70
1	AA	1162	C	N3-C4-N4	5.92	122.14	118.00
1	AA	1432	G	N3-C2-N2	5.92	124.04	119.90
27	B8	84	A	C5-C6-N6	-5.92	118.97	123.70
27	B8	310	A	C5-C6-N1	-5.92	114.74	117.70
27	B8	460	A	C4-C5-C6	5.92	119.96	117.00
27	B8	1010	A	C4-C5-C6	5.92	119.96	117.00
27	B8	1556	C	N3-C4-C5	-5.92	119.53	121.90
27	B8	1805	A	C4-C5-C6	5.92	119.96	117.00
27	B8	2767	C	N3-C4-N4	5.92	122.14	118.00
27	B8	2887	A	C5-C6-N6	-5.92	118.97	123.70
1	AA	796	C	N3-C4-N4	5.92	122.14	118.00
27	B8	19	A	C4-C5-C6	5.92	119.96	117.00
1	AA	344	A	C4-C5-C6	5.91	119.96	117.00
1	AA	581	G	N3-C2-N2	5.91	124.04	119.90
1	AA	896	C	N3-C4-N4	5.91	122.14	118.00
26	B7	119	A	C5-C6-N6	-5.91	118.97	123.70
27	B8	650	C	N3-C4-N4	5.91	122.14	118.00
27	B8	1998	A	C5-C6-N6	-5.91	118.97	123.70
27	B8	2317	A	C5-C6-N6	-5.91	118.97	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2435	A	O4'-C1'-N9	5.91	112.93	108.20
27	B8	2589	A	C5-C6-N1	-5.91	114.74	117.70
27	B8	2725	A	C4-C5-C6	5.91	119.96	117.00
27	B8	2813	A	C4-C5-C6	5.91	119.96	117.00
1	AA	136	C	N3-C4-N4	5.91	122.14	118.00
1	AA	1229	A	C5-C6-N6	-5.91	118.97	123.70
1	AA	1329	A	C4-C5-C6	5.91	119.96	117.00
27	B8	794	A	C4-C5-C6	5.91	119.96	117.00
27	B8	814	C	N3-C4-N4	5.91	122.14	118.00
1	AA	309	A	C4-C5-C6	5.91	119.96	117.00
1	AA	1236	A	C5-C6-N1	-5.91	114.75	117.70
1	AA	1524	C	N3-C4-N4	5.91	122.14	118.00
27	B8	103	A	C4-C5-C6	5.91	119.96	117.00
27	B8	838	C	N3-C4-N4	5.91	122.14	118.00
27	B8	1247	A	C5-C6-N1	-5.91	114.75	117.70
27	B8	1592	C	N3-C4-N4	5.91	122.14	118.00
27	B8	1745	A	C5-C6-N1	-5.91	114.75	117.70
27	B8	1863	G	O4'-C1'-N9	5.91	112.93	108.20
27	B8	1936	A	C5-C6-N6	-5.91	118.97	123.70
27	B8	1960	A	C4-C5-C6	5.91	119.95	117.00
1	AA	539	A	C5-C6-N6	-5.91	118.97	123.70
1	AA	985	C	N3-C4-N4	5.91	122.14	118.00
1	AA	1188	A	C5-C6-N6	-5.91	118.97	123.70
1	AA	1322	C	C6-N1-C1'	-5.91	113.71	120.80
27	B8	5	A	C4-C5-C6	5.91	119.95	117.00
27	B8	97	C	N3-C4-N4	5.91	122.14	118.00
27	B8	422	A	C4-C5-C6	5.91	119.95	117.00
27	B8	627	A	C4-C5-C6	5.91	119.95	117.00
27	B8	2662	A	C5-C6-N1	-5.91	114.75	117.70
27	B8	2829	A	C4-C5-C6	5.91	119.95	117.00
1	AA	131	A	C5-C6-N1	-5.91	114.75	117.70
1	AA	1019	A	O4'-C1'-N9	5.91	112.93	108.20
27	B8	435	C	N3-C4-C5	-5.91	119.54	121.90
27	B8	1450	G	O4'-C1'-N9	5.91	112.93	108.20
27	B8	2545	G	O4'-C1'-N9	5.91	112.93	108.20
1	AA	321	A	C5-C6-N1	-5.91	114.75	117.70
1	AA	1067	A	C4-C5-C6	5.91	119.95	117.00
27	B8	1243	C	N3-C4-N4	5.91	122.13	118.00
27	B8	2009	A	O4'-C1'-N9	5.91	112.92	108.20
27	B8	2147	A	C5-C6-N6	-5.91	118.98	123.70
1	AA	794	A	C4-C5-C6	5.90	119.95	117.00
1	AA	1067	A	C5-C6-N1	-5.90	114.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1250	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	1109	C	N3-C4-N4	5.90	122.13	118.00
27	B8	1677	A	C4-C5-C6	5.90	119.95	117.00
1	AA	328	C	C2-N1-C1'	5.90	125.29	118.80
27	B8	128	C	N3-C4-N4	5.90	122.13	118.00
27	B8	471	A	C5-C6-N1	-5.90	114.75	117.70
27	B8	599	A	C5-C6-N1	-5.90	114.75	117.70
27	B8	812	C	N3-C4-N4	5.90	122.13	118.00
27	B8	978	G	O4'-C1'-N9	5.90	112.92	108.20
27	B8	1039	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	1155	A	C4-C5-C6	5.90	119.95	117.00
27	B8	1241	A	C4-C5-C6	5.90	119.95	117.00
27	B8	1788	C	N3-C4-N4	5.90	122.13	118.00
1	AA	192	A	C5-C6-N1	-5.90	114.75	117.70
1	AA	396	C	N3-C4-N4	5.90	122.13	118.00
1	AA	462	G	O4'-C1'-N9	5.90	112.92	108.20
1	AA	1171	A	C4-C5-C6	5.90	119.95	117.00
1	AA	1364	U	C2-N1-C1'	5.90	124.78	117.70
1	AA	1480	A	C4-C5-C6	5.90	119.95	117.00
27	B8	211	C	N3-C4-N4	5.90	122.13	118.00
27	B8	749	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	789	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	994	C	N3-C4-N4	5.90	122.13	118.00
27	B8	1114	C	N3-C4-N4	5.90	122.13	118.00
27	B8	1334	G	O4'-C1'-N9	5.90	112.92	108.20
27	B8	1586	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	1615	C	O4'-C1'-N1	5.90	112.92	108.20
27	B8	2191	A	C4-C5-C6	5.90	119.95	117.00
27	B8	2710	C	N3-C4-N4	5.90	122.13	118.00
1	AA	11	G	O4'-C1'-N9	5.90	112.92	108.20
1	AA	1082	A	C5-C6-N1	-5.90	114.75	117.70
27	B8	181	A	O4'-C1'-N9	5.90	112.92	108.20
27	B8	404	A	C4-C5-C6	5.90	119.95	117.00
27	B8	624	C	N3-C4-C5	-5.90	119.54	121.90
1	AA	336	A	C4-C5-C6	5.90	119.95	117.00
27	B8	1194	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	1289	C	N3-C4-N4	5.90	122.13	118.00
27	B8	1760	C	N3-C4-N4	5.90	122.13	118.00
27	B8	2013	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	2133	G	O4'-C1'-N9	5.90	112.92	108.20
27	B8	2170	A	C5-C6-N6	-5.90	118.98	123.70
27	B8	2873	A	O4'-C1'-N9	5.90	112.92	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	800	G	C5-C6-O6	-5.90	125.06	128.60
1	AA	899	C	N3-C4-N4	5.90	122.13	118.00
27	B8	2810	A	C5-C6-N6	-5.90	118.98	123.70
1	AA	323	U	O4'-C1'-N1	5.89	112.92	108.20
1	AA	386	C	N3-C4-N4	5.89	122.13	118.00
1	AA	958	A	C5-C6-N1	-5.89	114.75	117.70
1	AA	1208	C	N3-C4-N4	5.89	122.13	118.00
1	AA	1374	A	C4-C5-C6	5.89	119.95	117.00
1	AA	1446	A	C4-C5-C6	5.89	119.95	117.00
27	B8	38	A	C5-C6-N6	-5.89	118.98	123.70
27	B8	322	A	C5-C6-N6	-5.89	118.98	123.70
27	B8	1208	C	N3-C4-N4	5.89	122.13	118.00
27	B8	1978	A	C5-C6-N6	-5.89	118.98	123.70
27	B8	2308	G	C5-C6-O6	-5.89	125.06	128.60
27	B8	2547	A	C4-C5-C6	5.89	119.95	117.00
1	AA	183	C	C2-N1-C1'	5.89	125.28	118.80
1	AA	938	A	C5-C6-N6	-5.89	118.99	123.70
1	AA	1031	C	N3-C4-C5	-5.89	119.54	121.90
27	B8	295	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	602	A	C4-C5-C6	5.89	119.95	117.00
27	B8	1191	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	1230	A	C5-C6-N6	-5.89	118.99	123.70
27	B8	1544	A	O4'-C1'-N9	5.89	112.91	108.20
27	B8	2075	U	O4'-C1'-N1	5.89	112.91	108.20
1	AA	68	G	C5-C6-O6	-5.89	125.06	128.60
1	AA	1214	C	O4'-C1'-N1	5.89	112.91	108.20
1	AA	1410	A	O4'-C1'-N9	5.89	112.91	108.20
27	B8	21	A	O4'-C1'-N9	5.89	112.91	108.20
27	B8	1446	C	N3-C4-N4	5.89	122.12	118.00
27	B8	1553	A	C4-C5-C6	5.89	119.94	117.00
27	B8	2837	A	C5-C6-N6	-5.89	118.99	123.70
1	AA	1049	U	O4'-C1'-N1	5.89	112.91	108.20
1	AA	1427	C	N3-C4-N4	5.89	122.12	118.00
1	AA	1429	A	C4-C5-C6	5.89	119.94	117.00
3	AV	59	A	C4-C5-C6	5.89	119.94	117.00
26	B7	118	C	N3-C4-N4	5.89	122.12	118.00
27	B8	382	A	C4-C5-C6	5.89	119.94	117.00
27	B8	605	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	855	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	910	A	C5-C6-N1	-5.89	114.75	117.70
27	B8	989	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	1090	A	O4'-C1'-N9	5.89	112.91	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1294	U	O4'-C1'-N1	5.89	112.91	108.20
27	B8	1639	C	O4'-C1'-N1	5.89	112.91	108.20
27	B8	1741	C	N3-C4-N4	5.89	122.12	118.00
27	B8	2317	A	O4'-C1'-N9	5.89	112.91	108.20
1	AA	7	A	C4-C5-C6	5.89	119.94	117.00
27	B8	904	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	1623	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	2132	U	C2-N1-C1'	5.89	124.77	117.70
1	AA	414	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1042	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1508	A	C4-C5-C6	5.89	119.94	117.00
26	B7	19	C	N3-C4-N4	5.89	122.12	118.00
27	B8	371	A	C5-C6-N1	-5.89	114.76	117.70
27	B8	1366	A	C5-C6-N6	-5.89	118.99	123.70
27	B8	2115	G	O4'-C1'-N9	5.89	112.91	108.20
27	B8	2200	C	N3-C4-C5	-5.89	119.55	121.90
27	B8	2250	G	C5-C6-O6	-5.89	125.07	128.60
27	B8	2630	G	O4'-C1'-N9	5.89	112.91	108.20
35	BG	108	PHE	CB-CG-CD1	-5.89	116.68	120.80
1	AA	45	G	O4'-C1'-N9	5.88	112.91	108.20
1	AA	694	A	C5-C6-N6	-5.88	118.99	123.70
1	AA	736	C	N3-C4-N4	5.88	122.12	118.00
1	AA	815	A	C4-C5-C6	5.88	119.94	117.00
1	AA	1246	A	C5-C6-N1	-5.88	114.76	117.70
1	AA	1358	U	O4'-C1'-N1	5.88	112.91	108.20
1	AA	1377	A	C5-C6-N6	-5.88	118.99	123.70
27	B8	410	G	N3-C2-N2	5.88	124.02	119.90
27	B8	691	C	N3-C4-N4	5.88	122.12	118.00
27	B8	2162	G	O4'-C1'-N9	5.88	112.91	108.20
27	B8	2198	A	C4-C5-C6	5.88	119.94	117.00
27	B8	2820	A	C4-C5-C6	5.88	119.94	117.00
27	B8	2823	A	C4-C5-C6	5.88	119.94	117.00
1	AA	1176	A	C4-C5-C6	5.88	119.94	117.00
27	B8	847	U	C2-N1-C1'	5.88	124.76	117.70
27	B8	982	C	C6-N1-C1'	-5.88	113.74	120.80
27	B8	1663	G	O4'-C1'-N9	5.88	112.91	108.20
27	B8	2252	G	O4'-C1'-N9	5.88	112.91	108.20
1	AA	301	G	O4'-C1'-N9	5.88	112.90	108.20
1	AA	1155	A	C5-C6-N1	-5.88	114.76	117.70
1	AA	1167	A	C4-C5-C6	5.88	119.94	117.00
1	AA	1339	A	O4'-C1'-N9	5.88	112.91	108.20
1	AA	1492	A	O4'-C1'-N9	5.88	112.91	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	127	A	C4-C5-C6	5.88	119.94	117.00
27	B8	961	C	O4'-C1'-N1	5.88	112.91	108.20
27	B8	2000	C	N3-C4-N4	5.88	122.12	118.00
27	B8	2191	A	C5-C6-N1	-5.88	114.76	117.70
27	B8	2281	A	O4'-C1'-N9	5.88	112.91	108.20
27	B8	2468	A	C4-C5-C6	5.88	119.94	117.00
27	B8	2636	C	N3-C4-N4	5.88	122.12	118.00
27	B8	2706	A	C5-C6-N6	-5.88	118.99	123.70
27	B8	2882	A	C4-C5-C6	5.88	119.94	117.00
1	AA	655	A	C5-C6-N1	-5.88	114.76	117.70
1	AA	949	A	C4-C5-C6	5.88	119.94	117.00
1	AA	1340	A	C4-C5-C6	5.88	119.94	117.00
27	B8	1325	U	O4'-C1'-N1	5.88	112.90	108.20
27	B8	1362	C	N3-C4-N4	5.88	122.12	118.00
27	B8	2169	A	C4-C5-C6	5.88	119.94	117.00
27	B8	455	C	N3-C4-C5	-5.88	119.55	121.90
27	B8	497	A	C5-C6-N1	-5.88	114.76	117.70
27	B8	905	A	O4'-C1'-N9	5.88	112.90	108.20
27	B8	1194	A	C4-C5-C6	5.88	119.94	117.00
27	B8	1768	C	N3-C4-N4	5.88	122.11	118.00
27	B8	2005	A	C4-C5-C6	5.88	119.94	117.00
27	B8	2090	A	C4-C5-C6	5.88	119.94	117.00
27	B8	2722	G	O4'-C1'-N9	5.88	112.90	108.20
1	AA	553	A	C5-C6-N6	-5.88	119.00	123.70
1	AA	974	A	C5-C6-N6	-5.88	119.00	123.70
27	B8	798	G	O4'-C1'-N9	5.88	112.90	108.20
27	B8	1260	A	O4'-C1'-N9	5.88	112.90	108.20
27	B8	1978	A	O4'-C1'-N9	5.88	112.90	108.20
27	B8	2021	C	N3-C4-N4	5.88	122.11	118.00
1	AA	300	A	C4-C5-C6	5.88	119.94	117.00
1	AA	533	A	C5-C6-N1	-5.88	114.76	117.70
1	AA	773	G	O4'-C1'-N9	5.88	112.90	108.20
27	B8	2359	C	N3-C4-N4	5.88	122.11	118.00
1	AA	19	A	C5-C6-N6	-5.87	119.00	123.70
1	AA	629	A	C5-C6-N6	-5.87	119.00	123.70
1	AA	687	A	C4-C5-C6	5.87	119.94	117.00
1	AA	946	A	C5-C6-N1	-5.87	114.76	117.70
27	B8	181	A	C4-C5-C6	5.87	119.94	117.00
27	B8	429	A	C5-C6-N6	-5.87	119.00	123.70
27	B8	544	C	C6-N1-C1'	-5.87	113.75	120.80
27	B8	1757	A	C5-C6-N6	-5.87	119.00	123.70
27	B8	1773	A	O4'-C1'-N9	5.87	112.90	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2059	A	C4-C5-C6	5.87	119.94	117.00
1	AA	65	A	C4-C5-C6	5.87	119.94	117.00
1	AA	263	A	C5-C6-N6	-5.87	119.00	123.70
1	AA	434	U	O4'-C1'-N1	5.87	112.90	108.20
1	AA	1063	C	O4'-C1'-N1	5.87	112.90	108.20
26	B7	54	G	O4'-C1'-N9	5.87	112.90	108.20
27	B8	746	U	O4'-C1'-N1	5.87	112.90	108.20
1	AA	441	A	C4-C5-C6	5.87	119.94	117.00
1	AA	1058	G	O4'-C1'-N9	5.87	112.90	108.20
27	B8	920	A	C5-C6-N1	-5.87	114.77	117.70
1	AA	223	A	C5-C6-N1	-5.87	114.77	117.70
27	B8	26	G	N3-C2-N2	5.87	124.01	119.90
27	B8	950	G	O4'-C1'-N9	5.87	112.89	108.20
27	B8	1615	C	N3-C4-N4	5.87	122.11	118.00
27	B8	1618	A	C5-C6-N6	-5.87	119.00	123.70
27	B8	1749	A	C5-C6-N1	-5.87	114.77	117.70
27	B8	1881	C	N3-C4-N4	5.87	122.11	118.00
27	B8	1969	A	C5-C6-N1	-5.87	114.77	117.70
27	B8	2108	A	C4-C5-C6	5.87	119.94	117.00
27	B8	2807	U	O4'-C1'-N1	5.87	112.89	108.20
1	AA	3	A	C5-C6-N6	-5.87	119.01	123.70
1	AA	525	C	N3-C4-N4	5.87	122.11	118.00
27	B8	2841	C	N3-C4-N4	5.87	122.11	118.00
1	AA	205	A	O4'-C1'-N9	5.87	112.89	108.20
1	AA	443	C	N3-C4-N4	5.87	122.11	118.00
1	AA	705	G	O4'-C1'-N9	5.87	112.89	108.20
1	AA	1237	C	N3-C4-N4	5.87	122.11	118.00
1	AA	1254	A	C4-C5-C6	5.87	119.93	117.00
1	AA	1513	A	C4-C5-C6	5.87	119.93	117.00
27	B8	395	U	O4'-C1'-N1	5.87	112.89	108.20
27	B8	480	A	O4'-C1'-N9	5.87	112.89	108.20
27	B8	716	A	C5-C6-N6	-5.87	119.01	123.70
27	B8	1126	A	C4-C5-C6	5.87	119.93	117.00
27	B8	2311	A	C5-C6-N1	-5.87	114.77	117.70
27	B8	2362	C	N3-C4-N4	5.87	122.11	118.00
27	B8	2369	A	C4-C5-C6	5.87	119.93	117.00
27	B8	2753	A	O4'-C1'-N9	5.87	112.89	108.20
27	B8	2756	U	P-O3'-C3'	5.87	126.74	119.70
1	AA	182	A	C5-C6-N1	-5.86	114.77	117.70
1	AA	382	A	C4-C5-C6	5.86	119.93	117.00
27	B8	191	A	C5-C6-N1	-5.86	114.77	117.70
27	B8	965	C	N3-C4-C5	-5.86	119.55	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	977	G	O4'-C1'-N9	5.86	112.89	108.20
27	B8	1771	C	N3-C4-N4	5.86	122.10	118.00
1	AA	453	G	O4'-C1'-N9	5.86	112.89	108.20
27	B8	1496	A	C4-C5-C6	5.86	119.93	117.00
1	AA	199	A	C5-C6-N1	-5.86	114.77	117.70
1	AA	346	G	O4'-C1'-N9	5.86	112.89	108.20
1	AA	1054	C	N3-C4-N4	5.86	122.10	118.00
27	B8	53	A	C5-C6-N6	-5.86	119.01	123.70
27	B8	2411	A	C5-C6-N6	-5.86	119.01	123.70
27	B8	2829	A	C5-C6-N1	-5.86	114.77	117.70
1	AA	1280	A	C4-C5-C6	5.86	119.93	117.00
27	B8	1050	A	C5-C6-N6	-5.86	119.01	123.70
27	B8	1408	G	O4'-C1'-N9	5.86	112.89	108.20
27	B8	2213	U	O4'-C1'-N1	5.86	112.89	108.20
27	B8	2791	G	O4'-C1'-N9	5.86	112.89	108.20
1	AA	350	G	O4'-C1'-N9	5.86	112.89	108.20
1	AA	441	A	O4'-C1'-N9	5.86	112.89	108.20
1	AA	553	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1021	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1157	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1204	A	C5-C6-N1	-5.86	114.77	117.70
1	AA	1388	C	N3-C4-N4	5.86	122.10	118.00
26	B7	73	A	C5-C6-N1	-5.86	114.77	117.70
27	B8	382	A	C5-C6-N1	-5.86	114.77	117.70
27	B8	421	C	N3-C4-N4	5.86	122.10	118.00
27	B8	1009	A	C5-C6-N6	-5.86	119.01	123.70
27	B8	1090	A	C4-C5-C6	5.86	119.93	117.00
27	B8	1244	A	C4-C5-C6	5.86	119.93	117.00
27	B8	1496	A	O4'-C1'-N9	5.86	112.89	108.20
27	B8	1690	A	O4'-C1'-N9	5.86	112.89	108.20
27	B8	2326	C	N3-C4-N4	5.86	122.10	118.00
27	B8	2518	A	C4-C5-C6	5.86	119.93	117.00
27	B8	2670	A	C5-C6-N6	-5.86	119.01	123.70
27	B8	2814	A	O4'-C1'-N9	5.86	112.89	108.20
1	AA	647	C	N3-C4-N4	5.86	122.10	118.00
1	AA	949	A	C5-C6-N1	-5.86	114.77	117.70
27	B8	945	A	C5-C6-N6	-5.86	119.02	123.70
27	B8	1558	C	N3-C4-C5	-5.86	119.56	121.90
27	B8	1952	A	C5-C6-N6	-5.86	119.02	123.70
27	B8	2206	C	N3-C4-N4	5.86	122.10	118.00
27	B8	2314	A	C5-C6-N1	-5.86	114.77	117.70
27	B8	2449	U	O4'-C1'-N1	5.86	112.89	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2570	G	O4'-C1'-N9	5.86	112.89	108.20
27	B8	2676	C	N3-C4-N4	5.86	122.10	118.00
26	B7	70	C	N3-C4-N4	5.85	122.10	118.00
27	B8	1014	A	C4-C5-C6	5.85	119.93	117.00
27	B8	2412	A	C5-C6-N6	-5.85	119.02	123.70
1	AA	504	C	N3-C4-C5	-5.85	119.56	121.90
1	AA	771	G	O4'-C1'-N9	5.85	112.88	108.20
1	AA	1377	A	O4'-C1'-N9	5.85	112.88	108.20
1	AA	1413	A	C5-C6-N1	-5.85	114.77	117.70
27	B8	549	G	O4'-C1'-N9	5.85	112.88	108.20
27	B8	715	A	C4-C5-C6	5.85	119.93	117.00
27	B8	1503	A	C5-C6-N1	-5.85	114.77	117.70
1	AA	560	A	C5-C6-N6	-5.85	119.02	123.70
1	AA	737	C	N3-C4-C5	-5.85	119.56	121.90
1	AA	1196	A	C5-C6-N6	-5.85	119.02	123.70
27	B8	429	A	C5-C6-N1	-5.85	114.77	117.70
27	B8	557	C	N3-C4-N4	5.85	122.09	118.00
27	B8	1490	A	C5-C6-N6	-5.85	119.02	123.70
27	B8	1928	A	O4'-C1'-N9	5.85	112.88	108.20
27	B8	2665	A	C5-C6-N6	-5.85	119.02	123.70
1	AA	171	A	O4'-C1'-N9	5.85	112.88	108.20
1	AA	217	C	N3-C4-N4	5.85	122.09	118.00
1	AA	384	G	O4'-C1'-N9	5.85	112.88	108.20
27	B8	1579	A	O4'-C1'-N9	5.85	112.88	108.20
1	AA	236	A	C5-C6-N6	-5.85	119.02	123.70
1	AA	341	C	N3-C4-N4	5.85	122.09	118.00
1	AA	414	A	O4'-C1'-N9	5.85	112.88	108.20
3	AV	63	C	N3-C4-C5	-5.85	119.56	121.90
27	B8	111	A	C5-C6-N6	-5.85	119.02	123.70
27	B8	209	C	N3-C4-N4	5.85	122.09	118.00
27	B8	679	C	N3-C4-N4	5.85	122.09	118.00
27	B8	951	C	N3-C4-N4	5.85	122.09	118.00
27	B8	1502	A	C4-C5-C6	5.85	119.92	117.00
27	B8	2268	A	C5-C6-N1	-5.85	114.78	117.70
27	B8	2781	A	C4-C5-C6	5.85	119.92	117.00
1	AA	1352	C	N3-C4-N4	5.85	122.09	118.00
26	B7	94	A	C5-C6-N6	-5.85	119.02	123.70
27	B8	1167	C	N3-C4-N4	5.85	122.09	118.00
27	B8	2052	A	C4-C5-C6	5.85	119.92	117.00
27	B8	2733	A	O4'-C1'-N9	5.85	112.88	108.20
27	B8	2740	A	C4-C5-C6	5.85	119.92	117.00
27	B8	2781	A	C5-C6-N6	-5.85	119.02	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	817	C	N3-C4-N4	5.84	122.09	118.00
27	B8	825	A	C4-C5-C6	5.84	119.92	117.00
27	B8	935	C	N3-C4-N4	5.84	122.09	118.00
27	B8	1609	A	C5-C6-N6	-5.84	119.02	123.70
27	B8	1965	C	N3-C4-N4	5.84	122.09	118.00
27	B8	2093	G	O4'-C1'-N9	5.84	112.88	108.20
27	B8	2386	A	C4-C5-C6	5.84	119.92	117.00
1	AA	959	A	C5-C6-N1	-5.84	114.78	117.70
27	B8	1764	C	N3-C4-N4	5.84	122.09	118.00
27	B8	2376	A	C5-C6-N6	-5.84	119.03	123.70
1	AA	51	A	C5-C6-N1	-5.84	114.78	117.70
1	AA	100	G	O4'-C1'-N9	5.84	112.87	108.20
1	AA	825	A	O4'-C1'-N9	5.84	112.87	108.20
26	B7	47	C	N3-C4-C5	-5.84	119.56	121.90
27	B8	599	A	C4-C5-C6	5.84	119.92	117.00
27	B8	2156	G	C5-C6-O6	-5.84	125.09	128.60
27	B8	2176	A	C4-C5-C6	5.84	119.92	117.00
1	AA	61	G	O4'-C1'-N9	5.84	112.87	108.20
1	AA	257	G	O4'-C1'-N9	5.84	112.87	108.20
1	AA	452	A	O4'-C1'-N9	5.84	112.87	108.20
1	AA	938	A	C4-C5-C6	5.84	119.92	117.00
1	AA	1322	C	N3-C4-C5	-5.84	119.56	121.90
27	B8	394	C	N3-C4-N4	5.84	122.09	118.00
27	B8	917	A	C5-C6-N1	-5.84	114.78	117.70
27	B8	1416	G	O4'-C1'-N9	5.84	112.87	108.20
27	B8	1595	C	N3-C4-N4	5.84	122.09	118.00
1	AA	32	A	C5-C6-N6	-5.84	119.03	123.70
27	B8	1142	A	C5'-C4'-O4'	5.84	116.11	109.10
27	B8	1272	A	O4'-C1'-N9	5.84	112.87	108.20
27	B8	1906	G	O4'-C1'-N9	5.84	112.87	108.20
27	B8	2313	C	N3-C4-N4	5.84	122.09	118.00
27	B8	2691	C	N3-C4-N4	5.84	122.09	118.00
1	AA	243	A	C4'-C3'-C2'	5.84	108.44	102.60
1	AA	1176	A	O4'-C1'-N9	5.84	112.87	108.20
27	B8	203	A	C5-C6-N6	-5.84	119.03	123.70
27	B8	272	A	C4-C5-C6	5.84	119.92	117.00
27	B8	539	G	C5-C6-O6	-5.84	125.10	128.60
27	B8	608	A	C5-C6-N6	-5.84	119.03	123.70
27	B8	764	A	C5-C6-N1	-5.84	114.78	117.70
27	B8	1585	C	N3-C4-N4	5.84	122.09	118.00
27	B8	2060	A	C4-C5-C6	5.84	119.92	117.00
1	AA	435	A	C5-C6-N6	-5.83	119.03	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1461	G	O4'-C1'-N9	5.83	112.87	108.20
27	B8	829	A	C4-C5-C6	5.83	119.92	117.00
27	B8	1077	A	O4'-C1'-N9	5.83	112.87	108.20
27	B8	1091	G	O4'-C1'-N9	5.83	112.87	108.20
27	B8	1161	C	N3-C4-N4	5.83	122.08	118.00
27	B8	2183	A	C5-C6-N6	-5.83	119.03	123.70
27	B8	2740	A	C5-C6-N6	-5.83	119.03	123.70
1	AA	246	A	C5-C6-N1	-5.83	114.78	117.70
1	AA	302	G	O4'-C1'-N9	5.83	112.87	108.20
1	AA	497	G	O4'-C1'-N9	5.83	112.87	108.20
1	AA	511	C	N3-C4-N4	5.83	122.08	118.00
1	AA	999	C	N3-C4-N4	5.83	122.08	118.00
1	AA	1155	A	C4-C5-C6	5.83	119.92	117.00
3	AV	52	A	C4-C5-C6	5.83	119.92	117.00
27	B8	146	A	C4-C5-C6	5.83	119.92	117.00
27	B8	203	A	C4-C5-C6	5.83	119.92	117.00
27	B8	949	G	O4'-C1'-N9	5.83	112.87	108.20
27	B8	1079	C	N3-C4-N4	5.83	122.08	118.00
27	B8	1338	G	O4'-C1'-N9	5.83	112.87	108.20
1	AA	819	A	C4-C5-C6	5.83	119.92	117.00
1	AA	1051	C	N3-C4-N4	5.83	122.08	118.00
1	AA	1331	G	N3-C2-N2	5.83	123.98	119.90
3	AV	6	C	N3-C4-N4	5.83	122.08	118.00
26	B7	67	G	C5-C6-O6	-5.83	125.10	128.60
27	B8	300	A	C5-C6-N6	-5.83	119.03	123.70
27	B8	695	G	O4'-C1'-N9	5.83	112.87	108.20
27	B8	1373	A	C5-C6-N1	-5.83	114.78	117.70
27	B8	1654	A	C5-C6-N6	-5.83	119.03	123.70
27	B8	1754	A	O4'-C1'-N9	5.83	112.86	108.20
27	B8	2594	C	N3-C4-N4	5.83	122.08	118.00
27	B8	2734	A	C4-C5-C6	5.83	119.92	117.00
1	AA	634	C	N3-C4-N4	5.83	122.08	118.00
1	AA	1107	C	N3-C4-N4	5.83	122.08	118.00
1	AA	1456	A	O4'-C1'-N9	5.83	112.86	108.20
27	B8	666	A	C4-C5-C6	5.83	119.92	117.00
1	AA	522	C	N3-C4-N4	5.83	122.08	118.00
1	AA	1184	G	O4'-C1'-N9	5.83	112.86	108.20
26	B7	39	A	O4'-C1'-N9	5.83	112.86	108.20
27	B8	320	A	C5-C6-N6	-5.83	119.04	123.70
27	B8	524	G	O4'-C1'-N9	5.83	112.86	108.20
27	B8	733	G	O4'-C1'-N9	5.83	112.86	108.20
27	B8	1129	A	C4-C5-C6	5.83	119.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1239	G	O4'-C1'-N9	5.83	112.86	108.20
27	B8	1499	C	N3-C4-N4	5.83	122.08	118.00
27	B8	1609	A	C4-C5-C6	5.83	119.91	117.00
27	B8	345	A	C5-C6-N6	-5.83	119.04	123.70
27	B8	1241	A	C5-C6-N6	-5.83	119.04	123.70
27	B8	1986	C	N3-C4-N4	5.83	122.08	118.00
1	AA	303	A	C5-C6-N1	-5.83	114.79	117.70
1	AA	487	A	C5-C6-N1	-5.83	114.79	117.70
1	AA	780	A	C4-C5-C6	5.83	119.91	117.00
1	AA	781	A	C5-C6-N1	-5.83	114.79	117.70
1	AA	787	A	C5-C6-N6	-5.83	119.04	123.70
3	AV	12	G	O4'-C1'-N9	5.83	112.86	108.20
27	B8	1009	A	C4-C5-C6	5.83	119.91	117.00
27	B8	1040	A	O4'-C1'-N9	5.83	112.86	108.20
27	B8	1359	A	C5-C6-N6	-5.83	119.04	123.70
27	B8	1504	A	C5-C6-N1	-5.83	114.79	117.70
27	B8	2091	C	N3-C4-N4	5.83	122.08	118.00
27	B8	2592	G	O4'-C1'-N9	5.83	112.86	108.20
1	AA	8	A	C5-C6-N6	-5.82	119.04	123.70
27	B8	655	A	C4-C5-C6	5.82	119.91	117.00
27	B8	1012	U	O4'-C1'-N1	5.82	112.86	108.20
27	B8	1257	C	N3-C4-N4	5.82	122.08	118.00
27	B8	2295	C	N3-C4-N4	5.82	122.08	118.00
27	B8	2642	G	O4'-C1'-N9	5.82	112.86	108.20
27	B8	2671	G	O4'-C1'-N9	5.82	112.86	108.20
1	AA	43	C	N3-C4-N4	5.82	122.08	118.00
1	AA	994	A	C5-C6-N6	-5.82	119.04	123.70
26	B7	102	G	O4'-C1'-N9	5.82	112.86	108.20
27	B8	1701	A	O4'-C1'-N9	5.82	112.86	108.20
27	B8	2618	G	O4'-C1'-N9	5.82	112.86	108.20
1	AA	349	A	C4-C5-C6	5.82	119.91	117.00
1	AA	1117	A	C4-C5-C6	5.82	119.91	117.00
26	B7	71	C	N3-C4-N4	5.82	122.07	118.00
27	B8	632	A	C5-C6-N6	-5.82	119.04	123.70
27	B8	717	C	N3-C4-N4	5.82	122.08	118.00
27	B8	1701	A	C4-C5-C6	5.82	119.91	117.00
27	B8	2891	U	O4'-C1'-N1	5.82	112.86	108.20
1	AA	1271	A	O4'-C1'-N9	5.82	112.86	108.20
27	B8	634	C	N3-C4-N4	5.82	122.07	118.00
27	B8	996	A	C5-C6-N6	-5.82	119.05	123.70
27	B8	1456	G	O4'-C1'-N9	5.82	112.86	108.20
1	AA	338	A	C5-C6-N1	-5.82	114.79	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	969	A	C4-C5-C6	5.82	119.91	117.00
27	B8	796	C	N3-C4-N4	5.82	122.07	118.00
27	B8	995	C	N3-C4-N4	5.82	122.07	118.00
27	B8	1028	A	C4-C5-C6	5.82	119.91	117.00
27	B8	1548	A	C5-C6-N6	-5.82	119.05	123.70
27	B8	1614	A	C4-C5-C6	5.82	119.91	117.00
27	B8	1711	A	C4-C5-C6	5.82	119.91	117.00
27	B8	1968	G	N3-C2-N2	5.82	123.97	119.90
27	B8	2264	C	N3-C4-N4	5.82	122.07	118.00
27	B8	2340	A	C4-C5-C6	5.82	119.91	117.00
27	B8	2794	C	N3-C4-N4	5.82	122.07	118.00
48	BT	99	ALA	N-CA-CB	5.82	118.24	110.10
1	AA	665	A	C4-C5-C6	5.82	119.91	117.00
1	AA	994	A	O4'-C1'-N9	5.82	112.85	108.20
27	B8	91	A	C5-C6-N1	-5.82	114.79	117.70
27	B8	618	G	O4'-C1'-N9	5.82	112.85	108.20
27	B8	1284	A	C4-C5-C6	5.82	119.91	117.00
27	B8	1480	C	N3-C4-N4	5.82	122.07	118.00
27	B8	1495	A	C5-C6-N6	-5.82	119.05	123.70
27	B8	2406	A	C5-C6-N6	-5.82	119.05	123.70
1	AA	816	A	C5-C6-N6	-5.81	119.05	123.70
27	B8	988	A	C5-C6-N1	-5.81	114.79	117.70
27	B8	1479	G	O4'-C1'-N9	5.81	112.85	108.20
1	AA	149	A	C5-C6-N6	-5.81	119.05	123.70
1	AA	393	A	C5-C6-N1	-5.81	114.79	117.70
1	AA	1140	C	N3-C4-N4	5.81	122.07	118.00
1	AA	1311	A	C4-C5-C6	5.81	119.91	117.00
27	B8	1075	C	N3-C4-N4	5.81	122.07	118.00
27	B8	1399	C	N3-C4-C5	-5.81	119.58	121.90
27	B8	2021	C	N3-C4-C5	-5.81	119.58	121.90
27	B8	2064	C	N3-C4-N4	5.81	122.07	118.00
27	B8	2600	A	C4-C5-C6	5.81	119.91	117.00
27	B8	2651	C	N3-C4-N4	5.81	122.07	118.00
27	B8	2057	G	O4'-C1'-N9	5.81	112.85	108.20
1	AA	124	C	N3-C4-N4	5.81	122.07	118.00
1	AA	411	A	C4-C5-C6	5.81	119.90	117.00
1	AA	1210	C	N3-C4-N4	5.81	122.07	118.00
26	B7	93	C	N3-C4-N4	5.81	122.07	118.00
27	B8	98	G	O4'-C1'-N9	5.81	112.85	108.20
27	B8	1226	A	C5-C6-N1	-5.81	114.80	117.70
27	B8	1276	A	C4-C5-C6	5.81	119.91	117.00
27	B8	1549	A	C4-C5-C6	5.81	119.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1591	A	C4-C5-C6	5.81	119.90	117.00
27	B8	2063	C	N3-C4-N4	5.81	122.07	118.00
1	AA	44	A	C5-C6-N1	-5.81	114.80	117.70
1	AA	76	G	P-O5'-C5'	5.81	130.19	120.90
1	AA	1007	U	O4'-C1'-N1	5.81	112.85	108.20
1	AA	1340	A	C5-C6-N1	-5.81	114.80	117.70
27	B8	180	G	O4'-C1'-N9	5.81	112.85	108.20
27	B8	466	A	C5-C6-N1	-5.81	114.80	117.70
27	B8	1679	A	C4-C5-C6	5.81	119.90	117.00
27	B8	2097	A	C4-C5-C6	5.81	119.90	117.00
27	B8	2146	C	N3-C4-C5	-5.81	119.58	121.90
1	AA	1081	A	C4-C5-C6	5.81	119.90	117.00
1	AA	1437	A	C5-C6-N1	-5.81	114.80	117.70
27	B8	608	A	O4'-C1'-N9	5.81	112.84	108.20
27	B8	1260	A	C4-C5-C6	5.81	119.90	117.00
27	B8	2051	A	C4-C5-C6	5.81	119.90	117.00
27	B8	2903	U	C6-N1-C1'	-5.81	113.07	121.20
1	AA	576	C	N3-C4-N4	5.80	122.06	118.00
1	AA	1519	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	146	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	742	A	O4'-C1'-N9	5.80	112.84	108.20
27	B8	1145	C	N3-C4-N4	5.80	122.06	118.00
27	B8	1433	A	C5-C6-N6	-5.80	119.06	123.70
26	B7	115	A	O4'-C1'-N9	5.80	112.84	108.20
27	B8	69	C	N3-C4-C5	-5.80	119.58	121.90
27	B8	299	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	1936	A	C5-C6-N1	-5.80	114.80	117.70
1	AA	353	A	C4-C5-C6	5.80	119.90	117.00
1	AA	1350	A	C4-C5-C6	5.80	119.90	117.00
26	B7	115	A	C4-C5-C6	5.80	119.90	117.00
27	B8	144	A	O4'-C1'-N9	5.80	112.84	108.20
27	B8	1048	A	C5-C6-N1	-5.80	114.80	117.70
27	B8	1293	C	N3-C4-N4	5.80	122.06	118.00
27	B8	1819	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	2158	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	2737	G	O4'-C1'-N9	5.80	112.84	108.20
1	AA	26	A	C5-C6-N6	-5.80	119.06	123.70
1	AA	44	A	C4-C5-C6	5.80	119.90	117.00
1	AA	579	A	C5-C6-N6	-5.80	119.06	123.70
1	AA	749	A	C4-C5-C6	5.80	119.90	117.00
1	AA	784	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	845	A	C5-C6-N6	-5.80	119.06	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1667	G	O4'-C1'-N9	5.80	112.84	108.20
27	B8	1952	A	C4-C5-C6	5.80	119.90	117.00
27	B8	2247	A	C4-C5-C6	5.80	119.90	117.00
1	AA	342	C	N3-C4-N4	5.80	122.06	118.00
26	B7	12	C	N3-C4-N4	5.80	122.06	118.00
27	B8	940	G	O4'-C1'-N9	5.80	112.84	108.20
27	B8	2020	A	C4-C5-C6	5.80	119.90	117.00
27	B8	2070	A	C4-C5-C6	5.80	119.90	117.00
1	AA	648	A	C4-C5-C6	5.80	119.90	117.00
1	AA	649	A	C5-C6-N1	-5.80	114.80	117.70
1	AA	805	C	N3-C4-N4	5.80	122.06	118.00
1	AA	1350	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	466	A	O4'-C1'-N9	5.80	112.84	108.20
27	B8	495	G	O4'-C1'-N9	5.80	112.84	108.20
27	B8	638	G	O4'-C1'-N9	5.80	112.84	108.20
27	B8	1616	A	C4-C5-C6	5.80	119.90	117.00
27	B8	2126	A	C5-C6-N6	-5.80	119.06	123.70
27	B8	2332	C	N3-C4-N4	5.80	122.06	118.00
27	B8	2700	A	C4-C5-C6	5.80	119.90	117.00
1	AA	752	G	O4'-C1'-N9	5.79	112.84	108.20
1	AA	1375	A	C5-C6-N1	-5.79	114.80	117.70
27	B8	226	A	O4'-C1'-N9	5.79	112.84	108.20
27	B8	1949	G	O4'-C1'-N9	5.79	112.84	108.20
27	B8	2328	A	C5-C6-N6	-5.79	119.06	123.70
27	B8	2418	A	C4-C5-C6	5.79	119.90	117.00
27	B8	2806	C	N3-C4-N4	5.79	122.06	118.00
1	AA	215	C	N3-C4-C5	-5.79	119.58	121.90
1	AA	535	A	C4-C5-C6	5.79	119.90	117.00
1	AA	635	A	C4-C5-C6	5.79	119.90	117.00
1	AA	935	A	C5-C6-N6	-5.79	119.06	123.70
27	B8	31	C	N3-C4-N4	5.79	122.06	118.00
27	B8	197	A	C5-C6-N6	-5.79	119.07	123.70
27	B8	238	C	N3-C4-N4	5.79	122.06	118.00
27	B8	256	A	C5-C6-N1	-5.79	114.80	117.70
27	B8	621	A	C4-C5-C6	5.79	119.90	117.00
27	B8	928	A	C4-C5-C6	5.79	119.90	117.00
27	B8	1150	C	N3-C4-C5	-5.79	119.58	121.90
27	B8	1444	G	O4'-C1'-N9	5.79	112.83	108.20
27	B8	1634	A	C5-C6-N6	-5.79	119.06	123.70
27	B8	1772	A	C4-C5-C6	5.79	119.90	117.00
27	B8	1903	G	O4'-C1'-N9	5.79	112.83	108.20
27	B8	2462	C	N3-C4-N4	5.79	122.06	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2626	C	N3-C4-N4	5.79	122.06	118.00
27	B8	2628	C	N3-C4-N4	5.79	122.06	118.00
1	AA	546	A	C5-C6-N6	-5.79	119.07	123.70
1	AA	825	A	C4-C5-C6	5.79	119.90	117.00
1	AA	1229	A	C5-C6-N1	-5.79	114.80	117.70
27	B8	590	A	C4-C5-C6	5.79	119.90	117.00
27	B8	1537	G	P-O3'-C3'	5.79	126.65	119.70
27	B8	1591	A	C5-C6-N1	-5.79	114.80	117.70
27	B8	2142	A	C4-C5-C6	5.79	119.90	117.00
27	B8	2456	C	N3-C4-N4	5.79	122.05	118.00
1	AA	33	A	O4'-C1'-N9	5.79	112.83	108.20
1	AA	802	A	C4-C5-C6	5.79	119.89	117.00
26	B7	98	G	O4'-C1'-N9	5.79	112.83	108.20
27	B8	706	A	C5-C6-N6	-5.79	119.07	123.70
1	AA	564	C	N3-C4-N4	5.79	122.05	118.00
1	AA	578	C	N3-C4-N4	5.79	122.05	118.00
1	AA	747	A	C4-C5-C6	5.79	119.89	117.00
1	AA	1271	A	C4-C5-C6	5.79	119.89	117.00
1	AA	1280	A	C5-C6-N6	-5.79	119.07	123.70
27	B8	473	G	O4'-C1'-N9	5.79	112.83	108.20
27	B8	1172	C	N3-C4-N4	5.79	122.05	118.00
27	B8	1197	G	O4'-C1'-N9	5.79	112.83	108.20
27	B8	1236	G	N3-C2-N2	5.79	123.95	119.90
27	B8	2273	A	O4'-C1'-N9	5.79	112.83	108.20
27	B8	2388	A	C5-C6-N1	-5.79	114.81	117.70
1	AA	1161	C	N3-C4-N4	5.79	122.05	118.00
27	B8	64	A	C4-C5-C6	5.79	119.89	117.00
27	B8	2761	A	C5-C6-N1	-5.79	114.81	117.70
1	AA	569	C	N3-C4-N4	5.79	122.05	118.00
1	AA	1141	C	N3-C4-N4	5.79	122.05	118.00
26	B7	46	A	C4-C5-C6	5.79	119.89	117.00
1	AA	959	A	C4-C5-C6	5.78	119.89	117.00
1	AA	1373	G	O4'-C1'-N9	5.78	112.83	108.20
27	B8	2296	U	O4'-C1'-N1	5.78	112.83	108.20
27	B8	2482	A	C5-C6-N1	-5.78	114.81	117.70
1	AA	1249	C	N3-C4-N4	5.78	122.05	118.00
1	AA	1332	A	C4-C5-C6	5.78	119.89	117.00
27	B8	1276	A	O4'-C1'-N9	5.78	112.83	108.20
27	B8	1367	A	C4-C5-C6	5.78	119.89	117.00
1	AA	600	A	C5-C6-N6	-5.78	119.08	123.70
27	B8	462	C	N3-C4-N4	5.78	122.05	118.00
27	B8	590	A	C5-C6-N6	-5.78	119.08	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	869	G	O4'-C1'-N9	5.78	112.82	108.20
27	B8	1111	A	C4-C5-C6	5.78	119.89	117.00
27	B8	1134	A	C5-C6-N6	-5.78	119.08	123.70
27	B8	1169	A	C4-C5-C6	5.78	119.89	117.00
27	B8	1759	A	C4-C5-C6	5.78	119.89	117.00
27	B8	2107	G	O4'-C1'-N9	5.78	112.82	108.20
27	B8	1028	A	O4'-C1'-N9	5.78	112.82	108.20
27	B8	1503	A	C4-C5-C6	5.78	119.89	117.00
1	AA	325	A	O4'-C1'-N9	5.78	112.82	108.20
1	AA	1275	A	O4'-C1'-N9	5.78	112.82	108.20
1	AA	1507	A	C5-C6-N6	-5.78	119.08	123.70
26	B7	90	C	N3-C4-N4	5.78	122.04	118.00
27	B8	689	A	C5-C6-N1	-5.78	114.81	117.70
27	B8	844	A	C5-C6-N1	-5.78	114.81	117.70
27	B8	982	C	N3-C4-N4	5.78	122.04	118.00
27	B8	1728	C	N3-C4-N4	5.78	122.04	118.00
27	B8	1790	C	N3-C4-N4	5.78	122.05	118.00
27	B8	2088	A	C5-C6-N6	-5.78	119.08	123.70
27	B8	2328	A	O4'-C1'-N9	5.78	112.82	108.20
1	AA	50	A	C4-C5-C6	5.78	119.89	117.00
1	AA	407	U	O4'-C1'-N1	5.78	112.82	108.20
1	AA	608	A	C4-C5-C6	5.78	119.89	117.00
1	AA	1106	G	O4'-C1'-N9	5.78	112.82	108.20
1	AA	1128	C	N3-C4-N4	5.78	122.04	118.00
1	AA	1384	C	N3-C4-N4	5.78	122.04	118.00
27	B8	76	C	N3-C4-N4	5.78	122.04	118.00
27	B8	217	A	O4'-C1'-N9	5.78	112.82	108.20
27	B8	783	A	C5-C6-N6	-5.78	119.08	123.70
27	B8	948	C	N3-C4-N4	5.78	122.04	118.00
27	B8	1143	A	C4-C5-C6	5.78	119.89	117.00
27	B8	1230	A	C4-C5-C6	5.78	119.89	117.00
27	B8	1383	A	C5-C6-N6	-5.78	119.08	123.70
27	B8	2058	A	C4-C5-C6	5.78	119.89	117.00
27	B8	2452	C	N3-C4-N4	5.78	122.04	118.00
27	B8	2727	A	C5-C6-N1	-5.78	114.81	117.70
1	AA	1274	A	C5-C6-N6	-5.77	119.08	123.70
27	B8	2119	A	C5-C6-N1	-5.77	114.81	117.70
1	AA	210	C	N3-C4-N4	5.77	122.04	118.00
1	AA	335	C	N3-C4-N4	5.77	122.04	118.00
1	AA	460	A	C4-C5-C6	5.77	119.89	117.00
1	AA	1171	A	C5-C6-N6	-5.77	119.08	123.70
3	AV	5	A	C5-C6-N6	-5.77	119.08	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	71	A	C5-C6-N1	-5.77	114.81	117.70
27	B8	532	A	C4-C5-C6	5.77	119.89	117.00
27	B8	1670	C	N3-C4-C5	-5.77	119.59	121.90
27	B8	66	C	N3-C4-C5	-5.77	119.59	121.90
27	B8	352	A	C5-C6-N6	-5.77	119.08	123.70
27	B8	582	A	O4'-C1'-N9	5.77	112.82	108.20
27	B8	783	A	C4-C5-C6	5.77	119.89	117.00
27	B8	1437	C	N3-C4-N4	5.77	122.04	118.00
1	AA	496	A	O4'-C1'-N9	5.77	112.81	108.20
1	AA	573	A	C5-C6-N6	-5.77	119.08	123.70
1	AA	1113	C	N3-C4-N4	5.77	122.04	118.00
1	AA	1277	C	N3-C4-N4	5.77	122.04	118.00
27	B8	269	C	N3-C4-N4	5.77	122.04	118.00
27	B8	721	A	C4-C5-C6	5.77	119.89	117.00
27	B8	1927	A	C5-C6-N6	-5.77	119.08	123.70
27	B8	1933	G	O4'-C1'-N9	5.77	112.81	108.20
27	B8	2325	G	O4'-C1'-N9	5.77	112.81	108.20
27	B8	2422	C	N3-C4-N4	5.77	122.04	118.00
27	B8	2542	A	C4-C5-C6	5.77	119.89	117.00
27	B8	2657	A	C4-C5-C6	5.77	119.89	117.00
1	AA	974	A	C5-C6-N1	-5.77	114.82	117.70
1	AA	1343	G	O4'-C1'-N9	5.77	112.81	108.20
27	B8	75	G	O4'-C1'-N9	5.77	112.81	108.20
27	B8	604	G	O4'-C1'-N9	5.77	112.81	108.20
27	B8	1077	A	C5-C6-N6	-5.77	119.09	123.70
27	B8	1585	C	N3-C4-C5	-5.77	119.59	121.90
27	B8	2365	G	O4'-C1'-N9	5.77	112.81	108.20
27	B8	2521	C	N3-C4-N4	5.77	122.04	118.00
27	B8	2726	A	O4'-C1'-N9	5.77	112.81	108.20
1	AA	228	A	O4'-C1'-N9	5.77	112.81	108.20
26	B7	50	A	C4-C5-C6	5.77	119.88	117.00
27	B8	475	C	N3-C4-N4	5.77	122.04	118.00
27	B8	1040	A	C4-C5-C6	5.77	119.88	117.00
27	B8	1211	C	N3-C4-C5	-5.77	119.59	121.90
27	B8	1246	A	C4-C5-C6	5.77	119.88	117.00
27	B8	2868	A	O4'-C1'-N9	5.77	112.81	108.20
1	AA	728	A	C5-C6-N6	-5.76	119.09	123.70
1	AA	1214	C	N3-C4-N4	5.76	122.03	118.00
1	AA	1507	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	233	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	1749	A	C4-C5-C6	5.76	119.88	117.00
27	B8	2179	C	N3-C4-N4	5.76	122.04	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2850	A	C5-C6-N6	-5.76	119.09	123.70
1	AA	1008	U	O4'-C1'-N1	5.76	112.81	108.20
27	B8	155	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	362	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	539	G	O4'-C1'-N9	5.76	112.81	108.20
27	B8	749	A	C4-C5-C6	5.76	119.88	117.00
27	B8	1413	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	1837	C	N3-C4-N4	5.76	122.03	118.00
27	B8	2200	C	N3-C4-N4	5.76	122.03	118.00
27	B8	2556	C	N3-C4-N4	5.76	122.03	118.00
27	B8	2741	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	2748	A	C5-C6-N1	-5.76	114.82	117.70
1	AA	572	A	C5-C6-N1	-5.76	114.82	117.70
1	AA	699	C	N3-C4-N4	5.76	122.03	118.00
1	AA	792	A	C4-C5-C6	5.76	119.88	117.00
1	AA	1041	G	O4'-C1'-N9	5.76	112.81	108.20
1	AA	1238	A	O4'-C1'-N9	5.76	112.81	108.20
1	AA	1323	G	O4'-C1'-N9	5.76	112.81	108.20
27	B8	223	A	C4-C5-C6	5.76	119.88	117.00
27	B8	553	G	O4'-C1'-N9	5.76	112.81	108.20
27	B8	782	A	C5-C6-N1	-5.76	114.82	117.70
27	B8	2309	A	O4'-C1'-N9	5.76	112.81	108.20
27	B8	2311	A	C5-C6-N6	-5.76	119.09	123.70
1	AA	706	A	O4'-C1'-N9	5.76	112.81	108.20
1	AA	760	G	O4'-C1'-N9	5.76	112.81	108.20
27	B8	227	A	C5-C6-N6	-5.76	119.09	123.70
27	B8	1525	A	C5-C6-N1	-5.76	114.82	117.70
1	AA	431	A	C4-C5-C6	5.76	119.88	117.00
1	AA	508	U	O4'-C1'-N1	5.76	112.81	108.20
1	AA	679	C	N3-C4-N4	5.76	122.03	118.00
1	AA	1201	A	C5-C6-N6	-5.76	119.09	123.70
1	AA	1366	C	N3-C4-N4	5.76	122.03	118.00
27	B8	142	A	C4-C5-C6	5.76	119.88	117.00
27	B8	176	A	C4-C5-C6	5.76	119.88	117.00
27	B8	515	A	C4-C5-C6	5.76	119.88	117.00
27	B8	1162	G	O4'-C1'-N9	5.76	112.81	108.20
27	B8	1353	A	C5-C6-N1	-5.76	114.82	117.70
27	B8	1472	C	N3-C4-N4	5.76	122.03	118.00
27	B8	1678	A	C5-C6-N6	-5.76	119.09	123.70
27	B8	1879	C	N3-C4-N4	5.76	122.03	118.00
27	B8	2116	G	O4'-C1'-N9	5.76	112.81	108.20
27	B8	2317	A	C4-C5-C6	5.76	119.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2808	G	O4'-C1'-N9	5.76	112.81	108.20
26	B7	11	C	N3-C4-C5	-5.75	119.60	121.90
27	B8	10	A	C5-C6-N1	-5.75	114.82	117.70
27	B8	944	C	N3-C4-N4	5.75	122.03	118.00
27	B8	1794	A	C5-C6-N6	-5.75	119.10	123.70
27	B8	1913	A	C5-C6-N6	-5.75	119.10	123.70
1	AA	783	C	N3-C4-N4	5.75	122.03	118.00
27	B8	742	A	C4-C5-C6	5.75	119.88	117.00
27	B8	1887	C	N3-C4-N4	5.75	122.03	118.00
27	B8	2451	A	C5-C6-N6	-5.75	119.10	123.70
1	AA	719	C	N3-C4-N4	5.75	122.03	118.00
1	AA	1367	C	N3-C4-N4	5.75	122.03	118.00
27	B8	423	A	O4'-C1'-N9	5.75	112.80	108.20
27	B8	557	C	N3-C4-C5	-5.75	119.60	121.90
27	B8	1445	G	O4'-C1'-N9	5.75	112.80	108.20
27	B8	1637	A	O4'-C1'-N9	5.75	112.80	108.20
27	B8	2682	A	C5-C6-N6	-5.75	119.10	123.70
27	B8	2809	A	C5-C6-N6	-5.75	119.10	123.70
1	AA	513	C	N3-C4-N4	5.75	122.03	118.00
1	AA	1476	A	O4'-C1'-N9	5.75	112.80	108.20
27	B8	601	C	N3-C4-N4	5.75	122.03	118.00
27	B8	2641	G	O4'-C1'-N9	5.75	112.80	108.20
1	AA	274	A	C4-C5-C6	5.75	119.88	117.00
27	B8	223	A	C5-C6-N6	-5.75	119.10	123.70
27	B8	376	G	O4'-C1'-N9	5.75	112.80	108.20
27	B8	693	A	C4-C5-C6	5.75	119.87	117.00
27	B8	1007	C	N3-C4-N4	5.75	122.02	118.00
27	B8	1569	A	C4-C5-C6	5.75	119.88	117.00
27	B8	262	A	C5-C6-N6	-5.75	119.10	123.70
27	B8	294	A	C4-C5-C6	5.75	119.87	117.00
27	B8	965	C	N3-C4-N4	5.75	122.02	118.00
27	B8	1127	A	O4'-C1'-N9	5.75	112.80	108.20
27	B8	1528	A	C5-C6-N1	-5.75	114.83	117.70
27	B8	1590	A	C5-C6-N1	-5.75	114.83	117.70
27	B8	1821	A	C5-C6-N1	-5.75	114.83	117.70
27	B8	2893	A	C5-C6-N1	-5.75	114.83	117.70
28	BA	340	ARG	N-CA-CB	5.75	120.94	110.60
1	AA	919	A	O4'-C1'-N9	5.75	112.80	108.20
27	B8	145	C	N3-C4-N4	5.75	122.02	118.00
27	B8	430	A	C4-C5-C6	5.75	119.87	117.00
1	AA	387	U	O4'-C1'-N1	5.74	112.80	108.20
1	AA	478	A	C4-C5-C6	5.74	119.87	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	499	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	902	G	O4'-C1'-N9	5.74	112.79	108.20
1	AA	1181	G	O4'-C1'-N9	5.74	112.80	108.20
1	AA	1293	C	N3-C4-N4	5.74	122.02	118.00
1	AA	1399	C	N3-C4-N4	5.74	122.02	118.00
27	B8	905	A	C5-C6-N6	-5.74	119.10	123.70
27	B8	1211	C	C6-N1-C1'	-5.74	113.91	120.80
27	B8	1600	C	N3-C4-N4	5.74	122.02	118.00
27	B8	1661	G	O4'-C1'-N9	5.74	112.79	108.20
27	B8	1804	C	N3-C4-N4	5.74	122.02	118.00
27	B8	1821	A	C4-C5-C6	5.74	119.87	117.00
27	B8	2184	A	O4'-C1'-N9	5.74	112.80	108.20
27	B8	2417	C	N3-C4-N4	5.74	122.02	118.00
27	B8	2443	C	N3-C4-N4	5.74	122.02	118.00
27	B8	2530	A	C4-C5-C6	5.74	119.87	117.00
27	B8	2733	A	C5-C6-N1	-5.74	114.83	117.70
1	AA	611	C	N3-C4-N4	5.74	122.02	118.00
27	B8	1637	A	C4-C5-C6	5.74	119.87	117.00
27	B8	2792	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	478	A	C5-C6-N1	-5.74	114.83	117.70
1	AA	663	A	C4-C5-C6	5.74	119.87	117.00
1	AA	790	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	807	A	O4'-C1'-N9	5.74	112.79	108.20
1	AA	907	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	1227	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	1433	A	C4-C5-C6	5.74	119.87	117.00
1	AA	1454	G	P-O5'-C5'	5.74	130.09	120.90
27	B8	933	A	C4-C5-C6	5.74	119.87	117.00
27	B8	1054	A	C5-C6-N6	-5.74	119.11	123.70
27	B8	2463	C	N3-C4-C5	-5.74	119.60	121.90
27	B8	2727	A	C5-C6-N6	-5.74	119.11	123.70
28	BA	217	PHE	CB-CG-CD1	5.74	124.82	120.80
1	AA	510	A	C5-C6-N1	-5.74	114.83	117.70
1	AA	583	A	C4-C5-C6	5.74	119.87	117.00
1	AA	669	G	O4'-C1'-N9	5.74	112.79	108.20
1	AA	691	G	N3-C2-N2	5.74	123.92	119.90
1	AA	706	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	815	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	1004	A	C5-C6-N1	-5.74	114.83	117.70
3	AV	67	C	N3-C4-N4	5.74	122.02	118.00
26	B7	50	A	C5-C6-N6	-5.74	119.11	123.70
27	B8	1398	C	N3-C4-N4	5.74	122.02	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1974	C	N3-C4-N4	5.74	122.02	118.00
27	B8	2136	G	O4'-C1'-N9	5.74	112.79	108.20
1	AA	526	C	N3-C4-N4	5.74	122.02	118.00
1	AA	753	A	C5-C6-N1	-5.74	114.83	117.70
1	AA	1152	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	1243	C	N3-C4-C5	-5.74	119.61	121.90
27	B8	79	C	N3-C4-C5	-5.74	119.61	121.90
27	B8	1030	C	N3-C4-N4	5.74	122.02	118.00
27	B8	1806	C	N3-C4-N4	5.74	122.02	118.00
27	B8	2857	G	N3-C2-N2	5.74	123.92	119.90
35	BG	108	PHE	CB-CG-CD2	5.74	124.82	120.80
1	AA	1221	G	O4'-C1'-N9	5.74	112.79	108.20
3	AV	63	C	N3-C4-N4	5.74	122.02	118.00
26	B7	104	A	C4-C5-C6	5.74	119.87	117.00
27	B8	44	A	O4'-C1'-N9	5.74	112.79	108.20
27	B8	282	A	C4-C5-C6	5.74	119.87	117.00
27	B8	1914	C	N3-C4-N4	5.74	122.01	118.00
27	B8	1987	A	C5-C6-N1	-5.74	114.83	117.70
27	B8	2882	A	O4'-C1'-N9	5.74	112.79	108.20
1	AA	635	A	C5-C6-N6	-5.73	119.11	123.70
27	B8	2003	A	C5-C6-N6	-5.73	119.11	123.70
27	B8	2234	G	O4'-C1'-N9	5.73	112.79	108.20
27	B8	2453	A	C5-C6-N1	-5.73	114.83	117.70
27	B8	2453	A	O4'-C1'-N9	5.73	112.79	108.20
1	AA	931	C	N3-C4-N4	5.73	122.01	118.00
1	AA	1071	C	N3-C4-C5	-5.73	119.61	121.90
27	B8	368	A	C5-C6-N6	-5.73	119.11	123.70
27	B8	654	A	C4-C5-C6	5.73	119.87	117.00
27	B8	2603	G	O4'-C1'-N9	5.73	112.79	108.20
1	AA	139	A	C4-C5-C6	5.73	119.86	117.00
1	AA	143	A	C5-C6-N1	-5.73	114.83	117.70
1	AA	415	A	C5-C6-N1	-5.73	114.83	117.70
1	AA	554	A	C4-C5-C6	5.73	119.87	117.00
1	AA	557	G	O4'-C1'-N9	5.73	112.78	108.20
1	AA	1431	A	C5-C6-N6	-5.73	119.11	123.70
1	AA	1446	A	C5-C6-N6	-5.73	119.12	123.70
27	B8	402	A	C5-C6-N1	-5.73	114.83	117.70
27	B8	1420	A	C5-C6-N6	-5.73	119.11	123.70
27	B8	2248	C	N3-C4-N4	5.73	122.01	118.00
27	B8	2619	C	N3-C4-N4	5.73	122.01	118.00
27	B8	2883	A	C4-C5-C6	5.73	119.86	117.00
1	AA	1513	A	O4'-C1'-N9	5.73	112.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1154	G	N3-C2-N2	5.73	123.91	119.90
27	B8	1794	A	C5-C6-N1	-5.73	114.84	117.70
1	AA	523	A	C4-C5-C6	5.73	119.86	117.00
1	AA	1328	C	N3-C4-N4	5.73	122.01	118.00
26	B7	81	G	O4'-C1'-N9	5.73	112.78	108.20
27	B8	53	A	O4'-C1'-N9	5.73	112.78	108.20
27	B8	422	A	C5-C6-N6	-5.73	119.12	123.70
27	B8	727	A	C4-C5-C6	5.73	119.86	117.00
27	B8	1165	A	C4-C5-C6	5.73	119.86	117.00
27	B8	1706	C	N3-C4-N4	5.73	122.01	118.00
27	B8	1772	A	O4'-C1'-N9	5.73	112.78	108.20
27	B8	2688	G	O4'-C1'-N9	5.73	112.78	108.20
1	AA	1011	C	N3-C4-N4	5.73	122.01	118.00
27	B8	14	A	C5-C6-N1	-5.73	114.84	117.70
27	B8	272	A	O4'-C1'-N9	5.73	112.78	108.20
27	B8	587	C	N3-C4-N4	5.73	122.01	118.00
27	B8	1046	A	C5-C6-N6	-5.73	119.12	123.70
27	B8	1339	G	O4'-C1'-N9	5.73	112.78	108.20
27	B8	1477	A	C5-C6-N1	-5.73	114.84	117.70
27	B8	2809	A	C4-C5-C6	5.73	119.86	117.00
1	AA	135	C	N3-C4-N4	5.72	122.01	118.00
1	AA	168	G	O4'-C1'-N9	5.72	112.78	108.20
1	AA	189	A	O4'-C1'-N9	5.72	112.78	108.20
1	AA	243	A	C5-C6-N6	-5.72	119.12	123.70
1	AA	746	A	O4'-C1'-N9	5.72	112.78	108.20
1	AA	807	A	C5-C6-N1	-5.72	114.84	117.70
1	AA	1171	A	C5-C6-N1	-5.72	114.84	117.70
27	B8	155	A	C5-C6-N6	-5.72	119.12	123.70
27	B8	2077	A	C5-C6-N1	-5.72	114.84	117.70
27	B8	2358	A	C5-C6-N6	-5.72	119.12	123.70
27	B8	2412	A	C5-C6-N1	-5.72	114.84	117.70
27	B8	2806	C	N3-C4-C5	-5.72	119.61	121.90
27	B8	2824	C	N3-C4-N4	5.72	122.01	118.00
1	AA	66	A	C5-C6-N1	-5.72	114.84	117.70
1	AA	78	A	C4-C5-C6	5.72	119.86	117.00
1	AA	1324	A	C5-C6-N6	-5.72	119.12	123.70
1	AA	1456	A	C5-C6-N6	-5.72	119.12	123.70
27	B8	622	G	O4'-C1'-N9	5.72	112.78	108.20
27	B8	677	A	C4-C5-C6	5.72	119.86	117.00
27	B8	1354	A	O4'-C1'-N9	5.72	112.78	108.20
27	B8	2005	A	C5-C6-N6	-5.72	119.12	123.70
27	B8	2065	C	N3-C4-C5	-5.72	119.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2475	C	O4'-C1'-N1	5.72	112.78	108.20
1	AA	22	G	O4'-C1'-N9	5.72	112.78	108.20
1	AA	602	A	C4-C5-C6	5.72	119.86	117.00
1	AA	1225	A	C5-C6-N1	-5.72	114.84	117.70
3	AV	59	A	C5-C6-N6	-5.72	119.12	123.70
27	B8	497	A	C5-C6-N6	-5.72	119.12	123.70
27	B8	980	A	C5-C6-N6	-5.72	119.12	123.70
1	AA	482	A	C4-C5-C6	5.72	119.86	117.00
1	AA	640	A	C4-C5-C6	5.72	119.86	117.00
1	AA	1346	A	C4-C5-C6	5.72	119.86	117.00
3	AV	37	G	O4'-C1'-N9	5.72	112.78	108.20
27	B8	485	C	N3-C4-N4	5.72	122.00	118.00
27	B8	943	A	C5-C6-N1	-5.72	114.84	117.70
27	B8	1107	G	O4'-C1'-N9	5.72	112.78	108.20
27	B8	1377	G	N3-C2-N2	5.72	123.90	119.90
27	B8	1650	A	C4-C5-C6	5.72	119.86	117.00
27	B8	2761	A	C4-C5-C6	5.72	119.86	117.00
27	B8	2840	C	N3-C4-N4	5.72	122.00	118.00
1	AA	587	G	O4'-C1'-N9	5.72	112.77	108.20
1	AA	1169	A	C5-C6-N6	-5.72	119.13	123.70
27	B8	1102	C	N3-C4-N4	5.72	122.00	118.00
27	B8	2298	A	O4'-C1'-N9	5.72	112.77	108.20
1	AA	926	G	O4'-C1'-N9	5.72	112.77	108.20
1	AA	1105	A	C4-C5-C6	5.72	119.86	117.00
1	AA	1216	A	C5-C6-N1	-5.72	114.84	117.70
27	B8	46	G	O4'-C1'-N9	5.72	112.77	108.20
27	B8	693	A	O4'-C1'-N9	5.72	112.77	108.20
27	B8	1196	C	N3-C4-N4	5.72	122.00	118.00
27	B8	1502	A	C5-C6-N6	-5.72	119.13	123.70
27	B8	2097	A	C5-C6-N6	-5.72	119.13	123.70
1	AA	290	C	N3-C4-N4	5.71	122.00	118.00
1	AA	876	C	N3-C4-N4	5.71	122.00	118.00
27	B8	1069	A	C5-C6-N6	-5.71	119.13	123.70
27	B8	1140	C	N3-C4-N4	5.71	122.00	118.00
27	B8	2205	A	C5-C6-N1	-5.71	114.84	117.70
27	B8	2385	C	N3-C4-C5	-5.71	119.61	121.90
27	B8	2572	A	C5-C6-N6	-5.71	119.13	123.70
1	AA	631	C	N3-C4-N4	5.71	122.00	118.00
1	AA	963	G	O4'-C1'-N9	5.71	112.77	108.20
27	B8	57	C	N3-C4-N4	5.71	122.00	118.00
27	B8	1551	A	C4-C5-C6	5.71	119.86	117.00
27	B8	1694	C	O4'-C1'-N1	5.71	112.77	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2482	A	C5-C6-N6	-5.71	119.13	123.70
27	B8	2515	C	N3-C4-N4	5.71	122.00	118.00
1	AA	389	A	C5-C6-N6	-5.71	119.13	123.70
1	AA	607	A	O4'-C1'-N9	5.71	112.77	108.20
27	B8	344	A	C4-C5-C6	5.71	119.86	117.00
27	B8	348	A	C4-C5-C6	5.71	119.86	117.00
27	B8	1493	C	N3-C4-N4	5.71	122.00	118.00
27	B8	1656	C	N3-C4-N4	5.71	122.00	118.00
27	B8	2340	A	C5-C6-N6	-5.71	119.13	123.70
27	B8	2377	A	C5-C6-N6	-5.71	119.13	123.70
27	B8	2407	A	C5-C6-N1	-5.71	114.84	117.70
27	B8	2418	A	O4'-C1'-N9	5.71	112.77	108.20
3	AV	49	C	N3-C4-C5	-5.71	119.62	121.90
27	B8	354	A	C4-C5-C6	5.71	119.86	117.00
27	B8	761	A	C4-C5-C6	5.71	119.86	117.00
27	B8	1387	A	C4-C5-C6	5.71	119.86	117.00
1	AA	655	A	C5-C6-N6	-5.71	119.13	123.70
1	AA	712	A	C4-C5-C6	5.71	119.86	117.00
1	AA	754	C	N3-C4-N4	5.71	122.00	118.00
1	AA	839	C	N3-C4-N4	5.71	122.00	118.00
1	AA	1103	C	N3-C4-C5	-5.71	119.62	121.90
27	B8	79	C	N3-C4-N4	5.71	122.00	118.00
27	B8	626	A	C5-C6-N1	-5.71	114.85	117.70
27	B8	851	C	N3-C4-N4	5.71	122.00	118.00
27	B8	1046	A	C4-C5-C6	5.71	119.85	117.00
27	B8	1928	A	C5-C6-N1	-5.71	114.85	117.70
27	B8	2602	A	C5-C6-N6	-5.71	119.13	123.70
1	AA	336	A	C5-C6-N6	-5.71	119.14	123.70
1	AA	759	A	C4-C5-C6	5.71	119.85	117.00
1	AA	1248	A	C5-C6-N6	-5.71	119.13	123.70
1	AA	1446	A	O4'-C1'-N9	5.71	112.76	108.20
27	B8	115	C	N3-C4-N4	5.71	122.00	118.00
27	B8	182	A	C5-C6-N6	-5.71	119.14	123.70
27	B8	878	A	C5-C6-N1	-5.71	114.85	117.70
27	B8	889	C	N3-C4-C5	-5.71	119.62	121.90
27	B8	1363	C	N3-C4-N4	5.71	121.99	118.00
27	B8	1735	A	C5-C6-N1	-5.71	114.85	117.70
27	B8	1908	C	N3-C4-N4	5.71	122.00	118.00
1	AA	60	A	C4-C5-C6	5.71	119.85	117.00
1	AA	983	A	C5-C6-N6	-5.71	119.14	123.70
27	B8	1305	C	N3-C4-N4	5.71	121.99	118.00
1	AA	67	C	N3-C4-C5	-5.70	119.62	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	308	C	N3-C4-N4	5.70	121.99	118.00
1	AA	1130	A	C4-C5-C6	5.70	119.85	117.00
27	B8	466	A	C4-C5-C6	5.70	119.85	117.00
27	B8	764	A	C4-C5-C6	5.70	119.85	117.00
27	B8	1426	G	N3-C2-N2	5.70	123.89	119.90
27	B8	2717	C	N3-C4-C5	-5.70	119.62	121.90
27	B8	129	C	N3-C4-N4	5.70	121.99	118.00
27	B8	943	A	C5-C6-N6	-5.70	119.14	123.70
27	B8	1221	C	N3-C4-N4	5.70	121.99	118.00
27	B8	1637	A	C5-C6-N6	-5.70	119.14	123.70
27	B8	2814	A	C5-C6-N6	-5.70	119.14	123.70
1	AA	169	C	N3-C4-C5	-5.70	119.62	121.90
1	AA	882	C	N3-C4-N4	5.70	121.99	118.00
1	AA	1256	A	O4'-C1'-N9	5.70	112.76	108.20
27	B8	163	C	N3-C4-N4	5.70	121.99	118.00
27	B8	245	G	O4'-C1'-N9	5.70	112.76	108.20
27	B8	1328	A	C4-C5-C6	5.70	119.85	117.00
27	B8	1434	A	C4-C5-C6	5.70	119.85	117.00
27	B8	1564	C	N3-C4-C5	-5.70	119.62	121.90
27	B8	1962	C	O4'-C1'-N1	5.70	112.76	108.20
27	B8	1978	A	C4-C5-C6	5.70	119.85	117.00
27	B8	1981	A	C4-C5-C6	5.70	119.85	117.00
27	B8	2624	G	O4'-C1'-N9	5.70	112.76	108.20
1	AA	253	A	C4-C5-C6	5.70	119.85	117.00
1	AA	388	G	O4'-C1'-N9	5.70	112.76	108.20
1	AA	456	A	C4-C5-C6	5.70	119.85	117.00
1	AA	1261	A	C5-C6-N1	-5.70	114.85	117.70
27	B8	981	A	C5-C6-N6	-5.70	119.14	123.70
27	B8	1142	A	C5-C6-N6	-5.70	119.14	123.70
27	B8	1144	A	C5-C6-N1	-5.70	114.85	117.70
27	B8	1225	G	O4'-C1'-N9	5.70	112.76	108.20
27	B8	1719	G	O4'-C1'-N9	5.70	112.76	108.20
27	B8	2156	G	N3-C2-N2	5.70	123.89	119.90
27	B8	2688	G	N3-C2-N2	5.70	123.89	119.90
1	AA	559	A	C5-C6-N6	-5.70	119.14	123.70
1	AA	1513	A	C5-C6-N1	-5.70	114.85	117.70
27	B8	1330	C	N3-C4-N4	5.70	121.99	118.00
27	B8	1901	A	O4'-C1'-N9	5.70	112.76	108.20
27	B8	1971	U	C2-N1-C1'	5.70	124.54	117.70
27	B8	2125	G	C5-C6-O6	-5.70	125.18	128.60
1	AA	222	C	N3-C4-N4	5.70	121.99	118.00
1	AA	901	A	C5-C6-N1	-5.70	114.85	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	217	A	C5-C6-N6	-5.70	119.14	123.70
27	B8	592	A	C4-C5-C6	5.70	119.85	117.00
27	B8	1607	C	N3-C4-C5	-5.70	119.62	121.90
27	B8	1784	A	C4-C5-C6	5.70	119.85	117.00
27	B8	2870	C	N3-C4-N4	5.70	121.99	118.00
27	B8	499	U	O4'-C1'-N1	5.69	112.75	108.20
27	B8	627	A	C5-C6-N6	-5.69	119.14	123.70
27	B8	1469	A	C5-C6-N1	-5.69	114.85	117.70
27	B8	1547	C	N3-C4-N4	5.69	121.99	118.00
1	AA	298	A	C4-C5-C6	5.69	119.85	117.00
1	AA	900	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	528	A	C5-C6-N1	-5.69	114.85	117.70
27	B8	1675	C	N3-C4-N4	5.69	121.98	118.00
27	B8	1685	C	N3-C4-N4	5.69	121.98	118.00
27	B8	1772	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	2288	A	C5-C6-N1	-5.69	114.85	117.70
27	B8	2516	A	C4-C5-C6	5.69	119.85	117.00
27	B8	2527	C	N3-C4-N4	5.69	121.98	118.00
1	AA	440	C	N3-C4-C5	-5.69	119.62	121.90
1	AA	1179	A	O4'-C1'-N9	5.69	112.75	108.20
1	AA	1250	A	C4-C5-C6	5.69	119.85	117.00
1	AA	1403	C	N3-C4-C5	-5.69	119.62	121.90
27	B8	131	A	C4-C5-C6	5.69	119.85	117.00
27	B8	466	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	507	A	C4-C5-C6	5.69	119.84	117.00
27	B8	1057	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	1502	A	C5-C6-N1	-5.69	114.86	117.70
27	B8	1916	A	C5-C6-N1	-5.69	114.85	117.70
27	B8	1966	A	O4'-C1'-N9	5.69	112.75	108.20
27	B8	2071	A	C5-C6-N6	-5.69	119.15	123.70
1	AA	649	A	C4-C5-C6	5.69	119.84	117.00
27	B8	1327	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	1705	A	C4-C5-C6	5.69	119.84	117.00
27	B8	1928	A	C5-C6-N6	-5.69	119.15	123.70
1	AA	1055	A	C5-C6-N6	-5.69	119.15	123.70
1	AA	1494	G	O4'-C1'-N9	5.69	112.75	108.20
3	AV	26	C	N3-C4-N4	5.69	121.98	118.00
27	B8	482	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	1032	A	C4-C5-C6	5.69	119.84	117.00
27	B8	1123	C	N3-C4-N4	5.69	121.98	118.00
27	B8	2013	A	C5-C6-N1	-5.69	114.86	117.70
27	B8	2055	C	N3-C4-N4	5.69	121.98	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2309	A	C5-C6-N6	-5.69	119.15	123.70
27	B8	2436	G	O4'-C1'-N9	5.69	112.75	108.20
27	B8	339	U	O4'-C1'-N1	5.69	112.75	108.20
27	B8	2434	A	C5-C6-N1	-5.69	114.86	117.70
27	B8	2663	G	O4'-C1'-N9	5.69	112.75	108.20
1	AA	153	C	N3-C4-N4	5.68	121.98	118.00
1	AA	321	A	C4-C5-C6	5.68	119.84	117.00
1	AA	972	C	N3-C4-C5	-5.68	119.63	121.90
1	AA	1240	U	O4'-C1'-N1	5.68	112.75	108.20
1	AA	1419	G	O4'-C1'-N9	5.68	112.75	108.20
1	AA	1534	A	C5-C6-N1	-5.68	114.86	117.70
3	AV	5	A	C4-C5-C6	5.68	119.84	117.00
3	AV	77	A	C5-C6-N1	-5.68	114.86	117.70
26	B7	109	A	C4-C5-C6	5.68	119.84	117.00
27	B8	619	G	N3-C2-N2	5.68	123.88	119.90
27	B8	920	A	C4-C5-C6	5.68	119.84	117.00
27	B8	1508	A	C5-C6-N6	-5.68	119.15	123.70
27	B8	1558	C	N3-C4-N4	5.68	121.98	118.00
27	B8	2320	U	O4'-C1'-N1	5.68	112.75	108.20
27	B8	2835	A	C5-C6-N6	-5.68	119.15	123.70
1	AA	199	A	C4-C5-C6	5.68	119.84	117.00
1	AA	914	A	C4-C5-C6	5.68	119.84	117.00
1	AA	934	C	O4'-C1'-N1	5.68	112.75	108.20
1	AA	1133	G	O4'-C1'-N9	5.68	112.75	108.20
1	AA	1380	U	O4'-C1'-N1	5.68	112.75	108.20
1	AA	1396	A	C5-C6-N6	-5.68	119.15	123.70
26	B7	38	C	N3-C4-C5	-5.68	119.63	121.90
27	B8	979	A	C5-C6-N6	-5.68	119.15	123.70
27	B8	1088	A	C5-C6-N1	-5.68	114.86	117.70
27	B8	1262	A	C5-C6-N1	-5.68	114.86	117.70
27	B8	1528	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	1570	A	C4-C5-C6	5.68	119.84	117.00
27	B8	1691	C	N3-C4-N4	5.68	121.98	118.00
27	B8	1895	C	N3-C4-C5	-5.68	119.63	121.90
27	B8	2015	A	C4-C5-C6	5.68	119.84	117.00
1	AA	1214	C	C2-N1-C1'	5.68	125.05	118.80
1	AA	1236	A	C4-C5-C6	5.68	119.84	117.00
27	B8	362	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	1711	A	C5-C6-N1	-5.68	114.86	117.70
1	AA	87	C	N3-C4-C5	-5.68	119.63	121.90
1	AA	122	G	O4'-C1'-N9	5.68	112.74	108.20
1	AA	167	A	C4-C5-C6	5.68	119.84	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	328	C	N3-C4-C5	-5.68	119.63	121.90
1	AA	549	C	N3-C4-C5	-5.68	119.63	121.90
1	AA	729	A	C4-C5-C6	5.68	119.84	117.00
1	AA	750	C	N3-C4-N4	5.68	121.98	118.00
1	AA	1082	A	O4'-C1'-N9	5.68	112.74	108.20
1	AA	1281	C	N3-C4-N4	5.68	121.97	118.00
3	AV	74	A	C4-C5-C6	5.68	119.84	117.00
27	B8	626	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	1151	A	O4'-C1'-N9	5.68	112.74	108.20
27	B8	1386	C	N3-C4-N4	5.68	121.98	118.00
27	B8	1895	C	N3-C4-N4	5.68	121.98	118.00
27	B8	1909	C	N3-C4-N4	5.68	121.98	118.00
27	B8	2173	A	C5-C6-N1	-5.68	114.86	117.70
27	B8	2434	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	2598	A	C4-C5-C6	5.68	119.84	117.00
1	AA	132	C	N3-C4-N4	5.68	121.97	118.00
1	AA	533	A	O4'-C1'-N9	5.68	112.74	108.20
1	AA	1517	G	O4'-C1'-N9	5.68	112.74	108.20
26	B7	34	A	C4-C5-C6	5.68	119.84	117.00
27	B8	415	A	O4'-C1'-N9	5.68	112.74	108.20
27	B8	478	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	1304	A	C4-C5-C6	5.68	119.84	117.00
27	B8	1319	C	N3-C4-N4	5.68	121.97	118.00
27	B8	1357	C	N3-C4-N4	5.68	121.97	118.00
27	B8	2088	A	C4-C5-C6	5.68	119.84	117.00
1	AA	246	A	C4-C5-C6	5.68	119.84	117.00
1	AA	1021	A	C5-C6-N6	-5.68	119.16	123.70
1	AA	1257	A	C5-C6-N6	-5.68	119.16	123.70
1	AA	1306	A	C5-C6-N1	-5.68	114.86	117.70
26	B7	18	G	O4'-C1'-N9	5.68	112.74	108.20
26	B7	52	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	722	A	C5-C6-N6	-5.68	119.16	123.70
27	B8	1096	A	C5-C6-N1	-5.68	114.86	117.70
28	BA	332	TYR	CB-CG-CD2	5.68	124.41	121.00
1	AA	510	A	C4-C5-C6	5.67	119.84	117.00
1	AA	696	A	C5-C6-N1	-5.67	114.86	117.70
1	AA	1203	C	N3-C4-N4	5.67	121.97	118.00
1	AA	1251	A	C5-C6-N6	-5.67	119.16	123.70
3	AV	2	G	O4'-C1'-N9	5.67	112.74	108.20
3	AV	61	U	O4'-C1'-N1	5.67	112.74	108.20
27	B8	617	G	O4'-C1'-N9	5.67	112.74	108.20
27	B8	946	C	N3-C4-N4	5.67	121.97	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1073	A	C4-C5-C6	5.67	119.84	117.00
27	B8	1762	A	C5-C6-N6	-5.67	119.16	123.70
27	B8	1783	A	C5-C6-N1	-5.67	114.86	117.70
27	B8	2212	A	C5-C6-N1	-5.67	114.86	117.70
27	B8	2258	C	N3-C4-N4	5.67	121.97	118.00
1	AA	648	A	C5-C6-N1	-5.67	114.86	117.70
1	AA	721	G	O4'-C1'-N9	5.67	112.74	108.20
27	B8	160	A	C5-C6-N6	-5.67	119.16	123.70
27	B8	523	C	N3-C4-N4	5.67	121.97	118.00
27	B8	2110	G	P-O3'-C3'	5.67	126.51	119.70
27	B8	2445	G	O4'-C1'-N9	5.67	112.74	108.20
27	B8	2608	G	N3-C2-N2	5.67	123.87	119.90
1	AA	189	A	C5-C6-N6	-5.67	119.16	123.70
1	AA	306	A	O4'-C1'-N9	5.67	112.74	108.20
1	AA	977	A	C5-C6-N6	-5.67	119.16	123.70
1	AA	1081	A	O4'-C1'-N9	5.67	112.74	108.20
27	B8	460	A	O4'-C1'-N9	5.67	112.74	108.20
27	B8	541	A	C5-C6-N1	-5.67	114.86	117.70
27	B8	631	A	C5-C6-N6	-5.67	119.16	123.70
27	B8	1127	A	C4-C5-C6	5.67	119.84	117.00
27	B8	1650	A	O4'-C1'-N9	5.67	112.74	108.20
27	B8	1843	C	N3-C4-N4	5.67	121.97	118.00
27	B8	2009	A	C4-C5-C6	5.67	119.84	117.00
27	B8	2772	C	N3-C4-N4	5.67	121.97	118.00
1	AA	131	A	O4'-C1'-N9	5.67	112.74	108.20
1	AA	408	A	C5-C6-N6	-5.67	119.16	123.70
26	B7	93	C	N3-C4-C5	-5.67	119.63	121.90
27	B8	479	A	P-O3'-C3'	5.67	126.50	119.70
27	B8	1566	A	C5-C6-N6	-5.67	119.16	123.70
27	B8	2080	A	C5-C6-N6	-5.67	119.16	123.70
1	AA	272	C	N3-C4-N4	5.67	121.97	118.00
1	AA	542	G	O4'-C1'-N9	5.67	112.73	108.20
1	AA	609	A	O4'-C1'-N9	5.67	112.73	108.20
1	AA	612	C	N3-C4-C5	-5.67	119.63	121.90
3	AV	28	C	N3-C4-N4	5.67	121.97	118.00
27	B8	143	C	N3-C4-N4	5.67	121.97	118.00
27	B8	366	C	N3-C4-N4	5.67	121.97	118.00
27	B8	922	C	N3-C4-C5	-5.67	119.63	121.90
27	B8	968	C	N3-C4-N4	5.67	121.97	118.00
27	B8	1330	C	N3-C4-C5	-5.67	119.63	121.90
27	B8	1678	A	O4'-C1'-N9	5.67	112.73	108.20
27	B8	1773	A	C4-C5-C6	5.67	119.83	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2205	A	C4-C5-C6	5.67	119.83	117.00
27	B8	2547	A	C5-C6-N1	-5.67	114.87	117.70
1	AA	101	A	C5-C6-N6	-5.67	119.17	123.70
1	AA	261	U	O4'-C1'-N1	5.67	112.73	108.20
1	AA	630	A	C5-C6-N6	-5.67	119.17	123.70
1	AA	978	A	C4-C5-C6	5.67	119.83	117.00
1	AA	1019	A	C5-C6-N6	-5.67	119.17	123.70
27	B8	781	A	C5-C6-N1	-5.67	114.87	117.70
27	B8	833	A	O4'-C1'-N9	5.67	112.73	108.20
27	B8	1307	A	C4-C5-C6	5.67	119.83	117.00
27	B8	1364	G	O4'-C1'-N9	5.67	112.73	108.20
27	B8	2082	A	O4'-C1'-N9	5.67	112.73	108.20
27	B8	2749	A	C4-C5-C6	5.67	119.83	117.00
1	AA	110	C	N3-C4-N4	5.67	121.97	118.00
1	AA	1467	C	N3-C4-N4	5.67	121.97	118.00
27	B8	42	A	C4-C5-C6	5.67	119.83	117.00
27	B8	368	A	C5-C6-N1	-5.67	114.87	117.70
27	B8	1385	A	C4-C5-C6	5.67	119.83	117.00
1	AA	518	C	N3-C4-N4	5.66	121.97	118.00
1	AA	580	C	N3-C4-N4	5.66	121.96	118.00
1	AA	1080	A	C5-C6-N1	-5.66	114.87	117.70
1	AA	1442	G	O4'-C1'-N9	5.66	112.73	108.20
27	B8	155	A	C4-C5-C6	5.66	119.83	117.00
27	B8	793	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	2426	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	44	A	C5-C6-N1	-5.66	114.87	117.70
27	B8	983	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	1384	A	C4-C5-C6	5.66	119.83	117.00
27	B8	1635	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	2703	C	N3-C4-N4	5.66	121.96	118.00
1	AA	394	G	O4'-C1'-N9	5.66	112.73	108.20
1	AA	507	C	N3-C4-N4	5.66	121.96	118.00
26	B7	62	C	N3-C4-C5	-5.66	119.64	121.90
27	B8	203	A	O4'-C1'-N9	5.66	112.73	108.20
27	B8	382	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	483	A	O4'-C1'-N9	5.66	112.73	108.20
27	B8	1246	A	C5-C6-N1	-5.66	114.87	117.70
27	B8	1557	C	N3-C4-C5	-5.66	119.64	121.90
27	B8	1679	A	O4'-C1'-N9	5.66	112.73	108.20
27	B8	1746	A	C4-C5-C6	5.66	119.83	117.00
27	B8	2036	C	N3-C4-N4	5.66	121.96	118.00
27	B8	2177	C	N3-C4-N4	5.66	121.96	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2182	U	O4'-C1'-N1	5.66	112.73	108.20
27	B8	2765	A	C5-C6-N1	-5.66	114.87	117.70
27	B8	2858	C	N3-C4-C5	-5.66	119.64	121.90
1	AA	436	C	N3-C4-N4	5.66	121.96	118.00
1	AA	1243	C	N3-C4-N4	5.66	121.96	118.00
1	AA	1302	C	O4'-C1'-N1	5.66	112.73	108.20
26	B7	50	A	C5-C6-N1	-5.66	114.87	117.70
27	B8	497	A	C4-C5-C6	5.66	119.83	117.00
27	B8	723	C	N3-C4-N4	5.66	121.96	118.00
27	B8	925	A	O4'-C1'-N9	5.66	112.73	108.20
27	B8	952	G	O4'-C1'-N9	5.66	112.73	108.20
27	B8	1138	G	O4'-C1'-N9	5.66	112.73	108.20
27	B8	1274	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	1458	U	O4'-C1'-N1	5.66	112.73	108.20
27	B8	2104	C	N3-C4-C5	-5.66	119.64	121.90
27	B8	2439	A	C5-C6-N1	-5.66	114.87	117.70
27	B8	2614	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	2623	G	O4'-C1'-N9	5.66	112.73	108.20
27	B8	2660	A	C5-C6-N6	-5.66	119.17	123.70
1	AA	23	C	N3-C4-C5	-5.66	119.64	121.90
1	AA	770	C	N3-C4-N4	5.66	121.96	118.00
1	AA	1411	C	N3-C4-N4	5.66	121.96	118.00
27	B8	1912	A	C5-C6-N1	-5.66	114.87	117.70
27	B8	1970	A	C5-C6-N6	-5.66	119.17	123.70
27	B8	2298	A	C4-C5-C6	5.66	119.83	117.00
27	B8	2713	U	O4'-C1'-N1	5.66	112.72	108.20
1	AA	106	C	N3-C4-C5	-5.66	119.64	121.90
1	AA	124	C	N3-C4-C5	-5.66	119.64	121.90
1	AA	174	A	C5-C6-N1	-5.66	114.87	117.70
1	AA	488	C	N3-C4-N4	5.66	121.96	118.00
1	AA	908	A	C5-C6-N1	-5.66	114.87	117.70
1	AA	1163	A	C5-C6-N6	-5.66	119.18	123.70
1	AA	1412	C	N3-C4-N4	5.66	121.96	118.00
26	B7	57	A	C4-C5-C6	5.66	119.83	117.00
27	B8	597	G	O4'-C1'-N9	5.66	112.72	108.20
27	B8	758	C	N3-C4-N4	5.66	121.96	118.00
27	B8	1686	C	N3-C4-N4	5.66	121.96	118.00
27	B8	1721	G	N3-C2-N2	5.66	123.86	119.90
27	B8	1786	A	C4-C5-C6	5.66	119.83	117.00
1	AA	689	C	N3-C4-N4	5.65	121.96	118.00
27	B8	455	C	N3-C4-N4	5.65	121.96	118.00
27	B8	809	G	O4'-C1'-N9	5.65	112.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	983	A	O4'-C1'-N9	5.65	112.72	108.20
27	B8	2763	G	O4'-C1'-N9	5.65	112.72	108.20
1	AA	277	C	N3-C4-C5	-5.65	119.64	121.90
1	AA	1500	A	C5-C6-N1	-5.65	114.87	117.70
1	AA	1518	A	C5-C6-N1	-5.65	114.87	117.70
27	B8	270	A	C5-C6-N6	-5.65	119.18	123.70
27	B8	1285	A	O4'-C1'-N9	5.65	112.72	108.20
27	B8	2851	A	O4'-C1'-N9	5.65	112.72	108.20
1	AA	823	C	N3-C4-C5	-5.65	119.64	121.90
1	AA	1248	A	C4-C5-C6	5.65	119.83	117.00
27	B8	101	A	O4'-C1'-N9	5.65	112.72	108.20
27	B8	250	G	C5-C6-O6	-5.65	125.21	128.60
27	B8	2108	A	C5-C6-N1	-5.65	114.87	117.70
27	B8	2224	G	O4'-C1'-N9	5.65	112.72	108.20
27	B8	2290	G	O4'-C1'-N9	5.65	112.72	108.20
27	B8	2439	A	C5-C6-N6	-5.65	119.18	123.70
27	B8	2716	C	N3-C4-N4	5.65	121.95	118.00
27	B8	151	C	N3-C4-N4	5.65	121.95	118.00
27	B8	343	C	N3-C4-N4	5.65	121.95	118.00
27	B8	602	A	O4'-C1'-N9	5.65	112.72	108.20
27	B8	660	C	N3-C4-N4	5.65	121.95	118.00
27	B8	668	A	C5-C6-N1	-5.65	114.88	117.70
27	B8	833	A	C5-C6-N1	-5.65	114.88	117.70
1	AA	503	C	N3-C4-N4	5.65	121.95	118.00
27	B8	239	C	N3-C4-N4	5.65	121.95	118.00
27	B8	247	G	O4'-C1'-N9	5.65	112.72	108.20
27	B8	281	C	N3-C4-C5	-5.65	119.64	121.90
27	B8	526	A	C4-C5-C6	5.65	119.82	117.00
27	B8	714	U	O4'-C1'-N1	5.65	112.72	108.20
27	B8	890	C	N3-C4-N4	5.65	121.95	118.00
27	B8	901	C	P-O5'-C5'	5.65	129.94	120.90
27	B8	1274	A	C5-C6-N1	-5.65	114.88	117.70
27	B8	1304	A	C5-C6-N1	-5.65	114.88	117.70
27	B8	2023	C	N3-C4-N4	5.65	121.95	118.00
27	B8	2164	C	O4'-C1'-N1	5.65	112.72	108.20
27	B8	2275	C	N3-C4-N4	5.65	121.95	118.00
27	B8	2856	A	C4-C5-C6	5.65	119.82	117.00
1	AA	58	C	N3-C4-C5	-5.65	119.64	121.90
1	AA	223	A	C5-C6-N6	-5.65	119.18	123.70
1	AA	885	G	O4'-C1'-N9	5.65	112.72	108.20
3	AV	43	G	O4'-C1'-N9	5.65	112.72	108.20
27	B8	800	A	C5-C6-N1	-5.65	114.88	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	866	A	C5-C6-N6	-5.65	119.18	123.70
27	B8	960	A	C5-C6-N6	-5.65	119.18	123.70
27	B8	2821	A	C5-C6-N6	-5.65	119.18	123.70
27	B8	2823	A	C5-C6-N6	-5.65	119.18	123.70
1	AA	130	A	C5-C6-N6	-5.64	119.19	123.70
1	AA	280	C	N3-C4-N4	5.64	121.95	118.00
1	AA	422	C	N3-C4-C5	-5.64	119.64	121.90
1	AA	602	A	C5-C6-N1	-5.64	114.88	117.70
1	AA	1204	A	C4-C5-C6	5.64	119.82	117.00
26	B7	108	A	C4-C5-C6	5.64	119.82	117.00
27	B8	1507	C	N3-C4-C5	-5.64	119.64	121.90
27	B8	2246	G	O4'-C1'-N9	5.64	112.72	108.20
1	AA	345	C	N3-C4-C5	-5.64	119.64	121.90
1	AA	716	A	C5-C6-N6	-5.64	119.19	123.70
1	AA	918	A	C5-C6-N6	-5.64	119.19	123.70
1	AA	1158	C	O4'-C1'-N1	5.64	112.71	108.20
27	B8	101	A	C5-C6-N6	-5.64	119.19	123.70
27	B8	324	A	C5-C6-N6	-5.64	119.19	123.70
27	B8	1938	A	C5-C6-N6	-5.64	119.19	123.70
27	B8	2423	U	O4'-C1'-N1	5.64	112.71	108.20
27	B8	2448	A	C5-C6-N6	-5.64	119.19	123.70
1	AA	315	A	C4-C5-C6	5.64	119.82	117.00
1	AA	676	A	C4-C5-C6	5.64	119.82	117.00
1	AA	1216	A	C4-C5-C6	5.64	119.82	117.00
1	AA	1460	C	N3-C4-N4	5.64	121.95	118.00
27	B8	1164	C	N3-C4-N4	5.64	121.95	118.00
27	B8	1525	A	C5-C6-N6	-5.64	119.19	123.70
27	B8	1677	A	C5-C6-N1	-5.64	114.88	117.70
27	B8	1744	A	C5-C6-N1	-5.64	114.88	117.70
1	AA	348	G	O4'-C1'-N9	5.64	112.71	108.20
1	AA	729	A	C5-C6-N6	-5.64	119.19	123.70
1	AA	928	G	O4'-C1'-N9	5.64	112.71	108.20
27	B8	625	G	O4'-C1'-N9	5.64	112.71	108.20
27	B8	739	A	C5-C6-N6	-5.64	119.19	123.70
27	B8	834	G	O4'-C1'-N9	5.64	112.71	108.20
27	B8	1211	C	P-O3'-C3'	5.64	126.47	119.70
27	B8	2005	A	O4'-C1'-N9	5.64	112.71	108.20
27	B8	2103	C	N3-C4-N4	5.64	121.95	118.00
27	B8	1699	G	O4'-C1'-N9	5.64	112.71	108.20
1	AA	58	C	N3-C4-N4	5.64	121.95	118.00
1	AA	197	A	C4-C5-C6	5.64	119.82	117.00
1	AA	363	A	C5-C6-N6	-5.64	119.19	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	946	A	C4-C5-C6	5.64	119.82	117.00
1	AA	968	A	O4'-C1'-N9	5.64	112.71	108.20
1	AA	1322	C	N3-C4-N4	5.64	121.94	118.00
27	B8	272	A	C5-C6-N1	-5.64	114.88	117.70
27	B8	1327	A	C4-C5-C6	5.64	119.82	117.00
27	B8	1672	A	C5-C6-N6	-5.64	119.19	123.70
27	B8	1727	C	N3-C4-N4	5.64	121.95	118.00
27	B8	2428	G	P-O3'-C3'	5.64	126.46	119.70
1	AA	238	A	O4'-C1'-N9	5.63	112.71	108.20
1	AA	620	C	N3-C4-N4	5.63	121.94	118.00
1	AA	747	A	C5-C6-N6	-5.63	119.19	123.70
1	AA	1155	A	C5-C6-N6	-5.63	119.19	123.70
1	AA	1327	C	N3-C4-N4	5.63	121.94	118.00
3	AV	38	G	O4'-C1'-N9	5.63	112.71	108.20
27	B8	88	G	C5-C6-O6	-5.63	125.22	128.60
27	B8	299	A	C5-C6-N1	-5.63	114.88	117.70
27	B8	430	A	C5-C6-N6	-5.63	119.19	123.70
27	B8	1037	G	O4'-C1'-N9	5.63	112.71	108.20
27	B8	1039	A	C5-C6-N1	-5.63	114.88	117.70
27	B8	2058	A	O4'-C1'-N9	5.63	112.71	108.20
27	B8	2705	A	C4-C5-C6	5.63	119.82	117.00
27	B8	2757	A	C4-C5-C6	5.63	119.82	117.00
1	AA	195	A	C4-C5-C6	5.63	119.82	117.00
1	AA	1246	A	C4-C5-C6	5.63	119.82	117.00
3	AV	40	G	O4'-C1'-N9	5.63	112.71	108.20
27	B8	2199	A	C5-C6-N6	-5.63	119.19	123.70
1	AA	395	C	N3-C4-N4	5.63	121.94	118.00
1	AA	600	A	C4-C5-C6	5.63	119.82	117.00
1	AA	1000	A	C4-C5-C6	5.63	119.81	117.00
3	AV	52	A	C5-C6-N1	-5.63	114.88	117.70
3	AV	77	A	C5-C6-N6	-5.63	119.19	123.70
27	B8	172	A	C5-C6-N6	-5.63	119.19	123.70
27	B8	507	A	C5-C6-N6	-5.63	119.19	123.70
27	B8	875	G	P-O3'-C3'	5.63	126.46	119.70
27	B8	1570	A	C5-C6-N6	-5.63	119.19	123.70
27	B8	2635	A	C5-C6-N6	-5.63	119.19	123.70
27	B8	2675	A	C4-C5-C6	5.63	119.81	117.00
1	AA	633	G	C5-C6-O6	-5.63	125.22	128.60
1	AA	913	A	C4-C5-C6	5.63	119.81	117.00
1	AA	959	A	C5-C6-N6	-5.63	119.20	123.70
1	AA	1274	A	C4-C5-C6	5.63	119.81	117.00
1	AA	1430	A	C5-C6-N1	-5.63	114.89	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1500	A	O4'-C1'-N9	5.63	112.70	108.20
27	B8	736	C	N3-C4-C5	-5.63	119.65	121.90
27	B8	819	A	C5-C6-N6	-5.63	119.20	123.70
27	B8	1014	A	C5-C6-N6	-5.63	119.20	123.70
27	B8	1353	A	C4-C5-C6	5.63	119.81	117.00
27	B8	1870	C	N3-C4-N4	5.63	121.94	118.00
27	B8	2450	A	C4-C5-C6	5.63	119.81	117.00
1	AA	910	C	N3-C4-N4	5.63	121.94	118.00
1	AA	983	A	C4-C5-C6	5.63	119.81	117.00
1	AA	1117	A	C5-C6-N6	-5.63	119.20	123.70
1	AA	1430	A	C4-C5-C6	5.63	119.81	117.00
27	B8	22	C	N3-C4-N4	5.63	121.94	118.00
27	B8	672	C	N3-C4-N4	5.63	121.94	118.00
27	B8	765	C	N3-C4-N4	5.63	121.94	118.00
1	AA	210	C	N3-C4-C5	-5.63	119.65	121.90
1	AA	978	A	C5-C6-N1	-5.63	114.89	117.70
1	AA	1004	A	C5-C6-N6	-5.63	119.20	123.70
27	B8	1378	A	C5-C6-N1	-5.63	114.89	117.70
27	B8	2104	C	N3-C4-N4	5.63	121.94	118.00
27	B8	2377	A	O4'-C1'-N9	5.63	112.70	108.20
27	B8	2510	C	N3-C4-N4	5.63	121.94	118.00
27	B8	2560	A	O4'-C1'-N9	5.63	112.70	108.20
27	B8	2876	G	O4'-C1'-N9	5.63	112.70	108.20
1	AA	155	A	P-O5'-C5'	5.62	129.90	120.90
1	AA	307	C	N3-C4-N4	5.62	121.94	118.00
1	AA	366	A	C5-C6-N1	-5.62	114.89	117.70
1	AA	1112	C	N3-C4-N4	5.62	121.94	118.00
1	AA	1134	G	O4'-C1'-N9	5.62	112.70	108.20
26	B7	31	C	N3-C4-N4	5.62	121.94	118.00
27	B8	1665	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	1805	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	2059	A	C5-C6-N6	-5.62	119.20	123.70
1	AA	1031	C	N3-C4-N4	5.62	121.94	118.00
1	AA	1203	C	N3-C4-C5	-5.62	119.65	121.90
3	AV	4	C	O4'-C1'-N1	5.62	112.70	108.20
3	AV	26	C	N3-C4-C5	-5.62	119.65	121.90
26	B7	30	C	N3-C4-N4	5.62	121.94	118.00
27	B8	1605	C	N3-C4-C5	-5.62	119.65	121.90
27	B8	1618	A	O4'-C1'-N9	5.62	112.70	108.20
27	B8	2010	G	O4'-C1'-N9	5.62	112.70	108.20
27	B8	2270	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	2306	C	N3-C4-N4	5.62	121.94	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2432	A	C5-C6-N6	-5.62	119.20	123.70
27	B8	2600	A	C5-C6-N1	-5.62	114.89	117.70
1	AA	74	A	C5-C6-N1	-5.62	114.89	117.70
1	AA	248	C	N3-C4-N4	5.62	121.93	118.00
1	AA	276	G	O4'-C1'-N9	5.62	112.70	108.20
1	AA	1430	A	O4'-C1'-N9	5.62	112.70	108.20
1	AA	1510	C	N3-C4-C5	-5.62	119.65	121.90
27	B8	62	U	P-O3'-C3'	5.62	126.45	119.70
27	B8	332	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	391	A	O4'-C1'-N9	5.62	112.70	108.20
27	B8	603	A	C5-C6-N6	-5.62	119.20	123.70
27	B8	890	C	N3-C4-C5	-5.62	119.65	121.90
27	B8	2025	C	N3-C4-N4	5.62	121.94	118.00
27	B8	2483	C	N3-C4-N4	5.62	121.94	118.00
27	B8	2635	A	O4'-C1'-N9	5.62	112.70	108.20
27	B8	2745	C	N3-C4-C5	-5.62	119.65	121.90
1	AA	495	A	O4'-C1'-N9	5.62	112.70	108.20
1	AA	651	C	N3-C4-C5	-5.62	119.65	121.90
1	AA	983	A	C5-C6-N1	-5.62	114.89	117.70
26	B7	11	C	N3-C4-N4	5.62	121.93	118.00
27	B8	226	A	C4-C5-C6	5.62	119.81	117.00
27	B8	1348	C	N3-C4-N4	5.62	121.93	118.00
27	B8	1795	C	N3-C4-N4	5.62	121.93	118.00
27	B8	2178	C	N3-C4-C5	-5.62	119.65	121.90
1	AA	518	C	N3-C4-C5	-5.62	119.65	121.90
1	AA	532	A	C5-C6-N6	-5.62	119.20	123.70
27	B8	131	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	244	A	C4-C5-C6	5.62	119.81	117.00
27	B8	470	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	542	C	N3-C4-N4	5.62	121.93	118.00
27	B8	941	A	C5-C6-N6	-5.62	119.20	123.70
27	B8	1008	A	C5-C6-N6	-5.62	119.20	123.70
27	B8	1912	A	C4-C5-C6	5.62	119.81	117.00
27	B8	2088	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	2101	A	C5-C6-N6	-5.62	119.20	123.70
26	B7	68	C	N3-C4-N4	5.62	121.93	118.00
27	B8	190	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	825	A	C5-C6-N1	-5.62	114.89	117.70
27	B8	1229	C	N3-C4-C5	-5.62	119.65	121.90
27	B8	1395	A	C5-C6-N1	-5.62	114.89	117.70
1	AA	105	G	O4'-C1'-N9	5.62	112.69	108.20
1	AA	712	A	C5-C6-N6	-5.62	119.21	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1383	C	N3-C4-N4	5.62	121.93	118.00
27	B8	804	A	O4'-C1'-N9	5.62	112.69	108.20
27	B8	900	A	C4-C5-C6	5.62	119.81	117.00
27	B8	1237	A	C5-C6-N6	-5.62	119.21	123.70
27	B8	1770	G	O4'-C1'-N9	5.62	112.69	108.20
27	B8	1801	A	O4'-C1'-N9	5.62	112.69	108.20
1	AA	456	A	C5-C6-N6	-5.61	119.21	123.70
1	AA	930	C	N3-C4-N4	5.61	121.93	118.00
1	AA	1400	C	C6-N1-C1'	-5.61	114.06	120.80
27	B8	792	A	C5-C6-N6	-5.61	119.21	123.70
27	B8	823	C	N3-C4-N4	5.61	121.93	118.00
27	B8	1284	A	C5-C6-N6	-5.61	119.21	123.70
27	B8	1354	A	C5-C6-N1	-5.61	114.89	117.70
27	B8	1689	A	O4'-C1'-N9	5.61	112.69	108.20
27	B8	1735	A	C5-C6-N6	-5.61	119.21	123.70
27	B8	2384	U	O4'-C1'-N1	5.61	112.69	108.20
27	B8	2607	G	O4'-C1'-N9	5.61	112.69	108.20
1	AA	66	A	C5-C6-N6	-5.61	119.21	123.70
1	AA	325	A	C4-C5-C6	5.61	119.81	117.00
1	AA	897	C	N3-C4-N4	5.61	121.93	118.00
1	AA	1428	A	C5-C6-N6	-5.61	119.21	123.70
27	B8	2164	C	C2-N1-C1'	5.61	124.97	118.80
31	B6	189	ALA	N-CA-CB	5.61	117.96	110.10
1	AA	807	A	C4-C5-C6	5.61	119.81	117.00
1	AA	1349	A	C4-C5-C6	5.61	119.81	117.00
27	B8	853	C	N3-C4-N4	5.61	121.93	118.00
27	B8	1172	C	N3-C4-C5	-5.61	119.66	121.90
27	B8	1428	C	O4'-C1'-N1	5.61	112.69	108.20
27	B8	2247	A	C5-C6-N6	-5.61	119.21	123.70
27	B8	2660	A	C5-C6-N1	-5.61	114.89	117.70
2	AX	21	A	C5-C6-N6	-5.61	119.21	123.70
3	AV	16	C	N3-C4-N4	5.61	121.93	118.00
27	B8	661	A	O4'-C1'-N9	5.61	112.69	108.20
27	B8	2369	A	O4'-C1'-N9	5.61	112.69	108.20
1	AA	187	G	N3-C2-N2	5.61	123.83	119.90
1	AA	461	A	O4'-C1'-N9	5.61	112.69	108.20
1	AA	728	A	C4-C5-C6	5.61	119.80	117.00
1	AA	1360	A	C5-C6-N1	-5.61	114.90	117.70
27	B8	946	C	N3-C4-C5	-5.61	119.66	121.90
27	B8	1597	A	C5-C6-N6	-5.61	119.21	123.70
27	B8	1833	C	N3-C4-C5	-5.61	119.66	121.90
27	B8	2578	G	O4'-C1'-N9	5.61	112.69	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2583	G	O4'-C1'-N9	5.61	112.69	108.20
27	B8	2590	A	C5-C6-N1	-5.61	114.90	117.70
27	B8	2785	C	N3-C4-N4	5.61	121.93	118.00
1	AA	438	U	O4'-C1'-N1	5.61	112.68	108.20
1	AA	1251	A	C5-C6-N1	-5.61	114.90	117.70
1	AA	1493	A	C5-C6-N6	-5.61	119.22	123.70
27	B8	2154	A	C5-C6-N1	-5.61	114.90	117.70
27	B8	2241	A	C5-C6-N1	-5.61	114.90	117.70
1	AA	1157	A	C5-C6-N1	-5.60	114.90	117.70
1	AA	1311	A	C5-C6-N6	-5.60	119.22	123.70
1	AA	1519	A	O4'-C1'-N9	5.60	112.68	108.20
1	AA	1542	A	C5-C6-N6	-5.60	119.22	123.70
27	B8	814	C	N3-C4-C5	-5.60	119.66	121.90
27	B8	1591	A	C5-C6-N6	-5.60	119.22	123.70
27	B8	1839	G	O4'-C1'-N9	5.60	112.68	108.20
1	AA	635	A	O4'-C1'-N9	5.60	112.68	108.20
27	B8	1987	A	C4-C5-C6	5.60	119.80	117.00
27	B8	2805	C	N3-C4-N4	5.60	121.92	118.00
1	AA	366	A	C5-C6-N6	-5.60	119.22	123.70
1	AA	1151	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	173	A	C4-C5-C6	5.60	119.80	117.00
27	B8	227	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	1322	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	2342	C	N3-C4-N4	5.60	121.92	118.00
1	AA	643	C	N3-C4-N4	5.60	121.92	118.00
1	AA	796	C	N3-C4-C5	-5.60	119.66	121.90
1	AA	1480	A	C5-C6-N1	-5.60	114.90	117.70
26	B7	6	G	O4'-C1'-N9	5.60	112.68	108.20
27	B8	563	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	749	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	1462	C	N3-C4-N4	5.60	121.92	118.00
27	B8	1806	C	N3-C4-C5	-5.60	119.66	121.90
27	B8	1824	G	O4'-C1'-N9	5.60	112.68	108.20
27	B8	2160	C	N3-C4-N4	5.60	121.92	118.00
27	B8	2317	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	2821	A	C5-C6-N1	-5.60	114.90	117.70
1	AA	1	A	C5-C6-N6	-5.60	119.22	123.70
1	AA	1378	C	N3-C4-N4	5.60	121.92	118.00
1	AA	1461	G	C5-C6-O6	-5.60	125.24	128.60
27	B8	63	A	C4-C5-C6	5.60	119.80	117.00
27	B8	128	C	N3-C4-C5	-5.60	119.66	121.90
27	B8	144	A	C5-C6-N1	-5.60	114.90	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	782	A	C5-C6-N6	-5.60	119.22	123.70
27	B8	2012	G	O4'-C1'-N9	5.60	112.68	108.20
1	AA	519	C	N3-C4-N4	5.60	121.92	118.00
3	AV	1	C	N3-C4-C5	-5.60	119.66	121.90
27	B8	1001	A	C5-C6-N1	-5.60	114.90	117.70
27	B8	1147	A	C4-C5-C6	5.60	119.80	117.00
27	B8	1615	C	N3-C4-C5	-5.60	119.66	121.90
27	B8	1989	G	O4'-C1'-N9	5.60	112.68	108.20
1	AA	520	A	C5-C6-N1	-5.59	114.90	117.70
1	AA	559	A	C5-C6-N1	-5.59	114.90	117.70
1	AA	648	A	C5-C6-N6	-5.59	119.22	123.70
1	AA	808	C	N3-C4-N4	5.59	121.92	118.00
1	AA	913	A	C5-C6-N1	-5.59	114.90	117.70
1	AA	1413	A	C4-C5-C6	5.59	119.80	117.00
27	B8	83	A	C5-C6-N1	-5.59	114.90	117.70
27	B8	199	A	O4'-C1'-N9	5.59	112.68	108.20
27	B8	240	C	N3-C4-N4	5.59	121.92	118.00
27	B8	332	A	C5-C6-N6	-5.59	119.22	123.70
27	B8	972	A	C5-C6-N6	-5.59	119.22	123.70
27	B8	1095	A	C5-C6-N1	-5.59	114.90	117.70
27	B8	1347	A	C4-C5-C6	5.59	119.80	117.00
27	B8	1349	C	N3-C4-N4	5.59	121.92	118.00
27	B8	1847	A	C5-C6-N6	-5.59	119.22	123.70
27	B8	2112	G	C5-C6-O6	-5.59	125.24	128.60
27	B8	2295	C	N3-C4-C5	-5.59	119.66	121.90
1	AA	1476	A	C4-C5-C6	5.59	119.80	117.00
27	B8	1090	A	C5-C6-N1	-5.59	114.90	117.70
27	B8	1877	A	C5-C6-N6	-5.59	119.23	123.70
27	B8	2178	C	N3-C4-N4	5.59	121.92	118.00
1	AA	372	C	N3-C4-C5	-5.59	119.66	121.90
1	AA	1100	C	N3-C4-N4	5.59	121.92	118.00
27	B8	89	A	C5-C6-N6	-5.59	119.23	123.70
27	B8	514	A	C4-C5-C6	5.59	119.80	117.00
27	B8	564	C	N3-C4-C5	-5.59	119.66	121.90
27	B8	903	C	N3-C4-C5	-5.59	119.66	121.90
27	B8	989	G	N3-C2-N2	5.59	123.81	119.90
27	B8	1583	A	C5-C6-N6	-5.59	119.23	123.70
27	B8	1858	A	C4-C5-C6	5.59	119.80	117.00
27	B8	1960	A	C5-C6-N1	-5.59	114.91	117.70
27	B8	2538	C	N3-C4-N4	5.59	121.91	118.00
27	B8	2758	A	C4-C5-C6	5.59	119.80	117.00
1	AA	206	C	N3-C4-C5	-5.59	119.66	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	267	C	N3-C4-C5	-5.59	119.66	121.90
1	AA	704	A	C5-C6-N6	-5.59	119.23	123.70
1	AA	718	A	C5-C6-N1	-5.59	114.91	117.70
1	AA	948	C	N3-C4-C5	-5.59	119.66	121.90
1	AA	1538	C	N3-C4-N4	5.59	121.91	118.00
26	B7	47	C	N3-C4-N4	5.59	121.91	118.00
26	B7	83	G	O4'-C1'-N9	5.59	112.67	108.20
27	B8	278	A	C5-C6-N1	-5.59	114.91	117.70
27	B8	541	A	O4'-C1'-N9	5.59	112.67	108.20
27	B8	753	A	O4'-C1'-N9	5.59	112.67	108.20
27	B8	962	G	N3-C2-N2	5.59	123.81	119.90
27	B8	1959	G	O4'-C1'-N9	5.59	112.67	108.20
27	B8	2055	C	N3-C4-C5	-5.59	119.67	121.90
27	B8	2314	A	C4-C5-C6	5.59	119.80	117.00
27	B8	2478	A	O4'-C1'-N9	5.59	112.67	108.20
1	AA	680	C	N3-C4-N4	5.59	121.91	118.00
1	AA	806	C	N3-C4-N4	5.59	121.91	118.00
27	B8	472	A	C5-C6-N6	-5.59	119.23	123.70
27	B8	592	A	C5-C6-N6	-5.59	119.23	123.70
27	B8	2283	C	P-O5'-C5'	5.59	129.84	120.90
27	B8	2307	G	O4'-C1'-N9	5.59	112.67	108.20
1	AA	510	A	O4'-C1'-N9	5.59	112.67	108.20
1	AA	600	A	C5-C6-N1	-5.59	114.91	117.70
1	AA	658	C	N3-C4-N4	5.59	121.91	118.00
1	AA	767	A	O4'-C1'-N9	5.59	112.67	108.20
1	AA	1005	A	C5-C6-N1	-5.59	114.91	117.70
1	AA	1192	C	N3-C4-N4	5.59	121.91	118.00
27	B8	300	A	C5-C6-N1	-5.59	114.91	117.70
27	B8	341	C	N3-C4-C5	-5.59	119.67	121.90
27	B8	382	A	O4'-C1'-N9	5.59	112.67	108.20
27	B8	693	A	C5-C6-N1	-5.59	114.91	117.70
27	B8	1284	A	O4'-C1'-N9	5.59	112.67	108.20
27	B8	1785	A	O4'-C1'-N9	5.59	112.67	108.20
1	AA	452	A	C4-C5-C6	5.58	119.79	117.00
1	AA	1524	C	N3-C4-C5	-5.58	119.67	121.90
27	B8	430	A	C5-C6-N1	-5.58	114.91	117.70
27	B8	1815	A	C4-C5-C6	5.58	119.79	117.00
27	B8	2254	C	N3-C4-N4	5.58	121.91	118.00
27	B8	2685	G	O4'-C1'-N9	5.58	112.67	108.20
27	B8	2813	A	C5-C6-N6	-5.58	119.23	123.70
1	AA	172	A	C4-C5-C6	5.58	119.79	117.00
1	AA	243	A	C2'-C3'-O3'	5.58	122.64	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	309	A	C5-C6-N6	-5.58	119.23	123.70
27	B8	559	G	O4'-C1'-N9	5.58	112.67	108.20
27	B8	1013	C	N3-C4-N4	5.58	121.91	118.00
27	B8	1913	A	C5-C6-N1	-5.58	114.91	117.70
27	B8	2498	C	N3-C4-N4	5.58	121.91	118.00
27	B8	2539	C	N3-C4-C5	-5.58	119.67	121.90
27	B8	2665	A	O4'-C1'-N9	5.58	112.67	108.20
1	AA	233	C	N3-C4-N4	5.58	121.91	118.00
1	AA	549	C	N3-C4-N4	5.58	121.91	118.00
27	B8	165	A	C5-C6-N1	-5.58	114.91	117.70
27	B8	309	A	O4'-C1'-N9	5.58	112.67	108.20
27	B8	745	G	N3-C2-N2	5.58	123.81	119.90
27	B8	901	C	N3-C4-N4	5.58	121.91	118.00
27	B8	1106	G	O4'-C1'-N9	5.58	112.67	108.20
27	B8	1392	A	C5-C6-N6	-5.58	119.23	123.70
27	B8	1418	G	N3-C2-N2	5.58	123.81	119.90
27	B8	1447	C	N3-C4-C5	-5.58	119.67	121.90
27	B8	2196	C	N3-C4-C5	-5.58	119.67	121.90
27	B8	2255	G	O4'-C1'-N9	5.58	112.66	108.20
27	B8	2310	C	N3-C4-C5	-5.58	119.67	121.90
27	B8	2540	C	N3-C4-N4	5.58	121.91	118.00
1	AA	87	C	N3-C4-N4	5.58	121.91	118.00
1	AA	263	A	C5-C6-N1	-5.58	114.91	117.70
1	AA	607	A	C5-C6-N6	-5.58	119.24	123.70
1	AA	1320	C	N3-C4-C5	-5.58	119.67	121.90
3	AV	24	C	N3-C4-C5	-5.58	119.67	121.90
27	B8	1033	U	O4'-C1'-N1	5.58	112.66	108.20
27	B8	1043	C	N3-C4-N4	5.58	121.91	118.00
27	B8	1548	A	C4-C5-C6	5.58	119.79	117.00
27	B8	1966	A	C5-C6-N6	-5.58	119.24	123.70
27	B8	2346	A	C5-C6-N6	-5.58	119.24	123.70
1	AA	80	A	C5-C6-N6	-5.58	119.24	123.70
1	AA	1147	C	N3-C4-C5	-5.58	119.67	121.90
1	AA	1462	C	N3-C4-N4	5.58	121.91	118.00
3	AV	18	U	O4'-C1'-N1	5.58	112.66	108.20
3	AV	49	C	N3-C4-N4	5.58	121.91	118.00
26	B7	97	C	N3-C4-N4	5.58	121.91	118.00
27	B8	173	A	C5-C6-N6	-5.58	119.24	123.70
27	B8	585	G	O4'-C1'-N9	5.58	112.66	108.20
27	B8	804	A	C5-C6-N6	-5.58	119.24	123.70
27	B8	1454	C	C2-N1-C1'	5.58	124.94	118.80
27	B8	1551	A	C5-C6-N6	-5.58	119.24	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1552	A	O4'-C1'-N9	5.58	112.66	108.20
27	B8	1967	C	N3-C4-N4	5.58	121.90	118.00
27	B8	2577	A	C5-C6-N1	-5.58	114.91	117.70
27	B8	2638	G	O4'-C1'-N9	5.58	112.66	108.20
27	B8	2747	G	O4'-C1'-N9	5.58	112.66	108.20
1	AA	1050	G	O4'-C1'-N9	5.58	112.66	108.20
26	B7	57	A	O4'-C1'-N9	5.58	112.66	108.20
27	B8	264	C	N3-C4-N4	5.58	121.90	118.00
27	B8	2335	A	C5-C6-N1	-5.58	114.91	117.70
1	AA	7	A	O4'-C1'-N9	5.58	112.66	108.20
1	AA	344	A	C5-C6-N6	-5.58	119.24	123.70
1	AA	351	G	O4'-C1'-N9	5.58	112.66	108.20
1	AA	754	C	N3-C4-C5	-5.58	119.67	121.90
3	AV	14	A	C5-C6-N1	-5.58	114.91	117.70
27	B8	719	C	N3-C4-N4	5.58	121.90	118.00
27	B8	1378	A	O4'-C1'-N9	5.58	112.66	108.20
1	AA	1110	A	C5-C6-N1	-5.57	114.91	117.70
1	AA	1198	G	O4'-C1'-N9	5.57	112.66	108.20
27	B8	7	G	O4'-C1'-N9	5.57	112.66	108.20
27	B8	504	A	C5-C6-N6	-5.57	119.24	123.70
27	B8	634	C	N3-C4-C5	-5.57	119.67	121.90
27	B8	1403	A	C5-C6-N1	-5.57	114.91	117.70
27	B8	1494	A	C4-C5-C6	5.57	119.79	117.00
27	B8	1494	A	C5-C6-N1	-5.57	114.91	117.70
27	B8	1518	C	N3-C4-N4	5.57	121.90	118.00
27	B8	1552	A	P-O5'-C5'	5.57	129.82	120.90
27	B8	1877	A	C5-C6-N1	-5.57	114.91	117.70
27	B8	2433	A	C5-C6-N6	-5.57	119.24	123.70
27	B8	795	C	N3-C4-C5	-5.57	119.67	121.90
27	B8	865	C	N3-C4-N4	5.57	121.90	118.00
27	B8	2417	C	N3-C4-C5	-5.57	119.67	121.90
29	BB	104	MET	CG-SD-CE	-5.57	91.28	100.20
1	AA	1382	C	N3-C4-N4	5.57	121.90	118.00
27	B8	163	C	N3-C4-C5	-5.57	119.67	121.90
27	B8	272	A	C5-C6-N6	-5.57	119.24	123.70
27	B8	351	C	N3-C4-N4	5.57	121.90	118.00
27	B8	1006	C	N3-C4-N4	5.57	121.90	118.00
27	B8	1052	C	N3-C4-C5	-5.57	119.67	121.90
27	B8	1218	G	O4'-C1'-N9	5.57	112.66	108.20
27	B8	1308	A	C4-C5-C6	5.57	119.78	117.00
27	B8	1786	A	C5-C6-N6	-5.57	119.24	123.70
27	B8	1794	A	C4-C5-C6	5.57	119.79	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2061	G	O4'-C1'-N9	5.57	112.66	108.20
27	B8	2314	A	O4'-C1'-N9	5.57	112.66	108.20
27	B8	2776	A	C5-C6-N6	-5.57	119.24	123.70
27	B8	41	C	N3-C4-N4	5.57	121.90	118.00
27	B8	262	A	O4'-C1'-N9	5.57	112.66	108.20
27	B8	344	A	C5-C6-N6	-5.57	119.25	123.70
27	B8	433	C	N3-C4-N4	5.57	121.90	118.00
27	B8	1414	C	N3-C4-N4	5.57	121.90	118.00
27	B8	2023	C	N3-C4-C5	-5.57	119.67	121.90
27	B8	2164	C	N3-C4-N4	5.57	121.90	118.00
1	AA	996	A	O4'-C1'-N9	5.57	112.66	108.20
3	AV	51	G	O4'-C1'-N9	5.57	112.66	108.20
27	B8	450	G	O4'-C1'-N9	5.57	112.65	108.20
27	B8	637	A	C5-C6-N1	-5.57	114.92	117.70
27	B8	1532	A	C5-C6-N1	-5.57	114.92	117.70
27	B8	2193	G	O4'-C1'-N9	5.57	112.65	108.20
1	AA	143	A	C5-C6-N6	-5.57	119.25	123.70
26	B7	101	A	C4-C5-C6	5.57	119.78	117.00
27	B8	833	A	C5-C6-N6	-5.57	119.25	123.70
27	B8	1020	A	C5-C6-N6	-5.57	119.25	123.70
27	B8	1169	A	C5-C6-N1	-5.57	114.92	117.70
27	B8	1214	A	C4-C5-C6	5.57	119.78	117.00
27	B8	1429	G	O4'-C1'-N9	5.57	112.65	108.20
27	B8	1937	A	C4-C5-C6	5.57	119.78	117.00
27	B8	1969	A	C5-C6-N6	-5.57	119.25	123.70
27	B8	2058	A	C5-C6-N6	-5.57	119.25	123.70
1	AA	1026	G	O4'-C1'-N9	5.56	112.65	108.20
1	AA	1191	A	C5-C6-N1	-5.56	114.92	117.70
27	B8	2114	A	C5-C6-N1	-5.56	114.92	117.70
27	B8	2699	C	N3-C4-N4	5.56	121.89	118.00
1	AA	104	G	O4'-C1'-N9	5.56	112.65	108.20
1	AA	503	C	N3-C4-C5	-5.56	119.67	121.90
1	AA	980	C	N3-C4-N4	5.56	121.89	118.00
1	AA	1302	C	N3-C4-C5	-5.56	119.67	121.90
26	B7	37	C	N3-C4-C5	-5.56	119.67	121.90
27	B8	739	A	O4'-C1'-N9	5.56	112.65	108.20
27	B8	908	C	N3-C4-C5	-5.56	119.67	121.90
27	B8	1027	A	C5-C6-N1	-5.56	114.92	117.70
27	B8	1211	C	O4'-C1'-N1	5.56	112.65	108.20
27	B8	1281	G	O4'-C1'-N9	5.56	112.65	108.20
27	B8	1654	A	C5-C6-N1	-5.56	114.92	117.70
27	B8	2047	C	N3-C4-C5	-5.56	119.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2712	C	N3-C4-N4	5.56	121.89	118.00
27	B8	1632	A	C5-C6-N6	-5.56	119.25	123.70
27	B8	2525	G	O4'-C1'-N9	5.56	112.65	108.20
27	B8	2799	A	C5-C6-N6	-5.56	119.25	123.70
1	AA	234	C	N3-C4-N4	5.56	121.89	118.00
1	AA	432	A	O4'-C1'-N9	5.56	112.65	108.20
1	AA	642	A	C5-C6-N1	-5.56	114.92	117.70
1	AA	924	C	N3-C4-C5	-5.56	119.68	121.90
1	AA	1408	A	C4-C5-C6	5.56	119.78	117.00
26	B7	30	C	N3-C4-C5	-5.56	119.68	121.90
27	B8	209	C	N3-C4-C5	-5.56	119.68	121.90
27	B8	334	C	N3-C4-N4	5.56	121.89	118.00
27	B8	643	A	C5-C6-N6	-5.56	119.25	123.70
27	B8	1291	C	N3-C4-N4	5.56	121.89	118.00
27	B8	1295	C	N3-C4-N4	5.56	121.89	118.00
27	B8	1403	A	C5-C6-N6	-5.56	119.25	123.70
27	B8	1431	A	O4'-C1'-N9	5.56	112.65	108.20
27	B8	1625	C	N3-C4-N4	5.56	121.89	118.00
1	AA	178	C	N3-C4-N4	5.56	121.89	118.00
1	AA	306	A	C5-C6-N6	-5.56	119.25	123.70
1	AA	573	A	C5-C6-N1	-5.56	114.92	117.70
27	B8	480	A	C5-C6-N6	-5.56	119.25	123.70
27	B8	882	G	O4'-C1'-N9	5.56	112.65	108.20
27	B8	1313	U	O4'-C1'-N1	5.56	112.65	108.20
27	B8	1323	C	N3-C4-N4	5.56	121.89	118.00
27	B8	1761	C	N3-C4-N4	5.56	121.89	118.00
27	B8	1890	A	O4'-C1'-N9	5.56	112.64	108.20
1	AA	749	A	C5-C6-N1	-5.56	114.92	117.70
1	AA	1516	G	O4'-C1'-N9	5.56	112.64	108.20
3	AV	14	A	C5-C6-N6	-5.56	119.25	123.70
27	B8	156	A	C5-C6-N6	-5.56	119.25	123.70
27	B8	610	C	N3-C4-N4	5.56	121.89	118.00
1	AA	392	C	N3-C4-N4	5.55	121.89	118.00
1	AA	767	A	C5-C6-N6	-5.55	119.26	123.70
1	AA	1389	C	N3-C4-N4	5.55	121.89	118.00
27	B8	788	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	1349	C	N3-C4-C5	-5.55	119.68	121.90
27	B8	2029	G	N3-C2-N2	5.55	123.79	119.90
27	B8	2705	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	2764	A	C5-C6-N1	-5.55	114.92	117.70
1	AA	78	A	C5-C6-N1	-5.55	114.92	117.70
27	B8	348	A	C5-C6-N1	-5.55	114.92	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	621	A	C5-C6-N6	-5.55	119.26	123.70
1	AA	965	U	O4'-C1'-N1	5.55	112.64	108.20
1	AA	1394	A	C5-C6-N1	-5.55	114.92	117.70
1	AA	1402	C	N3-C4-C5	-5.55	119.68	121.90
3	AV	10	G	O4'-C1'-N9	5.55	112.64	108.20
27	B8	218	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	731	C	N3-C4-C5	-5.55	119.68	121.90
27	B8	889	C	N3-C4-N4	5.55	121.89	118.00
27	B8	899	A	C4-C5-C6	5.55	119.78	117.00
27	B8	1000	A	C5-C6-N1	-5.55	114.92	117.70
27	B8	1005	C	N3-C4-N4	5.55	121.89	118.00
27	B8	1226	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	1569	A	O4'-C1'-N9	5.55	112.64	108.20
27	B8	1804	C	N3-C4-C5	-5.55	119.68	121.90
27	B8	1985	C	N3-C4-N4	5.55	121.89	118.00
27	B8	2171	A	C5-C6-N1	-5.55	114.92	117.70
1	AA	1092	A	C5-C6-N1	-5.55	114.92	117.70
1	AA	1479	C	N3-C4-N4	5.55	121.89	118.00
27	B8	959	A	C4-C5-C6	5.55	119.77	117.00
27	B8	1871	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	2134	A	C5-C6-N1	-5.55	114.92	117.70
27	B8	2425	A	C5-C6-N1	-5.55	114.92	117.70
27	B8	2480	C	N3-C4-N4	5.55	121.89	118.00
27	B8	2666	C	N3-C4-C5	-5.55	119.68	121.90
1	AA	744	C	N3-C4-N4	5.55	121.88	118.00
27	B8	727	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	1089	A	C5-C6-N1	-5.55	114.93	117.70
27	B8	1090	A	C5-C6-N6	-5.55	119.26	123.70
27	B8	1153	C	N3-C4-C5	-5.55	119.68	121.90
27	B8	1730	C	N3-C4-N4	5.55	121.88	118.00
27	B8	2019	A	C5-C6-N1	-5.55	114.93	117.70
27	B8	2418	A	C5-C6-N1	-5.55	114.93	117.70
1	AA	466	A	C5-C6-N6	-5.55	119.26	123.70
1	AA	622	A	C5-C6-N6	-5.55	119.26	123.70
1	AA	1421	G	O4'-C1'-N9	5.55	112.64	108.20
1	AA	1499	A	C5-C6-N6	-5.55	119.26	123.70
1	AA	1515	G	O4'-C1'-N9	5.55	112.64	108.20
27	B8	140	C	N3-C4-C5	-5.55	119.68	121.90
27	B8	157	C	N3-C4-N4	5.55	121.88	118.00
27	B8	195	A	O4'-C1'-N9	5.55	112.64	108.20
27	B8	650	C	N3-C4-C5	-5.55	119.68	121.90
27	B8	995	C	N3-C4-C5	-5.55	119.68	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1370	C	N3-C4-N4	5.55	121.88	118.00
27	B8	2152	G	C5'-C4'-O4'	5.55	115.76	109.10
27	B8	2886	A	C5-C6-N6	-5.55	119.26	123.70
1	AA	1186	G	O4'-C1'-N9	5.54	112.64	108.20
27	B8	318	C	N3-C4-C5	-5.54	119.68	121.90
27	B8	800	A	C4-C5-C6	5.54	119.77	117.00
27	B8	2241	A	C5-C6-N6	-5.54	119.26	123.70
27	B8	2475	C	N3-C4-N4	5.54	121.88	118.00
1	AA	280	C	C2-N1-C1'	5.54	124.90	118.80
1	AA	526	C	N3-C4-C5	-5.54	119.68	121.90
1	AA	646	G	O4'-C1'-N9	5.54	112.63	108.20
1	AA	869	G	N3-C2-N2	5.54	123.78	119.90
1	AA	1045	C	N3-C4-N4	5.54	121.88	118.00
1	AA	1136	C	N3-C4-N4	5.54	121.88	118.00
1	AA	1349	A	O4'-C1'-N9	5.54	112.63	108.20
27	B8	821	A	C4-C5-C6	5.54	119.77	117.00
27	B8	1439	A	O4'-C1'-N9	5.54	112.64	108.20
27	B8	2573	C	N3-C4-C5	-5.54	119.68	121.90
27	B8	2691	C	N3-C4-C5	-5.54	119.68	121.90
1	AA	702	A	C5-C6-N1	-5.54	114.93	117.70
26	B7	53	A	C5-C6-N1	-5.54	114.93	117.70
27	B8	772	C	N3-C4-C5	-5.54	119.68	121.90
27	B8	941	A	C4-C5-C6	5.54	119.77	117.00
27	B8	1205	A	C5-C6-N1	-5.54	114.93	117.70
27	B8	2322	A	C5-C6-N1	-5.54	114.93	117.70
1	AA	166	U	O4'-C1'-N1	5.54	112.63	108.20
1	AA	459	A	C5-C6-N6	-5.54	119.27	123.70
1	AA	1180	A	C5-C6-N6	-5.54	119.27	123.70
1	AA	1483	A	O4'-C1'-N9	5.54	112.63	108.20
27	B8	480	A	C5-C6-N1	-5.54	114.93	117.70
27	B8	896	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	1129	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	1151	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	2174	C	N3-C4-C5	-5.54	119.68	121.90
27	B8	2364	C	N3-C4-N4	5.54	121.88	118.00
27	B8	2889	C	N3-C4-N4	5.54	121.88	118.00
1	AA	1092	A	C5-C6-N6	-5.54	119.27	123.70
1	AA	1271	A	C5-C6-N1	-5.54	114.93	117.70
1	AA	1395	C	N3-C4-N4	5.54	121.88	118.00
27	B8	380	G	O4'-C1'-N9	5.54	112.63	108.20
27	B8	432	A	O4'-C1'-N9	5.54	112.63	108.20
27	B8	440	C	N3-C4-N4	5.54	121.88	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	849	A	C4-C5-C6	5.54	119.77	117.00
27	B8	861	A	C4-C5-C6	5.54	119.77	117.00
27	B8	2333	A	C4-C5-C6	5.54	119.77	117.00
27	B8	2670	A	C5-C6-N1	-5.54	114.93	117.70
1	AA	1046	A	C4-C5-C6	5.54	119.77	117.00
27	B8	311	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	1919	A	C5-C6-N6	-5.54	119.27	123.70
1	AA	213	G	O4'-C1'-N9	5.54	112.63	108.20
1	AA	668	G	O4'-C1'-N9	5.54	112.63	108.20
1	AA	936	C	N3-C4-N4	5.54	121.88	118.00
1	AA	1368	A	C4-C5-C6	5.54	119.77	117.00
27	B8	752	A	C5-C6-N1	-5.54	114.93	117.70
27	B8	1167	C	N3-C4-C5	-5.54	119.69	121.90
27	B8	1302	A	C4-C5-C6	5.54	119.77	117.00
27	B8	1805	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	1848	A	C5-C6-N1	-5.54	114.93	117.70
27	B8	2215	C	N3-C4-C5	-5.54	119.69	121.90
27	B8	2352	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	2858	C	N3-C4-N4	5.54	121.88	118.00
27	B8	2883	A	C5-C6-N6	-5.54	119.27	123.70
27	B8	2893	A	C5-C6-N6	-5.54	119.27	123.70
1	AA	36	C	N3-C4-C5	-5.53	119.69	121.90
1	AA	198	G	O4'-C1'-N9	5.53	112.63	108.20
1	AA	306	A	C5-C6-N1	-5.53	114.93	117.70
1	AA	811	C	N3-C4-C5	-5.53	119.69	121.90
26	B7	114	C	N3-C4-N4	5.53	121.87	118.00
27	B8	194	G	O4'-C1'-N9	5.53	112.63	108.20
27	B8	1028	A	C5-C6-N6	-5.53	119.27	123.70
27	B8	1816	C	N3-C4-N4	5.53	121.87	118.00
27	B8	1997	C	N3-C4-N4	5.53	121.87	118.00
27	B8	2082	A	C5-C6-N6	-5.53	119.27	123.70
27	B8	2163	A	O4'-C1'-N9	5.53	112.63	108.20
1	AA	298	A	C5-C6-N6	-5.53	119.27	123.70
1	AA	629	A	C5-C6-N1	-5.53	114.93	117.70
1	AA	1161	C	C6-N1-C2	-5.53	118.09	120.30
27	B8	992	C	N3-C4-N4	5.53	121.87	118.00
27	B8	1461	C	N3-C4-C5	-5.53	119.69	121.90
27	B8	2589	A	C5-C6-N6	-5.53	119.28	123.70
1	AA	74	A	C4-C5-C6	5.53	119.77	117.00
1	AA	490	C	N3-C4-N4	5.53	121.87	118.00
1	AA	909	A	C5-C6-N6	-5.53	119.28	123.70
1	AA	1094	G	O4'-C1'-N9	5.53	112.62	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B7	52	A	C4-C5-C6	5.53	119.77	117.00
27	B8	231	A	O4'-C1'-N9	5.53	112.62	108.20
27	B8	417	C	N3-C4-C5	-5.53	119.69	121.90
27	B8	590	A	O4'-C1'-N9	5.53	112.62	108.20
27	B8	1156	A	C5-C6-N6	-5.53	119.28	123.70
27	B8	1535	A	C5-C6-N6	-5.53	119.28	123.70
27	B8	1676	A	O4'-C1'-N9	5.53	112.62	108.20
27	B8	1817	G	O4'-C1'-N9	5.53	112.62	108.20
1	AA	161	A	C5-C6-N6	-5.53	119.28	123.70
1	AA	826	C	N3-C4-N4	5.53	121.87	118.00
27	B8	1869	G	N3-C2-N2	5.53	123.77	119.90
27	B8	2851	A	C4-C5-C6	5.53	119.76	117.00
1	AA	706	A	C5-C6-N1	-5.53	114.94	117.70
1	AA	747	A	O4'-C1'-N9	5.53	112.62	108.20
1	AA	1437	A	O4'-C1'-N9	5.53	112.62	108.20
1	AA	1523	G	O4'-C1'-N9	5.53	112.62	108.20
27	B8	14	A	C5-C6-N6	-5.53	119.28	123.70
27	B8	1051	G	O4'-C1'-N9	5.53	112.62	108.20
27	B8	1652	A	C4-C5-C6	5.53	119.76	117.00
27	B8	1732	C	N3-C4-C5	-5.53	119.69	121.90
27	B8	1990	C	N3-C4-C5	-5.53	119.69	121.90
27	B8	2425	A	C5-C6-N6	-5.53	119.28	123.70
27	B8	2634	A	C5-C6-N1	-5.53	114.94	117.70
1	AA	131	A	C5-C6-N6	-5.53	119.28	123.70
1	AA	182	A	C5-C6-N6	-5.53	119.28	123.70
1	AA	951	G	O4'-C1'-N9	5.53	112.62	108.20
1	AA	1371	G	O4'-C1'-N9	5.53	112.62	108.20
27	B8	49	A	C5-C6-N6	-5.53	119.28	123.70
27	B8	118	A	C4-C5-C6	5.53	119.76	117.00
27	B8	1343	G	O4'-C1'-N9	5.53	112.62	108.20
27	B8	1604	C	N3-C4-C5	-5.53	119.69	121.90
27	B8	1748	C	N3-C4-N4	5.53	121.87	118.00
27	B8	2129	C	N3-C4-N4	5.53	121.87	118.00
27	B8	2340	A	C5-C6-N1	-5.53	114.94	117.70
27	B8	2367	G	O4'-C1'-N9	5.53	112.62	108.20
27	B8	2459	A	C5-C6-N1	-5.53	114.94	117.70
1	AA	286	C	N3-C4-C5	-5.52	119.69	121.90
1	AA	711	G	O4'-C1'-N9	5.52	112.62	108.20
1	AA	1011	C	N3-C4-C5	-5.52	119.69	121.90
3	AV	9	A	C5-C6-N1	-5.52	114.94	117.70
26	B7	15	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	792	A	C5-C6-N1	-5.52	114.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	906	A	C4-C5-C6	5.52	119.76	117.00
1	AA	1176	A	C5-C6-N1	-5.52	114.94	117.70
26	B7	109	A	O4'-C1'-N9	5.52	112.62	108.20
27	B8	432	A	C5-C6-N6	-5.52	119.28	123.70
27	B8	804	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	1265	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	1328	A	C5-C6-N6	-5.52	119.28	123.70
27	B8	1376	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	1759	A	C5-C6-N6	-5.52	119.28	123.70
27	B8	1816	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	2469	A	C4-C5-C6	5.52	119.76	117.00
27	B8	2565	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	2646	C	N3-C4-C5	-5.52	119.69	121.90
2	AX	13	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	125	A	C5-C6-N6	-5.52	119.28	123.70
27	B8	547	A	C5-C6-N6	-5.52	119.28	123.70
27	B8	1274	A	C4-C5-C6	5.52	119.76	117.00
27	B8	2009	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	2559	C	N3-C4-N4	5.52	121.86	118.00
1	AA	403	C	N3-C4-C5	-5.52	119.69	121.90
1	AA	612	C	N3-C4-N4	5.52	121.86	118.00
26	B7	42	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	393	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	502	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	990	A	C4-C5-C6	5.52	119.76	117.00
27	B8	1013	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	1077	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	1899	A	C4-C5-C6	5.52	119.76	117.00
27	B8	2534	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	2812	G	O4'-C1'-N9	5.52	112.62	108.20
1	AA	719	C	N3-C4-C5	-5.52	119.69	121.90
1	AA	1069	C	N3-C4-N4	5.52	121.86	118.00
1	AA	1213	A	C5-C6-N1	-5.52	114.94	117.70
2	AX	16	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	449	A	C5-C6-N1	-5.52	114.94	117.70
27	B8	601	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	984	A	C5-C6-N6	-5.52	119.29	123.70
27	B8	1789	A	C5-C6-N6	-5.52	119.29	123.70
27	B8	2101	A	C5-C6-N1	-5.52	114.94	117.70
1	AA	117	G	O4'-C1'-N9	5.52	112.61	108.20
1	AA	777	A	C5-C6-N1	-5.52	114.94	117.70
1	AA	1180	A	C5-C6-N1	-5.52	114.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	201	C	N3-C4-C5	-5.52	119.69	121.90
27	B8	2019	A	C5-C6-N6	-5.52	119.29	123.70
27	B8	2146	C	N3-C4-N4	5.52	121.86	118.00
27	B8	2609	U	O4'-C1'-N1	5.52	112.61	108.20
1	AA	162	A	C5-C6-N6	-5.51	119.29	123.70
1	AA	171	A	C5-C6-N1	-5.51	114.94	117.70
1	AA	715	A	C5-C6-N6	-5.51	119.29	123.70
1	AA	1368	A	C5-C6-N1	-5.51	114.94	117.70
26	B7	46	A	O4'-C1'-N9	5.51	112.61	108.20
27	B8	91	A	C5-C6-N6	-5.51	119.29	123.70
27	B8	152	A	C5-C6-N1	-5.51	114.94	117.70
27	B8	543	G	O4'-C1'-N9	5.51	112.61	108.20
27	B8	1987	A	C5-C6-N6	-5.51	119.29	123.70
27	B8	2033	A	C5-C6-N1	-5.51	114.94	117.70
1	AA	1169	A	C5-C6-N1	-5.51	114.94	117.70
1	AA	1318	A	C5-C6-N6	-5.51	119.29	123.70
2	AX	15	C	N3-C4-N4	5.51	121.86	118.00
27	B8	1096	A	C5-C6-N6	-5.51	119.29	123.70
1	AA	217	C	N3-C4-C5	-5.51	119.69	121.90
1	AA	620	C	N3-C4-C5	-5.51	119.69	121.90
7	AC	36	PHE	CB-CG-CD2	5.51	124.66	120.80
27	B8	635	C	N3-C4-C5	-5.51	119.69	121.90
27	B8	661	A	C5-C6-N6	-5.51	119.29	123.70
27	B8	673	C	N3-C4-N4	5.51	121.86	118.00
27	B8	1610	A	C4-C5-C6	5.51	119.75	117.00
27	B8	2001	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	2094	A	O4'-C1'-N9	5.51	112.61	108.20
27	B8	2287	A	C5-C6-N1	-5.51	114.94	117.70
27	B8	2342	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	2711	A	C4-C5-C6	5.51	119.75	117.00
1	AA	655	A	O4'-C1'-N9	5.51	112.61	108.20
1	AA	907	A	C5-C6-N1	-5.51	114.94	117.70
1	AA	1093	A	O4'-C1'-N9	5.51	112.61	108.20
1	AA	1137	C	N3-C4-C5	-5.51	119.70	121.90
1	AA	1158	C	N3-C4-C5	-5.51	119.70	121.90
1	AA	1466	C	N3-C4-N4	5.51	121.86	118.00
27	B8	311	A	C5-C6-N1	-5.51	114.94	117.70
27	B8	477	A	O4'-C1'-N9	5.51	112.61	108.20
27	B8	645	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	668	A	C4-C5-C6	5.51	119.75	117.00
27	B8	1006	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	1942	C	N3-C4-C5	-5.51	119.70	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2332	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	2681	C	N3-C4-N4	5.51	121.86	118.00
26	B7	42	C	N3-C4-N4	5.51	121.86	118.00
27	B8	24	G	O4'-C1'-N9	5.51	112.61	108.20
27	B8	1160	G	O4'-C1'-N9	5.51	112.61	108.20
27	B8	1550	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	1610	A	O4'-C1'-N9	5.51	112.61	108.20
27	B8	1758	U	O4'-C1'-N1	5.51	112.61	108.20
27	B8	2870	C	N3-C4-C5	-5.51	119.70	121.90
1	AA	915	A	O4'-C1'-N9	5.51	112.61	108.20
1	AA	1303	C	N3-C4-N4	5.51	121.85	118.00
26	B7	36	C	N3-C4-N4	5.51	121.85	118.00
27	B8	301	G	O4'-C1'-N9	5.51	112.61	108.20
27	B8	520	G	O4'-C1'-N9	5.51	112.61	108.20
27	B8	815	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	951	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	1320	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	1854	A	C4-C5-C6	5.51	119.75	117.00
27	B8	2275	C	N3-C4-C5	-5.51	119.70	121.90
27	B8	2327	A	C5-C6-N1	-5.51	114.95	117.70
27	B8	2839	G	O4'-C1'-N9	5.51	112.61	108.20
1	AA	165	G	O4'-C1'-N9	5.50	112.60	108.20
26	B7	17	C	N3-C4-N4	5.50	121.85	118.00
27	B8	12	U	P-O3'-C3'	5.50	126.31	119.70
1	AA	823	C	N3-C4-N4	5.50	121.85	118.00
1	AA	912	C	N3-C4-C5	-5.50	119.70	121.90
1	AA	1093	A	C5-C6-N6	-5.50	119.30	123.70
27	B8	318	C	N3-C4-N4	5.50	121.85	118.00
27	B8	453	A	O4'-C1'-N9	5.50	112.60	108.20
27	B8	819	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	889	C	C6-N1-C1'	-5.50	114.20	120.80
27	B8	1158	C	N3-C4-C5	-5.50	119.70	121.90
27	B8	1169	A	C5-C6-N6	-5.50	119.30	123.70
27	B8	1351	C	N3-C4-N4	5.50	121.85	118.00
27	B8	1552	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	1748	C	N3-C4-C5	-5.50	119.70	121.90
27	B8	2020	A	C5-C6-N1	-5.50	114.95	117.70
1	AA	2	A	C5-C6-N6	-5.50	119.30	123.70
1	AA	10	A	C5-C6-N1	-5.50	114.95	117.70
1	AA	280	C	N3-C4-C5	-5.50	119.70	121.90
1	AA	1145	A	C4-C5-C6	5.50	119.75	117.00
1	AA	1195	C	N3-C4-C5	-5.50	119.70	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	17	G	O4'-C1'-N9	5.50	112.60	108.20
27	B8	454	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	1020	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	1901	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	2454	G	O4'-C1'-N9	5.50	112.60	108.20
27	B8	2820	A	C5-C6-N6	-5.50	119.30	123.70
1	AA	556	C	N3-C4-C5	-5.50	119.70	121.90
1	AA	1396	A	C5-C6-N1	-5.50	114.95	117.70
26	B7	94	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	384	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	563	A	C5-C6-N6	-5.50	119.30	123.70
27	B8	1230	A	O4'-C1'-N9	5.50	112.60	108.20
1	AA	83	C	N3-C4-N4	5.50	121.85	118.00
1	AA	260	G	O4'-C1'-N9	5.50	112.60	108.20
27	B8	716	A	O4'-C1'-N9	5.50	112.60	108.20
27	B8	772	C	N3-C4-N4	5.50	121.85	118.00
27	B8	1439	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	1548	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	2073	C	N3-C4-C5	-5.50	119.70	121.90
27	B8	2432	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	2781	A	C5-C6-N1	-5.50	114.95	117.70
1	AA	196	A	C4-C5-C6	5.50	119.75	117.00
1	AA	430	A	O4'-C1'-N9	5.50	112.60	108.20
1	AA	448	A	C4-C5-C6	5.50	119.75	117.00
1	AA	994	A	C5-C6-N1	-5.50	114.95	117.70
1	AA	1336	C	N3-C4-N4	5.50	121.85	118.00
27	B8	482	A	C5-C6-N1	-5.50	114.95	117.70
27	B8	1630	A	C4-C5-C6	5.50	119.75	117.00
27	B8	2801	G	O4'-C1'-N9	5.50	112.60	108.20
1	AA	336	A	O4'-C1'-N9	5.50	112.60	108.20
1	AA	630	A	C5-C6-N1	-5.50	114.95	117.70
1	AA	995	C	N3-C4-C5	-5.50	119.70	121.90
1	AA	1410	A	C5-C6-N1	-5.50	114.95	117.70
26	B7	88	C	N3-C4-C5	-5.50	119.70	121.90
27	B8	56	A	O4'-C1'-N9	5.50	112.60	108.20
1	AA	57	G	O4'-C1'-N9	5.49	112.59	108.20
1	AA	109	A	O4'-C1'-N9	5.49	112.59	108.20
1	AA	264	C	N3-C4-N4	5.49	121.84	118.00
1	AA	610	U	C6-N1-C1'	-5.49	113.51	121.20
1	AA	1013	G	N3-C2-N2	5.49	123.75	119.90
3	AV	58	A	C5-C6-N6	-5.49	119.31	123.70
27	B8	486	C	N3-C4-N4	5.49	121.85	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	908	C	N3-C4-N4	5.49	121.85	118.00
27	B8	1050	A	C4-C5-C6	5.49	119.75	117.00
27	B8	1496	A	P-O3'-C3'	5.49	126.29	119.70
27	B8	1833	C	N3-C4-N4	5.49	121.84	118.00
33	BE	85	PHE	CB-CG-CD1	5.49	124.64	120.80
27	B8	666	A	O4'-C1'-N9	5.49	112.59	108.20
27	B8	1626	A	C5-C6-N1	-5.49	114.95	117.70
1	AA	197	A	C5-C6-N1	-5.49	114.95	117.70
1	AA	925	G	O4'-C1'-N9	5.49	112.59	108.20
1	AA	1120	C	N3-C4-N4	5.49	121.84	118.00
1	AA	1456	A	C5-C6-N1	-5.49	114.95	117.70
3	AV	52	A	O4'-C1'-N9	5.49	112.59	108.20
27	B8	491	G	O4'-C1'-N9	5.49	112.59	108.20
27	B8	526	A	C5-C6-N6	-5.49	119.31	123.70
27	B8	888	C	N3-C4-N4	5.49	121.84	118.00
27	B8	1556	C	N3-C4-N4	5.49	121.84	118.00
27	B8	2003	A	O4'-C1'-N9	5.49	112.59	108.20
1	AA	322	C	N3-C4-N4	5.49	121.84	118.00
1	AA	510	A	C5-C6-N6	-5.49	119.31	123.70
1	AA	611	C	N3-C4-C5	-5.49	119.70	121.90
1	AA	784	A	C5-C6-N1	-5.49	114.96	117.70
27	B8	659	G	O4'-C1'-N9	5.49	112.59	108.20
27	B8	806	C	N3-C4-C5	-5.49	119.70	121.90
27	B8	837	C	N3-C4-N4	5.49	121.84	118.00
27	B8	1072	C	N3-C4-C5	-5.49	119.70	121.90
27	B8	1080	A	C5-C6-N1	-5.49	114.96	117.70
27	B8	1370	C	N3-C4-C5	-5.49	119.70	121.90
27	B8	1449	G	O4'-C1'-N9	5.49	112.59	108.20
27	B8	2407	A	C5-C6-N6	-5.49	119.31	123.70
27	B8	685	A	C4-C5-C6	5.49	119.74	117.00
1	AA	449	G	O4'-C1'-N9	5.49	112.59	108.20
1	AA	622	A	C4-C5-C6	5.49	119.74	117.00
1	AA	715	A	C5-C6-N1	-5.49	114.96	117.70
1	AA	1250	A	O4'-C1'-N9	5.49	112.59	108.20
26	B7	63	C	N3-C4-N4	5.49	121.84	118.00
27	B8	13	A	C5-C6-N1	-5.49	114.96	117.70
27	B8	218	A	C5-C6-N1	-5.49	114.96	117.70
27	B8	385	C	N3-C4-C5	-5.49	119.71	121.90
27	B8	715	A	C5-C6-N6	-5.49	119.31	123.70
27	B8	1286	A	C5-C6-N6	-5.49	119.31	123.70
27	B8	1994	C	N3-C4-C5	-5.49	119.71	121.90
27	B8	2067	G	P-O3'-C3'	5.49	126.28	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2281	A	C5-C6-N1	-5.49	114.96	117.70
27	B8	2346	A	C5-C6-N1	-5.49	114.96	117.70
1	AA	716	A	C4-C5-C6	5.48	119.74	117.00
1	AA	1271	A	C5-C6-N6	-5.48	119.31	123.70
27	B8	205	G	O4'-C1'-N9	5.48	112.59	108.20
27	B8	1509	A	C5-C6-N6	-5.48	119.31	123.70
27	B8	1990	C	N3-C4-N4	5.48	121.84	118.00
27	B8	2539	C	N3-C4-N4	5.48	121.84	118.00
1	AA	50	A	C5-C6-N6	-5.48	119.31	123.70
1	AA	1204	A	O4'-C1'-N9	5.48	112.59	108.20
27	B8	348	A	C5-C6-N6	-5.48	119.31	123.70
27	B8	420	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	848	C	N3-C4-N4	5.48	121.84	118.00
27	B8	1153	C	N3-C4-N4	5.48	121.84	118.00
27	B8	1647	U	O4'-C1'-N1	5.48	112.59	108.20
27	B8	2153	C	N3-C4-N4	5.48	121.84	118.00
27	B8	2232	C	N3-C4-N4	5.48	121.84	118.00
1	AA	623	C	N3-C4-C5	-5.48	119.71	121.90
1	AA	923	A	O4'-C1'-N9	5.48	112.58	108.20
1	AA	1146	A	O4'-C1'-N9	5.48	112.58	108.20
3	AV	16	C	N3-C4-C5	-5.48	119.71	121.90
26	B7	94	A	C4-C5-C6	5.48	119.74	117.00
26	B7	106	G	O4'-C1'-N9	5.48	112.58	108.20
27	B8	316	C	N3-C4-N4	5.48	121.84	118.00
27	B8	752	A	C5-C6-N6	-5.48	119.31	123.70
27	B8	1809	A	C4-C5-C6	5.48	119.74	117.00
27	B8	1925	C	N3-C4-N4	5.48	121.84	118.00
1	AA	411	A	C5-C6-N6	-5.48	119.32	123.70
1	AA	441	A	C5-C6-N6	-5.48	119.32	123.70
1	AA	1492	A	C4-C5-C6	5.48	119.74	117.00
27	B8	2497	A	C5-C6-N1	-5.48	114.96	117.70
27	B8	2823	A	C5-C6-N1	-5.48	114.96	117.70
1	AA	77	A	O4'-C1'-N9	5.48	112.58	108.20
1	AA	621	A	C5-C6-N1	-5.48	114.96	117.70
1	AA	1081	A	C5-C6-N1	-5.48	114.96	117.70
1	AA	1280	A	C5-C6-N1	-5.48	114.96	117.70
1	AA	1400	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	196	A	C5-C6-N6	-5.48	119.32	123.70
27	B8	302	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	351	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	369	U	O4'-C1'-N1	5.48	112.58	108.20
27	B8	423	A	C4-C5-C6	5.48	119.74	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	730	A	O4'-C1'-N9	5.48	112.58	108.20
27	B8	996	A	O4'-C1'-N9	5.48	112.58	108.20
27	B8	1169	A	O4'-C1'-N9	5.48	112.58	108.20
27	B8	1332	G	O4'-C1'-N9	5.48	112.58	108.20
27	B8	1360	G	C5-C6-O6	-5.48	125.31	128.60
27	B8	1800	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	2278	A	C5-C6-N1	-5.48	114.96	117.70
27	B8	2360	G	O4'-C1'-N9	5.48	112.58	108.20
27	B8	2572	A	O4'-C1'-N9	5.48	112.58	108.20
1	AA	975	A	C5-C6-N6	-5.48	119.32	123.70
1	AA	1170	A	O4'-C1'-N9	5.48	112.58	108.20
27	B8	631	A	O4'-C1'-N9	5.48	112.58	108.20
27	B8	1549	A	C5-C6-N6	-5.48	119.32	123.70
27	B8	1658	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	2063	C	N3-C4-C5	-5.48	119.71	121.90
27	B8	2386	A	O4'-C1'-N9	5.48	112.58	108.20
1	AA	303	A	C5-C6-N6	-5.47	119.32	123.70
1	AA	547	A	C5-C6-N1	-5.47	114.96	117.70
1	AA	1412	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	393	C	N3-C4-N4	5.47	121.83	118.00
27	B8	445	C	N3-C4-N4	5.47	121.83	118.00
27	B8	508	A	C5-C6-N6	-5.47	119.32	123.70
27	B8	886	A	C5-C6-N1	-5.47	114.96	117.70
27	B8	1590	A	C4-C5-C6	5.47	119.74	117.00
27	B8	1774	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	1810	A	C5-C6-N1	-5.47	114.96	117.70
27	B8	2165	C	N3-C4-N4	5.47	121.83	118.00
27	B8	2314	A	C5-C6-N6	-5.47	119.32	123.70
27	B8	2830	C	N3-C4-C5	-5.47	119.71	121.90
1	AA	307	C	N3-C4-C5	-5.47	119.71	121.90
1	AA	1431	A	C4-C5-C6	5.47	119.74	117.00
27	B8	475	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	502	A	C4-C5-C6	5.47	119.74	117.00
27	B8	943	A	O4'-C1'-N9	5.47	112.58	108.20
27	B8	1266	G	O4'-C1'-N9	5.47	112.58	108.20
27	B8	2526	G	O4'-C1'-N9	5.47	112.58	108.20
1	AA	839	C	N3-C4-C5	-5.47	119.71	121.90
1	AA	1042	A	O4'-C1'-N9	5.47	112.58	108.20
1	AA	1152	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	115	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	529	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	1694	C	N3-C4-C5	-5.47	119.71	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1802	A	O4'-C1'-N9	5.47	112.58	108.20
1	AA	535	A	O4'-C1'-N9	5.47	112.58	108.20
1	AA	845	A	C5-C6-N6	-5.47	119.32	123.70
1	AA	1109	C	N3-C4-N4	5.47	121.83	118.00
1	AA	1166	G	N3-C2-N2	5.47	123.73	119.90
3	AV	13	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	680	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	927	A	C5-C6-N6	-5.47	119.33	123.70
27	B8	985	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	1093	G	O4'-C1'-N9	5.47	112.58	108.20
27	B8	1981	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	2078	C	N3-C4-N4	5.47	121.83	118.00
27	B8	2565	A	C5-C6-N6	-5.47	119.32	123.70
27	B8	2718	G	O4'-C1'-N9	5.47	112.58	108.20
27	B8	2874	C	N3-C4-C5	-5.47	119.71	121.90
32	BD	127	PHE	CB-CG-CD2	5.47	124.63	120.80
1	AA	935	A	O4'-C1'-N9	5.47	112.58	108.20
1	AA	1093	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	111	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	961	C	N3-C4-N4	5.47	121.83	118.00
27	B8	1871	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	2369	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	2422	C	N3-C4-C5	-5.47	119.71	121.90
1	AA	163	C	N3-C4-N4	5.47	121.83	118.00
1	AA	640	A	C5-C6-N1	-5.47	114.97	117.70
1	AA	654	G	O4'-C1'-N9	5.47	112.57	108.20
26	B7	59	A	O4'-C1'-N9	5.47	112.57	108.20
27	B8	345	A	C4-C5-C6	5.47	119.73	117.00
27	B8	624	C	N3-C4-N4	5.47	121.83	118.00
27	B8	863	A	O4'-C1'-N9	5.47	112.57	108.20
27	B8	981	A	C5-C6-N1	-5.47	114.97	117.70
27	B8	1348	C	N3-C4-C5	-5.47	119.71	121.90
27	B8	1622	G	O4'-C1'-N9	5.47	112.57	108.20
27	B8	2038	G	O4'-C1'-N9	5.47	112.57	108.20
1	AA	95	C	C6-N1-C2	-5.46	118.11	120.30
1	AA	968	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	1191	A	O4'-C1'-N9	5.46	112.57	108.20
27	B8	9	G	O4'-C1'-N9	5.46	112.57	108.20
27	B8	1010	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1544	A	C5-C6-N6	-5.46	119.33	123.70
27	B8	1665	A	C5-C6-N6	-5.46	119.33	123.70
34	BF	7	TYR	CB-CG-CD1	-5.46	117.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	364	A	C5-C6-N6	-5.46	119.33	123.70
27	B8	142	A	C5-C6-N1	-5.46	114.97	117.70
1	AA	233	C	N3-C4-C5	-5.46	119.72	121.90
1	AA	397	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	1311	A	C5-C6-N1	-5.46	114.97	117.70
2	AX	18	C	N3-C4-C5	-5.46	119.72	121.90
27	B8	964	C	N3-C4-C5	-5.46	119.72	121.90
27	B8	1981	A	C5-C6-N6	-5.46	119.33	123.70
27	B8	2358	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	2749	A	O4'-C1'-N9	5.46	112.57	108.20
1	AA	821	G	O4'-C1'-N9	5.46	112.57	108.20
2	AX	22	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	443	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1111	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1808	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	269	C	N3-C4-C5	-5.46	119.72	121.90
1	AA	694	A	C5-C6-N1	-5.46	114.97	117.70
1	AA	1257	A	O4'-C1'-N9	5.46	112.57	108.20
1	AA	1395	C	N3-C4-C5	-5.46	119.72	121.90
3	AV	76	C	N3-C4-C5	-5.46	119.72	121.90
27	B8	1135	C	N3-C4-N4	5.46	121.82	118.00
27	B8	1918	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	2368	C	N3-C4-N4	5.46	121.82	118.00
27	B8	2873	A	C5-C6-N1	-5.46	114.97	117.70
1	AA	452	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	461	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	490	C	N3-C4-C5	-5.46	119.72	121.90
1	AA	935	A	C5-C6-N1	-5.46	114.97	117.70
1	AA	1213	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	1317	C	N3-C4-N4	5.46	121.82	118.00
1	AA	1357	A	O4'-C1'-N9	5.46	112.56	108.20
1	AA	1499	A	O4'-C1'-N9	5.46	112.57	108.20
26	B7	12	C	N3-C4-C5	-5.46	119.72	121.90
27	B8	255	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	314	C	N3-C4-N4	5.46	121.82	118.00
27	B8	668	A	C5-C6-N6	-5.46	119.33	123.70
27	B8	1175	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1365	A	C5-C6-N6	-5.46	119.33	123.70
27	B8	1759	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1801	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1878	G	O4'-C1'-N9	5.46	112.56	108.20
27	B8	2798	U	C2-N1-C1'	5.46	124.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BA	158	PHE	CB-CG-CD1	5.46	124.62	120.80
3	AV	52	A	C5-C6-N6	-5.46	119.34	123.70
27	B8	492	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1000	A	C5-C6-N6	-5.46	119.34	123.70
27	B8	1419	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1570	A	C5-C6-N1	-5.46	114.97	117.70
27	B8	1837	C	N3-C4-C5	-5.46	119.72	121.90
1	AA	330	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	1218	C	N3-C4-N4	5.45	121.82	118.00
27	B8	176	A	C5-C6-N1	-5.45	114.97	117.70
27	B8	1505	A	C5-C6-N6	-5.45	119.34	123.70
27	B8	2062	A	C5-C6-N6	-5.45	119.34	123.70
27	B8	2872	A	C5-C6-N6	-5.45	119.34	123.70
1	AA	279	A	C4-C5-C6	5.45	119.73	117.00
1	AA	325	A	C5-C6-N6	-5.45	119.34	123.70
1	AA	1027	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	1452	C	N3-C4-C5	-5.45	119.72	121.90
27	B8	1024	G	O4'-C1'-N9	5.45	112.56	108.20
27	B8	1251	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	66	A	O4'-C1'-N9	5.45	112.56	108.20
1	AA	67	C	N3-C4-N4	5.45	121.81	118.00
1	AA	73	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	708	C	N3-C4-N4	5.45	121.82	118.00
1	AA	1267	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	1503	A	C5-C6-N1	-5.45	114.97	117.70
27	B8	544	C	N3-C4-N4	5.45	121.81	118.00
27	B8	1125	G	O4'-C1'-N9	5.45	112.56	108.20
27	B8	1301	A	C5-C6-N6	-5.45	119.34	123.70
27	B8	1614	A	C5-C6-N6	-5.45	119.34	123.70
27	B8	2736	A	C5-C6-N6	-5.45	119.34	123.70
1	AA	722	G	O4'-C1'-N9	5.45	112.56	108.20
1	AA	1179	A	C5-C6-N6	-5.45	119.34	123.70
1	AA	1480	A	C5-C6-N6	-5.45	119.34	123.70
3	AV	74	A	C5-C6-N6	-5.45	119.34	123.70
27	B8	472	A	C5-C6-N1	-5.45	114.98	117.70
27	B8	632	A	O4'-C1'-N9	5.45	112.56	108.20
27	B8	805	G	O4'-C1'-N9	5.45	112.56	108.20
27	B8	857	G	O4'-C1'-N9	5.45	112.56	108.20
27	B8	1951	U	O4'-C1'-N1	5.45	112.56	108.20
27	B8	2411	A	C5-C6-N1	-5.45	114.98	117.70
27	B8	2442	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	470	C	N3-C4-C5	-5.45	119.72	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AV	42	C	N3-C4-C5	-5.45	119.72	121.90
27	B8	1549	A	C5-C6-N1	-5.45	114.98	117.70
27	B8	1626	A	C5-C6-N6	-5.45	119.34	123.70
27	B8	2001	C	N3-C4-N4	5.45	121.81	118.00
27	B8	2322	A	C5-C6-N6	-5.45	119.34	123.70
1	AA	113	G	O4'-C1'-N9	5.45	112.56	108.20
1	AA	774	G	O4'-C1'-N9	5.45	112.56	108.20
26	B7	35	C	N3-C4-N4	5.45	121.81	118.00
27	B8	161	A	C4-C5-C6	5.45	119.72	117.00
27	B8	217	A	C5-C6-N1	-5.45	114.98	117.70
27	B8	1670	C	N3-C4-N4	5.45	121.81	118.00
27	B8	1808	A	C5-C6-N1	-5.45	114.98	117.70
27	B8	2159	G	O4'-C1'-N9	5.45	112.56	108.20
27	B8	2516	A	C5-C6-N1	-5.45	114.98	117.70
28	BA	314	GLN	CA-C-N	5.45	132.35	117.10
1	AA	8	A	C5-C6-N1	-5.44	114.98	117.70
1	AA	1042	A	C5-C6-N6	-5.44	119.34	123.70
1	AA	1362	A	C4-C5-C6	5.44	119.72	117.00
27	B8	1762	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	2260	C	N3-C4-C5	-5.44	119.72	121.90
27	B8	2776	A	C5-C6-N1	-5.44	114.98	117.70
33	BE	85	PHE	CB-CG-CD2	-5.44	116.99	120.80
1	AA	385	C	N3-C4-C5	-5.44	119.72	121.90
1	AA	775	G	O4'-C1'-N9	5.44	112.55	108.20
1	AA	1024	G	N3-C2-N2	5.44	123.71	119.90
1	AA	1363	A	C5-C6-N1	-5.44	114.98	117.70
1	AA	1394	A	C5-C6-N6	-5.44	119.35	123.70
2	AX	13	C	N3-C4-N4	5.44	121.81	118.00
27	B8	61	C	N3-C4-N4	5.44	121.81	118.00
27	B8	836	G	O4'-C1'-N9	5.44	112.55	108.20
27	B8	1536	C	N3-C4-C5	-5.44	119.72	121.90
1	AA	197	A	C5-C6-N6	-5.44	119.35	123.70
1	AA	265	G	C5-C6-O6	-5.44	125.33	128.60
1	AA	443	C	N3-C4-C5	-5.44	119.72	121.90
1	AA	778	G	O4'-C1'-N9	5.44	112.55	108.20
1	AA	845	A	P-O3'-C3'	5.44	126.23	119.70
1	AA	1137	C	C6-N1-C1'	-5.44	114.27	120.80
1	AA	1256	A	C5-C6-N6	-5.44	119.35	123.70
1	AA	1483	A	C5-C6-N6	-5.44	119.35	123.70
1	AA	1539	C	N3-C4-C5	-5.44	119.72	121.90
2	AX	22	A	C5-C6-N6	-5.44	119.35	123.70
27	B8	716	A	C5-C6-N1	-5.44	114.98	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	749	A	O4'-C1'-N9	5.44	112.55	108.20
27	B8	1246	A	C5-C6-N6	-5.44	119.35	123.70
27	B8	1253	A	C5-C6-N6	-5.44	119.35	123.70
27	B8	1366	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	1893	C	N3-C4-N4	5.44	121.81	118.00
27	B8	2235	G	O4'-C1'-N9	5.44	112.55	108.20
27	B8	2654	A	C4-C5-C6	5.44	119.72	117.00
27	B8	2829	A	O4'-C1'-N9	5.44	112.55	108.20
1	AA	967	C	N3-C4-C5	-5.44	119.72	121.90
27	B8	330	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	444	C	N3-C4-N4	5.44	121.81	118.00
27	B8	1612	C	N3-C4-N4	5.44	121.81	118.00
27	B8	2158	A	C5-C6-N1	-5.44	114.98	117.70
1	AA	7	A	C5-C6-N6	-5.44	119.35	123.70
1	AA	665	A	C5-C6-N6	-5.44	119.35	123.70
1	AA	1163	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	1254	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	1321	A	O4'-C1'-N9	5.44	112.55	108.20
27	B8	1597	A	O4'-C1'-N9	5.44	112.55	108.20
27	B8	1914	C	N3-C4-C5	-5.44	119.72	121.90
27	B8	1920	C	N3-C4-C5	-5.44	119.72	121.90
27	B8	1940	U	O4'-C1'-N1	5.44	112.55	108.20
27	B8	2579	C	N3-C4-C5	-5.44	119.72	121.90
27	B8	2675	A	O4'-C1'-N9	5.44	112.55	108.20
27	B8	2753	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	2894	G	O4'-C1'-N9	5.44	112.55	108.20
1	AA	430	A	C4-C5-C6	5.44	119.72	117.00
1	AA	1416	G	O4'-C1'-N9	5.44	112.55	108.20
27	B8	1935	G	O4'-C1'-N9	5.44	112.55	108.20
27	B8	2665	A	C5-C6-N1	-5.44	114.98	117.70
27	B8	2841	C	N3-C4-C5	-5.44	119.73	121.90
1	AA	44	A	C5-C6-N6	-5.43	119.35	123.70
1	AA	640	A	O4'-C1'-N9	5.43	112.55	108.20
1	AA	900	A	C5-C6-N1	-5.43	114.98	117.70
1	AA	1491	G	O4'-C1'-N9	5.43	112.55	108.20
27	B8	531	C	N3-C4-N4	5.43	121.81	118.00
27	B8	574	A	C5-C6-N6	-5.43	119.35	123.70
27	B8	1071	G	O4'-C1'-N9	5.43	112.55	108.20
27	B8	1173	U	O4'-C1'-N1	5.43	112.55	108.20
27	B8	1447	C	N3-C4-N4	5.43	121.81	118.00
27	B8	2070	A	C5-C6-N6	-5.43	119.35	123.70
27	B8	2147	A	C5-C6-N1	-5.43	114.98	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2170	A	O4'-C1'-N9	5.43	112.55	108.20
27	B8	2288	A	C5-C6-N6	-5.43	119.35	123.70
27	B8	2601	C	O4'-C1'-N1	5.43	112.55	108.20
27	B8	2644	G	O4'-C1'-N9	5.43	112.55	108.20
1	AA	90	C	N3-C4-C5	-5.43	119.73	121.90
1	AA	749	A	C5-C6-N6	-5.43	119.35	123.70
1	AA	840	C	N3-C4-N4	5.43	121.80	118.00
1	AA	1132	C	N3-C4-C5	-5.43	119.73	121.90
1	AA	1136	C	N3-C4-C5	-5.43	119.73	121.90
1	AA	1137	C	N3-C4-N4	5.43	121.80	118.00
1	AA	1346	A	C5-C6-N1	-5.43	114.98	117.70
27	B8	69	C	N3-C4-N4	5.43	121.80	118.00
27	B8	140	C	N3-C4-N4	5.43	121.80	118.00
27	B8	1102	C	N3-C4-C5	-5.43	119.73	121.90
27	B8	1109	C	N3-C4-C5	-5.43	119.73	121.90
27	B8	1290	C	N3-C4-C5	-5.43	119.73	121.90
27	B8	1489	C	O4'-C1'-N1	5.43	112.55	108.20
27	B8	2451	A	C4-C5-C6	5.43	119.72	117.00
27	B8	2634	A	C5-C6-N6	-5.43	119.35	123.70
1	AA	167	A	C5-C6-N6	-5.43	119.36	123.70
1	AA	339	C	N3-C4-N4	5.43	121.80	118.00
1	AA	392	C	N3-C4-C5	-5.43	119.73	121.90
1	AA	468	A	C5-C6-N6	-5.43	119.36	123.70
1	AA	810	C	N3-C4-N4	5.43	121.80	118.00
27	B8	478	A	C4-C5-C6	5.43	119.72	117.00
27	B8	1658	C	N3-C4-N4	5.43	121.80	118.00
27	B8	2266	A	C5-C6-N6	-5.43	119.36	123.70
1	AA	183	C	N3-C4-N4	5.43	121.80	118.00
1	AA	1217	C	N3-C4-N4	5.43	121.80	118.00
27	B8	10	A	C5-C6-N6	-5.43	119.36	123.70
27	B8	384	A	C5-C6-N6	-5.43	119.36	123.70
27	B8	733	G	N3-C2-N2	5.43	123.70	119.90
27	B8	903	C	N3-C4-N4	5.43	121.80	118.00
27	B8	1175	A	C5-C6-N6	-5.43	119.36	123.70
27	B8	1490	A	C5-C6-N1	-5.43	114.98	117.70
27	B8	1690	A	C5-C6-N1	-5.43	114.99	117.70
27	B8	2459	A	C5-C6-N6	-5.43	119.36	123.70
27	B8	2830	C	N3-C4-N4	5.43	121.80	118.00
1	AA	72	A	C5-C6-N1	-5.43	114.99	117.70
1	AA	277	C	N3-C4-N4	5.43	121.80	118.00
27	B8	160	A	C5-C6-N1	-5.43	114.99	117.70
27	B8	222	A	C5-C6-N6	-5.43	119.36	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1114	C	N3-C4-C5	-5.43	119.73	121.90
27	B8	2250	G	N3-C2-N2	5.43	123.70	119.90
27	B8	2381	A	C5-C6-N1	-5.43	114.99	117.70
1	AA	546	A	O4'-C1'-N9	5.43	112.54	108.20
1	AA	602	A	C5-C6-N6	-5.43	119.36	123.70
1	AA	970	C	N3-C4-N4	5.43	121.80	118.00
1	AA	1228	C	N3-C4-N4	5.43	121.80	118.00
1	AA	1483	A	C5-C6-N1	-5.43	114.99	117.70
3	AV	33	A	C5-C6-N6	-5.43	119.36	123.70
22	AR	4	PHE	CB-CG-CD2	-5.43	117.00	120.80
27	B8	671	C	C5'-C4'-C3'	-5.43	107.32	116.00
27	B8	1358	G	N3-C2-N2	5.43	123.70	119.90
27	B8	1746	A	C5-C6-N6	-5.43	119.36	123.70
27	B8	2005	A	C5-C6-N1	-5.43	114.99	117.70
27	B8	2042	A	C5-C6-N1	-5.43	114.99	117.70
27	B8	2184	A	C5-C6-N1	-5.43	114.99	117.70
27	B8	2201	G	O4'-C1'-N9	5.43	112.54	108.20
27	B8	2573	C	N3-C4-N4	5.43	121.80	118.00
1	AA	110	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	616	G	O4'-C1'-N9	5.42	112.54	108.20
1	AA	1285	A	C5'-C4'-C3'	-5.42	107.32	116.00
1	AA	1484	C	N3-C4-N4	5.42	121.80	118.00
3	AV	24	C	N3-C4-N4	5.42	121.80	118.00
27	B8	979	A	O4'-C1'-N9	5.42	112.54	108.20
27	B8	1708	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	984	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	1003	G	O4'-C1'-N9	5.42	112.54	108.20
1	AA	1037	C	N3-C4-N4	5.42	121.80	118.00
27	B8	873	C	N3-C4-N4	5.42	121.80	118.00
27	B8	1008	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	1801	A	C5-C6-N6	-5.42	119.36	123.70
1	AA	236	A	C5-C6-N1	-5.42	114.99	117.70
1	AA	330	C	N3-C4-N4	5.42	121.79	118.00
3	AV	5	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	845	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	1262	A	C5-C6-N6	-5.42	119.36	123.70
27	B8	1592	C	N3-C4-C5	-5.42	119.73	121.90
27	B8	1819	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	2734	A	O4'-C1'-N9	5.42	112.54	108.20
1	AA	492	C	N3-C4-N4	5.42	121.79	118.00
1	AA	1045	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	1226	C	N3-C4-N4	5.42	121.79	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1484	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	1503	A	C5-C6-N6	-5.42	119.36	123.70
27	B8	73	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	412	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	1505	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	1708	C	N3-C4-N4	5.42	121.79	118.00
1	AA	640	A	C5-C6-N6	-5.42	119.36	123.70
1	AA	688	G	O4'-C1'-N9	5.42	112.53	108.20
1	AA	1118	U	O4'-C1'-N1	5.42	112.54	108.20
27	B8	517	C	N3-C4-N4	5.42	121.79	118.00
27	B8	865	C	N3-C4-C5	-5.42	119.73	121.90
27	B8	1049	C	N3-C4-N4	5.42	121.79	118.00
27	B8	1136	G	O4'-C1'-N9	5.42	112.53	108.20
27	B8	1194	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	1780	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	1889	A	C5-C6-N6	-5.42	119.36	123.70
27	B8	2117	A	C5-C6-N6	-5.42	119.36	123.70
27	B8	2467	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	32	A	C5-C6-N1	-5.42	114.99	117.70
1	AA	225	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	250	A	C5-C6-N1	-5.42	114.99	117.70
1	AA	660	C	N3-C4-N4	5.42	121.79	118.00
1	AA	1408	A	C5-C6-N6	-5.42	119.37	123.70
27	B8	42	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	125	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	233	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	342	A	C5-C6-N1	-5.42	114.99	117.70
27	B8	363	G	P-O5'-C5'	5.42	129.56	120.90
27	B8	735	A	C4-C5-C6	5.42	119.71	117.00
27	B8	1313	U	C6-N1-C1'	-5.42	113.62	121.20
27	B8	1353	A	C5-C6-N6	-5.42	119.37	123.70
27	B8	2530	A	C5-C6-N6	-5.42	119.37	123.70
27	B8	2710	C	N3-C4-C5	-5.42	119.73	121.90
27	B8	1953	A	C5-C6-N6	-5.42	119.37	123.70
1	AA	129	A	C5-C6-N1	-5.41	114.99	117.70
1	AA	1410	A	C4-C5-C6	5.41	119.71	117.00
1	AA	1467	C	N3-C4-C5	-5.41	119.73	121.90
1	AA	1538	C	N3-C4-C5	-5.41	119.73	121.90
27	B8	692	C	N3-C4-C5	-5.41	119.73	121.90
27	B8	1269	A	O4'-C1'-N9	5.41	112.53	108.20
27	B8	1665	A	O4'-C1'-N9	5.41	112.53	108.20
27	B8	1739	A	C4-C5-C6	5.41	119.71	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2805	C	N3-C4-C5	-5.41	119.73	121.90
1	AA	811	C	N3-C4-N4	5.41	121.79	118.00
27	B8	542	C	N3-C4-C5	-5.41	119.73	121.90
27	B8	1161	C	N3-C4-C5	-5.41	119.73	121.90
27	B8	1588	G	O4'-C1'-N9	5.41	112.53	108.20
27	B8	2037	A	C5-C6-N1	-5.41	114.99	117.70
27	B8	2300	C	N3-C4-C5	-5.41	119.73	121.90
3	AV	29	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	1569	A	C5-C6-N6	-5.41	119.37	123.70
27	B8	817	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	984	A	C5-C6-N1	-5.41	115.00	117.70
27	B8	1014	A	C5-C6-N1	-5.41	115.00	117.70
27	B8	1079	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	1493	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	2208	C	N3-C4-N4	5.41	121.79	118.00
27	B8	2542	A	C5-C6-N6	-5.41	119.37	123.70
27	B8	2721	A	C5-C6-N6	-5.41	119.37	123.70
27	B8	509	C	N3-C4-N4	5.41	121.78	118.00
27	B8	1889	A	C5-C6-N1	-5.41	115.00	117.70
27	B8	2328	A	C5-C6-N1	-5.41	115.00	117.70
1	AA	250	A	C5-C6-N6	-5.41	119.38	123.70
1	AA	264	C	N3-C4-C5	-5.41	119.74	121.90
1	AA	777	A	C5-C6-N6	-5.41	119.38	123.70
1	AA	1362	A	C5-C6-N6	-5.41	119.38	123.70
1	AA	1536	C	N3-C4-N4	5.41	121.78	118.00
2	AX	15	C	N3-C4-C5	-5.41	119.74	121.90
3	AV	29	C	N3-C4-N4	5.41	121.78	118.00
27	B8	63	A	O4'-C1'-N9	5.41	112.53	108.20
27	B8	207	A	C4-C5-C6	5.41	119.70	117.00
27	B8	323	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	456	C	N3-C4-N4	5.41	121.78	118.00
27	B8	888	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	1655	A	C4-C5-C6	5.41	119.70	117.00
27	B8	1938	A	C5-C6-N1	-5.41	115.00	117.70
27	B8	2064	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	2145	C	O4'-C1'-N1	5.41	112.52	108.20
27	B8	2177	C	N3-C4-C5	-5.41	119.74	121.90
27	B8	2183	A	C5-C6-N1	-5.41	115.00	117.70
27	B8	2226	C	N3-C4-N4	5.41	121.78	118.00
27	B8	2468	A	C5-C6-N6	-5.41	119.38	123.70
27	B8	2824	C	N3-C4-C5	-5.41	119.74	121.90
1	AA	378	G	O4'-C1'-N9	5.40	112.52	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	878	A	C5-C6-N6	-5.40	119.38	123.70
1	AA	1149	C	N3-C4-C5	-5.40	119.74	121.90
1	AA	1333	A	C5-C6-N6	-5.40	119.38	123.70
1	AA	1441	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	307	G	O4'-C1'-N9	5.40	112.52	108.20
27	B8	645	C	N3-C4-N4	5.40	121.78	118.00
27	B8	2285	C	N3-C4-C5	-5.40	119.74	121.90
27	B8	2347	C	N3-C4-N4	5.40	121.78	118.00
27	B8	2731	G	O4'-C1'-N9	5.40	112.52	108.20
1	AA	305	G	O4'-C1'-N9	5.40	112.52	108.20
1	AA	582	C	N3-C4-N4	5.40	121.78	118.00
27	B8	236	C	N3-C4-C5	-5.40	119.74	121.90
27	B8	632	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	1596	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	1685	C	N3-C4-C5	-5.40	119.74	121.90
27	B8	1733	G	O4'-C1'-N9	5.40	112.52	108.20
27	B8	2073	C	N3-C4-N4	5.40	121.78	118.00
27	B8	2388	A	C5-C6-N6	-5.40	119.38	123.70
1	AA	339	C	N3-C4-C5	-5.40	119.74	121.90
1	AA	505	G	O4'-C1'-N9	5.40	112.52	108.20
1	AA	509	A	C5-C6-N1	-5.40	115.00	117.70
1	AA	548	G	O4'-C1'-N9	5.40	112.52	108.20
1	AA	1141	C	N3-C4-C5	-5.40	119.74	121.90
1	AA	1174	G	O4'-C1'-N9	5.40	112.52	108.20
1	AA	1214	C	N3-C4-C5	-5.40	119.74	121.90
26	B7	43	C	N3-C4-N4	5.40	121.78	118.00
27	B8	753	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	1566	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	1597	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	2705	A	O4'-C1'-N9	5.40	112.52	108.20
27	B8	2736	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	2835	A	C4-C5-C6	5.40	119.70	117.00
1	AA	1430	A	C5-C6-N6	-5.40	119.38	123.70
27	B8	84	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	2762	C	N3-C4-N4	5.40	121.78	118.00
27	B8	2889	C	N3-C4-C5	-5.40	119.74	121.90
1	AA	381	C	N3-C4-C5	-5.40	119.74	121.90
1	AA	1114	C	N3-C4-C5	-5.40	119.74	121.90
1	AA	1509	C	N3-C4-N4	5.40	121.78	118.00
1	AA	1531	A	C5-C6-N1	-5.40	115.00	117.70
26	B7	31	C	N3-C4-C5	-5.40	119.74	121.90
26	B7	58	A	C5-C6-N1	-5.40	115.00	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	675	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	1453	A	C5-C6-N6	-5.40	119.38	123.70
27	B8	1586	A	C5-C6-N1	-5.40	115.00	117.70
27	B8	2176	A	C5-C6-N6	-5.40	119.38	123.70
1	AA	661	G	O4'-C1'-N9	5.40	112.52	108.20
27	B8	21	A	C5-C6-N6	-5.40	119.38	123.70
27	B8	893	C	N3-C4-C5	-5.40	119.74	121.90
27	B8	2266	A	C5-C6-N1	-5.40	115.00	117.70
1	AA	183	C	N3-C4-C5	-5.39	119.74	121.90
1	AA	618	C	N3-C4-C5	-5.39	119.74	121.90
1	AA	1179	A	C5-C6-N1	-5.39	115.00	117.70
1	AA	1542	A	C5-C6-N1	-5.39	115.00	117.70
26	B7	59	A	C5-C6-N6	-5.39	119.39	123.70
27	B8	255	A	O4'-C1'-N9	5.39	112.52	108.20
27	B8	334	C	N3-C4-C5	-5.39	119.74	121.90
27	B8	575	A	C5-C6-N6	-5.39	119.38	123.70
27	B8	1274	A	O4'-C1'-N9	5.39	112.52	108.20
27	B8	1418	G	O4'-C1'-N9	5.39	112.52	108.20
27	B8	2209	G	O4'-C1'-N9	5.39	112.52	108.20
27	B8	2251	G	O4'-C1'-N9	5.39	112.52	108.20
1	AA	163	C	N3-C4-C5	-5.39	119.74	121.90
1	AA	992	U	O4'-C1'-N1	5.39	112.51	108.20
3	AV	1	C	N3-C4-N4	5.39	121.78	118.00
3	AV	22	A	O4'-C1'-N9	5.39	112.51	108.20
27	B8	196	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	627	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	1133	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	1420	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	1565	C	N3-C4-N4	5.39	121.78	118.00
27	B8	1925	C	N3-C4-C5	-5.39	119.74	121.90
27	B8	2031	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	2496	C	N3-C4-N4	5.39	121.78	118.00
28	BA	158	PHE	CB-CG-CD2	-5.39	117.03	120.80
1	AA	107	G	O4'-C1'-N9	5.39	112.51	108.20
1	AA	1097	C	N3-C4-C5	-5.39	119.74	121.90
27	B8	404	A	C5-C6-N6	-5.39	119.39	123.70
27	B8	761	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	2009	A	C5-C6-N6	-5.39	119.39	123.70
27	B8	2129	C	C6-N1-C1'	-5.39	114.33	120.80
27	B8	2191	A	C5-C6-N6	-5.39	119.39	123.70
27	B8	2792	A	C5-C6-N1	-5.39	115.00	117.70
1	AA	26	A	C4-C5-C6	5.39	119.69	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	379	C	N3-C4-N4	5.39	121.77	118.00
1	AA	412	A	C5-C6-N6	-5.39	119.39	123.70
1	AA	460	A	C5-C6-N6	-5.39	119.39	123.70
1	AA	532	A	C5-C6-N1	-5.39	115.01	117.70
3	AV	65	C	N3-C4-N4	5.39	121.77	118.00
27	B8	22	C	N3-C4-C5	-5.39	119.74	121.90
27	B8	226	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	947	A	O4'-C1'-N9	5.39	112.51	108.20
27	B8	1129	A	C5-C6-N1	-5.39	115.00	117.70
27	B8	1877	A	O4'-C1'-N9	5.39	112.51	108.20
27	B8	2476	A	C5-C6-N1	-5.39	115.01	117.70
27	B8	2541	A	C5-C6-N1	-5.39	115.01	117.70
27	B8	537	G	O4'-C1'-N9	5.39	112.51	108.20
27	B8	550	C	N3-C4-N4	5.39	121.77	118.00
27	B8	1044	C	N3-C4-N4	5.39	121.77	118.00
27	B8	2339	C	N3-C4-N4	5.39	121.77	118.00
1	AA	356	A	C4-C5-C6	5.39	119.69	117.00
1	AA	412	A	C5-C6-N1	-5.39	115.01	117.70
1	AA	535	A	C5-C6-N1	-5.39	115.01	117.70
1	AA	566	G	C5-C6-O6	-5.39	125.37	128.60
1	AA	1080	A	C4-C5-C6	5.39	119.69	117.00
1	AA	1226	C	N3-C4-C5	-5.39	119.75	121.90
27	B8	453	A	C5-C6-N6	-5.39	119.39	123.70
27	B8	915	C	N3-C4-C5	-5.39	119.75	121.90
27	B8	1583	A	C4-C5-C6	5.39	119.69	117.00
27	B8	2092	U	C2-N1-C1'	5.39	124.16	117.70
1	AA	568	G	O4'-C1'-N9	5.38	112.51	108.20
1	AA	705	G	N1-C6-O6	5.38	123.13	119.90
1	AA	996	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	483	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	1503	A	C5-C6-N6	-5.38	119.39	123.70
27	B8	1521	G	N3-C2-N2	5.38	123.67	119.90
27	B8	2030	A	C5-C6-N6	-5.38	119.39	123.70
27	B8	2058	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	2448	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	2572	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	2712	C	N3-C4-C5	-5.38	119.75	121.90
1	AA	1509	C	N3-C4-C5	-5.38	119.75	121.90
27	B8	914	G	O4'-C1'-N9	5.38	112.51	108.20
27	B8	944	C	N3-C4-C5	-5.38	119.75	121.90
27	B8	1595	C	N3-C4-C5	-5.38	119.75	121.90
27	B8	1745	A	O4'-C1'-N9	5.38	112.51	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2052	A	O4'-C1'-N9	5.38	112.51	108.20
27	B8	2364	C	N3-C4-C5	-5.38	119.75	121.90
1	AA	1192	C	N3-C4-C5	-5.38	119.75	121.90
27	B8	972	A	C4-C5-C6	5.38	119.69	117.00
27	B8	979	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	1463	C	N3-C4-N4	5.38	121.77	118.00
27	B8	1847	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	2002	G	O4'-C1'-N9	5.38	112.50	108.20
27	B8	2751	G	O4'-C1'-N9	5.38	112.51	108.20
1	AA	2	A	C5-C6-N1	-5.38	115.01	117.70
1	AA	212	G	O4'-C1'-N9	5.38	112.50	108.20
1	AA	381	C	N3-C4-N4	5.38	121.77	118.00
1	AA	880	C	N3-C4-C5	-5.38	119.75	121.90
3	AV	46	G	O4'-C1'-N9	5.38	112.50	108.20
27	B8	1287	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	1488	C	N3-C4-N4	5.38	121.77	118.00
27	B8	1947	C	N3-C4-N4	5.38	121.77	118.00
1	AA	207	C	N3-C4-N4	5.38	121.77	118.00
1	AA	335	C	N3-C4-C5	-5.38	119.75	121.90
1	AA	584	G	O4'-C1'-N9	5.38	112.50	108.20
1	AA	969	A	C5-C6-N6	-5.38	119.40	123.70
26	B7	66	A	C4-C5-C6	5.38	119.69	117.00
27	B8	302	C	N3-C4-N4	5.38	121.77	118.00
27	B8	442	G	O4'-C1'-N9	5.38	112.50	108.20
27	B8	484	C	N3-C4-C5	-5.38	119.75	121.90
27	B8	565	C	N3-C4-C5	-5.38	119.75	121.90
27	B8	1048	A	C5-C6-N6	-5.38	119.40	123.70
27	B8	1419	A	C5-C6-N6	-5.38	119.40	123.70
27	B8	1545	A	C4-C5-C6	5.38	119.69	117.00
27	B8	1763	G	O4'-C1'-N9	5.38	112.50	108.20
27	B8	1966	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	1970	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	2205	A	C5-C6-N6	-5.38	119.40	123.70
27	B8	2815	C	N3-C4-N4	5.38	121.77	118.00
27	B8	2868	A	C5-C6-N1	-5.38	115.01	117.70
1	AA	383	A	C5-C6-N6	-5.38	119.40	123.70
1	AA	447	G	O4'-C1'-N9	5.38	112.50	108.20
1	AA	566	G	O4'-C1'-N9	5.38	112.50	108.20
1	AA	807	A	C5-C6-N6	-5.38	119.40	123.70
1	AA	1324	A	C5-C6-N1	-5.38	115.01	117.70
1	AA	1408	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	176	A	C5-C6-N6	-5.38	119.40	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	854	C	N3-C4-N4	5.38	121.76	118.00
27	B8	1307	A	C5-C6-N6	-5.38	119.40	123.70
27	B8	1598	A	O4'-C1'-N9	5.38	112.50	108.20
27	B8	1645	G	O4'-C1'-N9	5.38	112.50	108.20
27	B8	1757	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	2276	G	O4'-C1'-N9	5.38	112.50	108.20
27	B8	2501	C	O4'-C1'-N1	5.38	112.50	108.20
1	AA	363	A	C5-C6-N1	-5.38	115.01	117.70
1	AA	663	A	O4'-C1'-N9	5.38	112.50	108.20
1	AA	764	C	N3-C4-C5	-5.38	119.75	121.90
1	AA	1539	C	N3-C4-N4	5.38	121.76	118.00
27	B8	49	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	1272	A	C5-C6-N1	-5.38	115.01	117.70
27	B8	1451	C	N3-C4-N4	5.38	121.76	118.00
27	B8	2799	A	C5-C6-N1	-5.38	115.01	117.70
1	AA	160	A	C5-C6-N1	-5.37	115.01	117.70
1	AA	482	A	O4'-C1'-N9	5.37	112.50	108.20
1	AA	1265	C	N3-C4-N4	5.37	121.76	118.00
27	B8	44	A	C5-C6-N6	-5.37	119.40	123.70
27	B8	320	A	O4'-C1'-N9	5.37	112.50	108.20
27	B8	1005	C	N3-C4-C5	-5.37	119.75	121.90
27	B8	1134	A	C5-C6-N1	-5.37	115.01	117.70
27	B8	1276	A	C5-C6-N6	-5.37	119.40	123.70
27	B8	1985	C	N3-C4-C5	-5.37	119.75	121.90
1	AA	1493	A	C5-C6-N1	-5.37	115.01	117.70
1	AA	1499	A	C5-C6-N1	-5.37	115.01	117.70
27	B8	537	G	N3-C2-N2	5.37	123.66	119.90
27	B8	928	A	O4'-C1'-N9	5.37	112.50	108.20
27	B8	1511	G	O4'-C1'-N9	5.37	112.50	108.20
27	B8	1596	A	C4-C5-C6	5.37	119.69	117.00
27	B8	1944	U	O4'-C1'-N1	5.37	112.50	108.20
27	B8	2126	A	C5-C6-N1	-5.37	115.01	117.70
27	B8	2307	G	C5-C6-O6	-5.37	125.38	128.60
27	B8	2336	A	C5-C6-N6	-5.37	119.40	123.70
27	B8	2476	A	C5-C6-N6	-5.37	119.40	123.70
1	AA	488	C	N3-C4-C5	-5.37	119.75	121.90
1	AA	635	A	C5-C6-N1	-5.37	115.02	117.70
1	AA	794	A	C5-C6-N6	-5.37	119.40	123.70
3	AV	42	C	N3-C4-N4	5.37	121.76	118.00
27	B8	1126	A	C5-C6-N6	-5.37	119.40	123.70
1	AA	1319	A	C5-C6-N1	-5.37	115.02	117.70
1	AA	1366	C	N3-C4-C5	-5.37	119.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1448	C	N3-C4-C5	-5.37	119.75	121.90
26	B7	100	G	O4'-C1'-N9	5.37	112.50	108.20
27	B8	73	A	C5-C6-N6	-5.37	119.41	123.70
27	B8	470	A	C5-C6-N6	-5.37	119.40	123.70
27	B8	692	C	N3-C4-N4	5.37	121.76	118.00
27	B8	909	A	C4-C5-C6	5.37	119.68	117.00
27	B8	1010	A	C5-C6-N6	-5.37	119.41	123.70
27	B8	1522	A	C5-C6-N6	-5.37	119.41	123.70
27	B8	2462	C	N3-C4-C5	-5.37	119.75	121.90
27	B8	2874	C	N3-C4-N4	5.37	121.76	118.00
1	AA	397	A	C5-C6-N1	-5.37	115.02	117.70
27	B8	848	C	N3-C4-C5	-5.37	119.75	121.90
27	B8	1080	A	C5-C6-N6	-5.37	119.41	123.70
27	B8	1538	G	O4'-C1'-N9	5.37	112.49	108.20
27	B8	1787	A	C5-C6-N1	-5.37	115.02	117.70
1	AA	298	A	O4'-C1'-N9	5.37	112.49	108.20
1	AA	374	A	C5-C6-N1	-5.37	115.02	117.70
1	AA	720	C	N3-C4-N4	5.37	121.76	118.00
1	AA	819	A	C5-C6-N6	-5.37	119.41	123.70
1	AA	1536	C	N3-C4-C5	-5.37	119.75	121.90
27	B8	1889	A	O4'-C1'-N9	5.37	112.49	108.20
27	B8	2327	A	O4'-C1'-N9	5.37	112.49	108.20
27	B8	2759	G	O4'-C1'-N9	5.37	112.49	108.20
1	AA	186	C	N3-C4-C5	-5.36	119.75	121.90
1	AA	189	A	C5-C6-N1	-5.36	115.02	117.70
1	AA	1036	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	147	C	N3-C4-C5	-5.36	119.75	121.90
27	B8	404	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	516	C	N3-C4-N4	5.36	121.75	118.00
27	B8	603	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	1040	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	1057	A	O4'-C1'-N9	5.36	112.49	108.20
27	B8	1672	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	2117	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	2468	A	C5-C6-N1	-5.36	115.02	117.70
1	AA	374	A	C5-C6-N6	-5.36	119.41	123.70
1	AA	907	A	O4'-C1'-N9	5.36	112.49	108.20
1	AA	1347	G	O4'-C1'-N9	5.36	112.49	108.20
27	B8	840	C	N3-C4-C5	-5.36	119.75	121.90
27	B8	1170	C	N3-C4-C5	-5.36	119.75	121.90
27	B8	2327	A	C5-C6-N6	-5.36	119.41	123.70
1	AA	153	C	N3-C4-C5	-5.36	119.76	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	161	A	C5-C6-N1	-5.36	115.02	117.70
1	AA	489	C	N3-C4-N4	5.36	121.75	118.00
1	AA	528	C	N3-C4-C5	-5.36	119.75	121.90
1	AA	841	C	N3-C4-N4	5.36	121.75	118.00
1	AA	972	C	N3-C4-N4	5.36	121.75	118.00
1	AA	1227	A	C4-C5-C6	5.36	119.68	117.00
1	AA	1363	A	C5-C6-N6	-5.36	119.41	123.70
3	AV	57	C	N3-C4-N4	5.36	121.75	118.00
27	B8	762	U	O4'-C1'-N1	5.36	112.49	108.20
27	B8	922	C	N3-C4-N4	5.36	121.75	118.00
27	B8	1335	C	N3-C4-N4	5.36	121.75	118.00
27	B8	1392	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	2094	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	2788	C	N3-C4-C5	-5.36	119.76	121.90
1	AA	815	A	C5-C6-N1	-5.36	115.02	117.70
1	AA	967	C	N3-C4-N4	5.36	121.75	118.00
1	AA	1012	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	1151	A	C5-C6-N1	-5.36	115.02	117.70
1	AA	567	G	O4'-C1'-N9	5.36	112.49	108.20
26	B7	76	G	O4'-C1'-N9	5.36	112.49	108.20
27	B8	729	G	O4'-C1'-N9	5.36	112.49	108.20
27	B8	753	A	C5-C6-N6	-5.36	119.41	123.70
27	B8	820	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	1086	A	C4-C5-C6	5.36	119.68	117.00
27	B8	1140	C	N3-C4-C5	-5.36	119.76	121.90
27	B8	1451	C	N3-C4-C5	-5.36	119.76	121.90
27	B8	1761	C	N3-C4-C5	-5.36	119.76	121.90
27	B8	1876	A	C4-C5-C6	5.36	119.68	117.00
27	B8	2066	C	N3-C4-C5	-5.36	119.76	121.90
27	B8	2066	C	N3-C4-N4	5.36	121.75	118.00
27	B8	2347	C	N3-C4-C5	-5.36	119.76	121.90
1	AA	172	A	C5-C6-N1	-5.36	115.02	117.70
1	AA	889	A	C4-C5-C6	5.36	119.68	117.00
1	AA	1110	A	O4'-C1'-N9	5.36	112.48	108.20
27	B8	742	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	788	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	1537	G	O4'-C1'-N9	5.36	112.48	108.20
27	B8	1952	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	2170	A	C5-C6-N1	-5.36	115.02	117.70
27	B8	2730	C	N3-C4-C5	-5.36	119.76	121.90
1	AA	779	C	N3-C4-C5	-5.35	119.76	121.90
27	B8	764	A	C5-C6-N6	-5.35	119.42	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1605	C	N3-C4-N4	5.35	121.75	118.00
27	B8	1958	C	N3-C4-C5	-5.35	119.76	121.90
27	B8	2522	U	O4'-C1'-N1	5.35	112.48	108.20
1	AA	167	A	O4'-C1'-N9	5.35	112.48	108.20
1	AA	401	C	N3-C4-N4	5.35	121.75	118.00
1	AA	783	C	N3-C4-C5	-5.35	119.76	121.90
1	AA	919	A	C5-C6-N6	-5.35	119.42	123.70
1	AA	968	A	C5-C6-N1	-5.35	115.02	117.70
1	AA	1089	G	O4'-C1'-N9	5.35	112.48	108.20
1	AA	1111	A	C5-C6-N1	-5.35	115.02	117.70
1	AA	1201	A	C5-C6-N1	-5.35	115.02	117.70
1	AA	1296	C	N3-C4-N4	5.35	121.75	118.00
1	AA	1389	C	N3-C4-C5	-5.35	119.76	121.90
1	AA	1535	C	N3-C4-N4	5.35	121.75	118.00
3	AV	67	C	N3-C4-C5	-5.35	119.76	121.90
27	B8	118	A	O4'-C1'-N9	5.35	112.48	108.20
27	B8	446	G	N3-C2-N2	5.35	123.65	119.90
27	B8	636	G	O4'-C1'-N9	5.35	112.48	108.20
27	B8	802	A	C5-C6-N6	-5.35	119.42	123.70
27	B8	996	A	C5-C6-N1	-5.35	115.02	117.70
27	B8	2284	A	C5-C6-N1	-5.35	115.02	117.70
1	AA	188	C	N3-C4-N4	5.35	121.75	118.00
27	B8	1746	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	2331	G	O4'-C1'-N9	5.35	112.48	108.20
1	AA	1377	A	C5-C6-N1	-5.35	115.03	117.70
3	AV	17	C	N3-C4-C5	-5.35	119.76	121.90
27	B8	173	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	249	C	N3-C4-C5	-5.35	119.76	121.90
27	B8	446	G	O4'-C1'-N9	5.35	112.48	108.20
27	B8	477	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	614	A	C5-C6-N6	-5.35	119.42	123.70
27	B8	666	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	1495	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	1522	A	O4'-C1'-N9	5.35	112.48	108.20
1	AA	244	U	O4'-C1'-N1	5.35	112.48	108.20
3	AV	65	C	N3-C4-C5	-5.35	119.76	121.90
3	AV	75	C	N3-C4-N4	5.35	121.74	118.00
5	A0	192	TYR	CB-CG-CD1	-5.35	117.79	121.00
26	B7	66	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	348	A	O4'-C1'-N9	5.35	112.48	108.20
27	B8	761	A	O4'-C1'-N9	5.35	112.48	108.20
27	B8	1235	G	N3-C2-N2	5.35	123.64	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1554	U	O4'-C1'-N1	5.35	112.48	108.20
27	B8	1580	A	O4'-C1'-N9	5.35	112.48	108.20
27	B8	1631	G	O4'-C1'-N9	5.35	112.48	108.20
27	B8	1707	G	O4'-C1'-N9	5.35	112.48	108.20
27	B8	2070	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	2377	A	C5-C6-N1	-5.35	115.03	117.70
27	B8	2855	C	N3-C4-C5	-5.35	119.76	121.90
1	AA	901	A	O4'-C1'-N9	5.35	112.48	108.20
1	AA	792	A	C5-C6-N6	-5.34	119.42	123.70
1	AA	1054	C	C2-N1-C1'	5.34	124.68	118.80
26	B7	101	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	608	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	937	C	N3-C4-C5	-5.34	119.76	121.90
27	B8	2096	C	N3-C4-N4	5.34	121.74	118.00
27	B8	2108	A	O4'-C1'-N9	5.34	112.48	108.20
27	B8	2771	C	N3-C4-C5	-5.34	119.76	121.90
27	B8	19	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	1076	C	N3-C4-N4	5.34	121.74	118.00
27	B8	1357	C	N3-C4-C5	-5.34	119.76	121.90
27	B8	1436	G	O4'-C1'-N9	5.34	112.47	108.20
27	B8	1785	A	C4-C5-C6	5.34	119.67	117.00
27	B8	2261	C	N3-C4-C5	-5.34	119.76	121.90
1	AA	240	G	O4'-C1'-N9	5.34	112.47	108.20
1	AA	465	A	C4-C5-C6	5.34	119.67	117.00
1	AA	523	A	C5-C6-N6	-5.34	119.43	123.70
1	AA	720	C	N3-C4-C5	-5.34	119.76	121.90
1	AA	1195	C	P-O3'-C3'	5.34	126.11	119.70
27	B8	38	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	1275	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	1321	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	2247	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	2394	C	N3-C4-C5	-5.34	119.76	121.90
27	B8	2727	A	O4'-C1'-N9	5.34	112.47	108.20
1	AA	768	A	C5-C6-N1	-5.34	115.03	117.70
1	AA	1054	C	N3-C4-C5	-5.34	119.77	121.90
1	AA	1508	A	C5-C6-N6	-5.34	119.43	123.70
27	B8	1053	C	N3-C4-C5	-5.34	119.76	121.90
27	B8	1327	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	2080	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	2472	G	O4'-C1'-N9	5.34	112.47	108.20
27	B8	2875	C	N3-C4-N4	5.34	121.74	118.00
1	AA	806	C	N3-C4-C5	-5.34	119.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1211	C	N3-C4-N4	5.34	121.74	118.00
27	B8	1809	A	O4'-C1'-N9	5.34	112.47	108.20
27	B8	2403	C	N3-C4-C5	-5.34	119.77	121.90
1	AA	28	A	C5-C6-N1	-5.34	115.03	117.70
1	AA	609	A	C5-C6-N6	-5.34	119.43	123.70
1	AA	853	C	N3-C4-N4	5.34	121.74	118.00
1	AA	892	A	C5-C6-N1	-5.34	115.03	117.70
1	AA	985	C	N3-C4-C5	-5.34	119.77	121.90
1	AA	1342	C	N3-C4-N4	5.34	121.73	118.00
1	AA	1369	C	N3-C4-C5	-5.34	119.77	121.90
27	B8	161	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	942	G	O4'-C1'-N9	5.34	112.47	108.20
27	B8	1232	G	O4'-C1'-N9	5.34	112.47	108.20
27	B8	1789	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	1870	C	N3-C4-C5	-5.34	119.77	121.90
27	B8	2095	A	C5-C6-N1	-5.34	115.03	117.70
27	B8	2497	A	C5-C6-N6	-5.34	119.43	123.70
27	B8	2507	C	N3-C4-C5	-5.34	119.77	121.90
27	B8	2610	C	N3-C4-C5	-5.34	119.77	121.90
27	B8	2699	C	N3-C4-C5	-5.34	119.77	121.90
1	AA	167	A	C5-C6-N1	-5.33	115.03	117.70
1	AA	1329	A	C5-C6-N1	-5.33	115.03	117.70
27	B8	340	A	C5-C6-N6	-5.33	119.43	123.70
27	B8	2406	A	C5-C6-N1	-5.33	115.03	117.70
27	B8	2814	A	C5-C6-N1	-5.33	115.03	117.70
1	AA	1396	A	C4-C5-C6	5.33	119.67	117.00
1	AA	1510	C	N3-C4-N4	5.33	121.73	118.00
27	B8	717	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	948	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	1204	A	C5-C6-N1	-5.33	115.03	117.70
27	B8	2124	G	O4'-C1'-N9	5.33	112.47	108.20
27	B8	2469	A	C5-C6-N6	-5.33	119.43	123.70
27	B8	2534	A	C5-C6-N6	-5.33	119.43	123.70
1	AA	18	C	N3-C4-C5	-5.33	119.77	121.90
1	AA	309	A	C5-C6-N1	-5.33	115.03	117.70
1	AA	321	A	C5-C6-N6	-5.33	119.44	123.70
1	AA	344	A	C5-C6-N1	-5.33	115.03	117.70
1	AA	595	A	C5-C6-N1	-5.33	115.03	117.70
1	AA	781	A	C5-C6-N6	-5.33	119.44	123.70
27	B8	490	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	778	G	O4'-C1'-N9	5.33	112.47	108.20
27	B8	1273	U	O4'-C1'-N1	5.33	112.47	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1314	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	1518	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	2394	C	N3-C4-N4	5.33	121.73	118.00
27	B8	2602	A	C5-C6-N1	-5.33	115.03	117.70
3	AV	11	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	968	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	1040	A	C5-C6-N6	-5.33	119.44	123.70
27	B8	1616	A	C5-C6-N1	-5.33	115.03	117.70
27	B8	2161	C	N3-C4-N4	5.33	121.73	118.00
1	AA	214	C	N3-C4-C5	-5.33	119.77	121.90
1	AA	958	A	C5-C6-N6	-5.33	119.44	123.70
27	B8	203	A	C5-C6-N1	-5.33	115.04	117.70
27	B8	251	A	C5-C6-N6	-5.33	119.44	123.70
27	B8	487	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	501	A	C5-C6-N1	-5.33	115.04	117.70
27	B8	1103	A	C5-C6-N1	-5.33	115.04	117.70
27	B8	1322	A	C5-C6-N6	-5.33	119.44	123.70
27	B8	1570	A	O4'-C1'-N9	5.33	112.46	108.20
27	B8	1611	C	N3-C4-N4	5.33	121.73	118.00
27	B8	1679	A	C5-C6-N1	-5.33	115.03	117.70
1	AA	787	A	C5-C6-N1	-5.33	115.04	117.70
1	AA	1021	A	C5-C6-N1	-5.33	115.04	117.70
1	AA	1384	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	213	A	O4'-C1'-N9	5.33	112.46	108.20
27	B8	536	G	O4'-C1'-N9	5.33	112.46	108.20
27	B8	1069	A	C5-C6-N1	-5.33	115.04	117.70
27	B8	1342	A	C5-C6-N1	-5.33	115.04	117.70
27	B8	2478	A	C5-C6-N1	-5.33	115.04	117.70
1	AA	228	A	C5-C6-N1	-5.33	115.04	117.70
1	AA	1507	A	C5-C6-N1	-5.33	115.04	117.70
1	AA	1519	A	C5-C6-N1	-5.33	115.04	117.70
3	AV	57	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	278	A	O4'-C1'-N9	5.33	112.46	108.20
27	B8	354	A	C5-C6-N6	-5.33	119.44	123.70
27	B8	1941	C	N3-C4-C5	-5.33	119.77	121.90
27	B8	2513	A	O4'-C1'-N9	5.33	112.46	108.20
27	B8	2547	A	C5-C6-N6	-5.33	119.44	123.70
1	AA	382	A	C5-C6-N1	-5.32	115.04	117.70
1	AA	624	C	N3-C4-C5	-5.32	119.77	121.90
1	AA	627	G	O4'-C1'-N9	5.32	112.46	108.20
1	AA	934	C	N3-C4-N4	5.32	121.73	118.00
1	AA	975	A	C5-C6-N1	-5.32	115.04	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1260	G	N3-C2-N2	5.32	123.63	119.90
27	B8	63	A	C5-C6-N6	-5.32	119.44	123.70
27	B8	213	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	685	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	751	A	O4'-C1'-N9	5.32	112.46	108.20
27	B8	1147	A	C5-C6-N6	-5.32	119.44	123.70
27	B8	1553	A	O4'-C1'-N9	5.32	112.46	108.20
27	B8	1629	U	O4'-C1'-N1	5.32	112.46	108.20
27	B8	1998	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	2553	G	O4'-C1'-N9	5.32	112.46	108.20
27	B8	1461	C	N3-C4-N4	5.32	121.72	118.00
1	AA	889	A	C5-C6-N1	-5.32	115.04	117.70
1	AA	1293	C	N3-C4-C5	-5.32	119.77	121.90
27	B8	126	A	C5-C6-N6	-5.32	119.44	123.70
27	B8	527	C	C2-N1-C1'	5.32	124.65	118.80
27	B8	1328	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	1727	C	N3-C4-C5	-5.32	119.77	121.90
27	B8	891	G	C5'-C4'-O4'	5.32	115.48	109.10
1	AA	34	C	N3-C4-C5	-5.32	119.77	121.90
1	AA	499	A	C5-C6-N1	-5.32	115.04	117.70
1	AA	546	A	C5-C6-N1	-5.32	115.04	117.70
1	AA	1327	C	N3-C4-C5	-5.32	119.77	121.90
27	B8	28	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	616	A	O4'-C1'-N9	5.32	112.45	108.20
27	B8	1204	A	O4'-C1'-N9	5.32	112.45	108.20
27	B8	1853	A	C5-C6-N6	-5.32	119.45	123.70
27	B8	1947	C	N3-C4-C5	-5.32	119.77	121.90
27	B8	2309	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	2520	C	N3-C4-N4	5.32	121.72	118.00
1	AA	585	G	O4'-C1'-N9	5.32	112.45	108.20
1	AA	815	A	O4'-C1'-N9	5.32	112.45	108.20
27	B8	11	C	N3-C4-N4	5.32	121.72	118.00
27	B8	104	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	613	A	C5-C6-N6	-5.32	119.45	123.70
27	B8	1509	A	C5-C6-N1	-5.32	115.04	117.70
27	B8	2662	A	O4'-C1'-N9	5.32	112.45	108.20
27	B8	2682	A	C5-C6-N1	-5.32	115.04	117.70
1	AA	1274	A	C5-C6-N1	-5.31	115.04	117.70
1	AA	1518	A	C5-C6-N6	-5.31	119.45	123.70
27	B8	1067	A	C5-C6-N1	-5.31	115.04	117.70
27	B8	1514	G	O4'-C1'-N9	5.31	112.45	108.20
27	B8	1853	A	C4-C5-C6	5.31	119.66	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	338	A	C5-C6-N6	-5.31	119.45	123.70
1	AA	702	A	O4'-C1'-N9	5.31	112.45	108.20
1	AA	1288	A	C5-C6-N1	-5.31	115.04	117.70
1	AA	1399	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	2270	A	C5-C6-N6	-5.31	119.45	123.70
27	B8	2651	C	N3-C4-C5	-5.31	119.78	121.90
1	AA	54	C	N3-C4-N4	5.31	121.72	118.00
1	AA	1069	C	N3-C4-C5	-5.31	119.78	121.90
2	AX	20	G	O4'-C1'-N9	5.31	112.45	108.20
27	B8	252	G	O4'-C1'-N9	5.31	112.45	108.20
27	B8	1156	A	C5-C6-N1	-5.31	115.05	117.70
27	B8	1606	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	2380	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	2427	C	N3-C4-N4	5.31	121.72	118.00
1	AA	395	C	N3-C4-C5	-5.31	119.78	121.90
1	AA	844	G	C5'-C4'-O4'	5.31	115.47	109.10
1	AA	1117	A	C5-C6-N1	-5.31	115.05	117.70
1	AA	1332	A	C5-C6-N6	-5.31	119.45	123.70
27	B8	106	C	N3-C4-N4	5.31	121.72	118.00
27	B8	322	A	O4'-C1'-N9	5.31	112.45	108.20
27	B8	1125	G	N3-C2-N2	5.31	123.62	119.90
27	B8	1428	C	N3-C4-N4	5.31	121.72	118.00
27	B8	1792	G	O4'-C1'-N9	5.31	112.45	108.20
1	AA	1238	A	C4-C5-C6	5.31	119.65	117.00
27	B8	74	A	C5-C6-N6	-5.31	119.45	123.70
27	B8	238	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	1009	A	C5-C6-N1	-5.31	115.05	117.70
27	B8	1270	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	2239	G	O4'-C1'-N9	5.31	112.45	108.20
27	B8	2273	A	C5-C6-N1	-5.31	115.05	117.70
1	AA	135	C	N3-C4-C5	-5.31	119.78	121.90
1	AA	1427	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	74	A	C5-C6-N1	-5.31	115.05	117.70
27	B8	512	G	O4'-C1'-N9	5.31	112.44	108.20
27	B8	713	G	N3-C2-N2	5.31	123.61	119.90
27	B8	715	A	C5-C6-N1	-5.31	115.05	117.70
27	B8	748	G	O4'-C1'-N9	5.31	112.44	108.20
27	B8	960	A	C5-C6-N1	-5.31	115.05	117.70
27	B8	1822	C	N3-C4-C5	-5.31	119.78	121.90
27	B8	2376	A	C5-C6-N1	-5.31	115.05	117.70
27	B8	2577	A	C5-C6-N6	-5.31	119.45	123.70
1	AA	78	A	C5-C6-N6	-5.30	119.46	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	99	C	N3-C4-N4	5.30	121.71	118.00
1	AA	637	C	N3-C4-C5	-5.30	119.78	121.90
1	AA	701	U	O4'-C1'-N1	5.30	112.44	108.20
1	AA	1429	A	C5-C6-N1	-5.30	115.05	117.70
26	B7	88	C	N3-C4-N4	5.30	121.71	118.00
27	B8	361	G	N3-C2-N2	5.30	123.61	119.90
27	B8	445	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	829	A	C5-C6-N1	-5.30	115.05	117.70
27	B8	961	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	1365	A	C5-C6-N1	-5.30	115.05	117.70
27	B8	1800	C	O4'-C1'-N1	5.30	112.44	108.20
27	B8	2501	C	N3-C4-N4	5.30	121.71	118.00
27	B8	2763	G	N3-C2-N2	5.30	123.61	119.90
28	BA	217	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	AA	422	C	N3-C4-N4	5.30	121.71	118.00
1	AA	845	A	C5-C6-N1	-5.30	115.05	117.70
1	AA	55	A	C5-C6-N1	-5.30	115.05	117.70
1	AA	136	C	N3-C4-C5	-5.30	119.78	121.90
1	AA	242	G	O4'-C1'-N9	5.30	112.44	108.20
3	AV	72	C	N3-C4-N4	5.30	121.71	118.00
27	B8	52	A	O4'-C1'-N9	5.30	112.44	108.20
27	B8	94	A	C5-C6-N1	-5.30	115.05	117.70
27	B8	208	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	2084	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	2129	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	2282	G	C2'-C3'-O3'	5.30	122.18	113.70
27	B8	2726	A	C5-C6-N1	-5.30	115.05	117.70
1	AA	3	A	C5-C6-N1	-5.30	115.05	117.70
1	AA	65	A	C5-C6-N1	-5.30	115.05	117.70
1	AA	432	A	C5-C6-N6	-5.30	119.46	123.70
1	AA	1404	C	N3-C4-C5	-5.30	119.78	121.90
3	AV	58	A	O4'-C1'-N9	5.30	112.44	108.20
26	B7	4	C	N3-C4-N4	5.30	121.71	118.00
27	B8	127	A	C5'-C4'-C3'	-5.30	107.52	116.00
27	B8	191	A	C5-C6-N6	-5.30	119.46	123.70
27	B8	398	C	N3-C4-N4	5.30	121.71	118.00
27	B8	614	A	C5-C6-N1	-5.30	115.05	117.70
27	B8	1243	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	1376	C	N3-C4-N4	5.30	121.71	118.00
27	B8	1744	A	C5-C6-N6	-5.30	119.46	123.70
27	B8	1960	A	C5-C6-N6	-5.30	119.46	123.70
27	B8	2420	C	N3-C4-C5	-5.30	119.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	856	C	N3-C4-N4	5.30	121.71	118.00
1	AA	1152	A	O4'-C1'-N9	5.30	112.44	108.20
27	B8	264	C	N3-C4-C5	-5.30	119.78	121.90
27	B8	368	A	O4'-C1'-N9	5.30	112.44	108.20
27	B8	527	C	N3-C4-N4	5.30	121.71	118.00
27	B8	1575	C	N3-C4-N4	5.30	121.71	118.00
27	B8	172	A	C5-C6-N1	-5.30	115.05	117.70
27	B8	555	G	N3-C2-N2	5.30	123.61	119.90
27	B8	846	U	C2-N1-C1'	5.30	124.06	117.70
27	B8	1133	A	C5-C6-N6	-5.30	119.46	123.70
27	B8	1254	A	C5-C6-N6	-5.30	119.46	123.70
27	B8	1698	A	C5-C6-N1	-5.30	115.05	117.70
27	B8	2095	A	C5-C6-N6	-5.30	119.46	123.70
27	B8	2338	C	N3-C4-N4	5.30	121.71	118.00
27	B8	2840	C	N3-C4-C5	-5.30	119.78	121.90
1	AA	1102	A	O4'-C1'-N9	5.29	112.44	108.20
1	AA	1188	A	C5-C6-N1	-5.29	115.05	117.70
27	B8	11	C	N3-C4-C5	-5.29	119.78	121.90
1	AA	40	C	N3-C4-C5	-5.29	119.78	121.90
1	AA	160	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	685	G	O4'-C1'-N9	5.29	112.44	108.20
3	AV	3	G	O4'-C1'-N9	5.29	112.43	108.20
26	B7	44	G	O4'-C1'-N9	5.29	112.44	108.20
27	B8	546	U	O4'-C1'-N1	5.29	112.44	108.20
27	B8	697	G	O4'-C1'-N9	5.29	112.44	108.20
27	B8	1616	A	C5-C6-N6	-5.29	119.47	123.70
27	B8	1760	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	1965	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	2395	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	2440	C	N3-C4-N4	5.29	121.71	118.00
1	AA	72	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	101	A	C5-C6-N1	-5.29	115.05	117.70
1	AA	158	G	O4'-C1'-N9	5.29	112.43	108.20
1	AA	572	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	607	A	C5-C6-N1	-5.29	115.05	117.70
1	AA	675	A	C5-C6-N1	-5.29	115.05	117.70
1	AA	1167	A	C5-C6-N1	-5.29	115.06	117.70
1	AA	1410	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	1535	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	308	G	O4'-C1'-N9	5.29	112.43	108.20
27	B8	352	A	C5-C6-N1	-5.29	115.05	117.70
27	B8	1939	U	O4'-C1'-N1	5.29	112.43	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2078	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	2821	A	O4'-C1'-N9	5.29	112.43	108.20
27	B8	2853	C	N3-C4-C5	-5.29	119.78	121.90
1	AA	1109	C	N3-C4-C5	-5.29	119.78	121.90
1	AA	1531	A	C5-C6-N6	-5.29	119.47	123.70
27	B8	137	U	P-O5'-C5'	5.29	129.36	120.90
27	B8	1701	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	576	C	N3-C4-C5	-5.29	119.78	121.90
1	AA	1270	G	O4'-C1'-N9	5.29	112.43	108.20
1	AA	1342	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	342	A	O4'-C1'-N9	5.29	112.43	108.20
27	B8	1057	A	C5-C6-N1	-5.29	115.06	117.70
27	B8	1146	C	N3-C4-N4	5.29	121.70	118.00
27	B8	1176	U	O4'-C1'-N1	5.29	112.43	108.20
27	B8	1213	A	C5-C6-N6	-5.29	119.47	123.70
27	B8	1489	C	N3-C4-N4	5.29	121.70	118.00
27	B8	2425	A	O4'-C1'-N9	5.29	112.43	108.20
27	B8	2426	A	C5-C6-N1	-5.29	115.06	117.70
1	AA	676	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	1360	A	O4'-C1'-N9	5.29	112.43	108.20
27	B8	897	C	N3-C4-C5	-5.29	119.78	121.90
27	B8	1395	A	O4'-C1'-N9	5.29	112.43	108.20
27	B8	1710	G	O4'-C1'-N9	5.29	112.43	108.20
27	B8	2287	A	C5-C6-N6	-5.29	119.47	123.70
1	AA	415	A	C5-C6-N6	-5.29	119.47	123.70
3	AV	58	A	C5-C6-N1	-5.29	115.06	117.70
27	B8	32	C	N3-C4-C5	-5.29	119.79	121.90
27	B8	1303	G	O4'-C1'-N9	5.29	112.43	108.20
27	B8	1504	A	C5-C6-N6	-5.29	119.47	123.70
27	B8	1942	C	N3-C4-N4	5.29	121.70	118.00
27	B8	2267	A	C5-C6-N1	-5.29	115.06	117.70
27	B8	2628	C	N3-C4-C5	-5.29	119.79	121.90
1	AA	523	A	C5-C6-N1	-5.28	115.06	117.70
27	B8	751	A	C5-C6-N6	-5.28	119.47	123.70
27	B8	1067	A	C5-C6-N6	-5.28	119.47	123.70
27	B8	1322	A	C4-C5-C6	5.28	119.64	117.00
27	B8	1803	A	O4'-C1'-N9	5.28	112.43	108.20
27	B8	2090	A	C5-C6-N1	-5.28	115.06	117.70
1	AA	461	A	C5-C6-N1	-5.28	115.06	117.70
27	B8	579	G	O4'-C1'-N9	5.28	112.43	108.20
1	AA	238	A	C5-C6-N1	-5.28	115.06	117.70
1	AA	466	A	C5-C6-N1	-5.28	115.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	946	A	C5-C6-N6	-5.28	119.47	123.70
27	B8	118	A	C5-C6-N6	-5.28	119.48	123.70
27	B8	309	A	C5-C6-N1	-5.28	115.06	117.70
27	B8	354	A	O4'-C1'-N9	5.28	112.42	108.20
27	B8	750	A	O4'-C1'-N9	5.28	112.42	108.20
27	B8	1271	G	O4'-C1'-N9	5.28	112.42	108.20
27	B8	1381	G	O4'-C1'-N9	5.28	112.42	108.20
27	B8	2468	A	O4'-C1'-N9	5.28	112.42	108.20
27	B8	2619	C	N3-C4-C5	-5.28	119.79	121.90
27	B8	2652	C	N3-C4-N4	5.28	121.70	118.00
27	B8	2823	A	O4'-C1'-N9	5.28	112.42	108.20
1	AA	609	A	C5-C6-N1	-5.28	115.06	117.70
1	AA	1012	A	C4-C5-C6	5.28	119.64	117.00
1	AA	51	A	C5-C6-N6	-5.28	119.48	123.70
1	AA	235	C	N3-C4-C5	-5.28	119.79	121.90
1	AA	1216	A	C5-C6-N6	-5.28	119.48	123.70
1	AA	1402	C	N3-C4-N4	5.28	121.69	118.00
26	B7	57	A	C5-C6-N6	-5.28	119.48	123.70
27	B8	504	A	C5-C6-N1	-5.28	115.06	117.70
27	B8	1212	G	N3-C2-N2	5.28	123.59	119.90
27	B8	1602	U	O4'-C1'-N1	5.28	112.42	108.20
27	B8	1730	C	N3-C4-C5	-5.28	119.79	121.90
27	B8	2019	A	O4'-C1'-N9	5.28	112.42	108.20
27	B8	2164	C	N3-C4-C5	-5.28	119.79	121.90
27	B8	2890	G	O4'-C1'-N9	5.28	112.42	108.20
1	AA	704	A	O4'-C1'-N9	5.28	112.42	108.20
1	AA	1359	C	N3-C4-C5	-5.28	119.79	121.90
2	AX	21	A	C5-C6-N1	-5.28	115.06	117.70
27	B8	660	C	N3-C4-C5	-5.28	119.79	121.90
1	AA	162	A	C8-N9-C4	-5.27	103.69	105.80
1	AA	410	G	C5-C6-O6	-5.27	125.44	128.60
27	B8	357	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	1790	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	2849	U	O4'-C1'-N1	5.27	112.42	108.20
1	AA	74	A	C5-C6-N6	-5.27	119.48	123.70
1	AA	149	A	C5-C6-N1	-5.27	115.06	117.70
1	AA	382	A	C5-C6-N6	-5.27	119.48	123.70
1	AA	736	C	N3-C4-C5	-5.27	119.79	121.90
1	AA	825	A	C5-C6-N1	-5.27	115.06	117.70
1	AA	1101	A	C4-C5-C6	5.27	119.64	117.00
27	B8	383	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	436	C	N3-C4-C5	-5.27	119.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	508	A	C5-C6-N1	-5.27	115.06	117.70
27	B8	921	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	1272	A	C5-C6-N6	-5.27	119.48	123.70
27	B8	1500	G	O4'-C1'-N9	5.27	112.42	108.20
27	B8	1983	G	O4'-C1'-N9	5.27	112.42	108.20
27	B8	2051	A	C5-C6-N1	-5.27	115.06	117.70
1	AA	580	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	1924	C	N3-C4-C5	-5.27	119.79	121.90
1	AA	352	C	N3-C4-C5	-5.27	119.79	121.90
1	AA	949	A	O4'-C1'-N9	5.27	112.42	108.20
1	AA	1428	A	O4'-C1'-N9	5.27	112.42	108.20
3	AV	4	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	27	G	N3-C2-N2	5.27	123.59	119.90
27	B8	41	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	182	A	O4'-C1'-N9	5.27	112.42	108.20
27	B8	793	A	O4'-C1'-N9	5.27	112.42	108.20
27	B8	1103	A	C5-C6-N6	-5.27	119.48	123.70
27	B8	1968	G	O4'-C1'-N9	5.27	112.42	108.20
27	B8	2161	C	N3-C4-C5	-5.27	119.79	121.90
1	AA	373	A	C5-C6-N6	-5.27	119.49	123.70
1	AA	380	G	O4'-C1'-N9	5.27	112.41	108.20
1	AA	861	G	O4'-C1'-N9	5.27	112.41	108.20
26	B7	53	A	C5-C6-N6	-5.27	119.49	123.70
27	B8	739	A	C5-C6-N1	-5.27	115.07	117.70
27	B8	925	A	C5-C6-N6	-5.27	119.49	123.70
27	B8	959	A	O4'-C1'-N9	5.27	112.42	108.20
27	B8	1089	A	C5-C6-N6	-5.27	119.49	123.70
27	B8	1254	A	O4'-C1'-N9	5.27	112.41	108.20
27	B8	1498	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	1780	A	C4-C5-C6	5.27	119.63	117.00
27	B8	2405	G	O4'-C1'-N9	5.27	112.41	108.20
27	B8	2450	A	O4'-C1'-N9	5.27	112.41	108.20
27	B8	2564	A	C5-C6-N6	-5.27	119.49	123.70
17	AM	105	ALA	N-CA-CB	5.27	117.47	110.10
27	B8	279	A	C5-C6-N1	-5.27	115.07	117.70
27	B8	2681	C	N3-C4-C5	-5.27	119.79	121.90
27	B8	2887	A	C5-C6-N1	-5.27	115.07	117.70
1	AA	47	C	N3-C4-C5	-5.26	119.80	121.90
1	AA	90	C	N3-C4-N4	5.26	121.69	118.00
1	AA	511	C	P-O3'-C3'	5.26	126.02	119.70
27	B8	270	A	O4'-C1'-N9	5.26	112.41	108.20
27	B8	514	A	C5-C6-N6	-5.26	119.49	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1689	A	C5-C6-N1	-5.26	115.07	117.70
1	AA	119	A	C5-C6-N6	-5.26	119.49	123.70
1	AA	691	G	O4'-C1'-N9	5.26	112.41	108.20
1	AA	1059	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	943	A	C4-C5-C6	5.26	119.63	117.00
27	B8	1032	A	C5-C6-N1	-5.26	115.07	117.70
27	B8	1810	A	O4'-C1'-N9	5.26	112.41	108.20
1	AA	1004	A	O4'-C1'-N9	5.26	112.41	108.20
1	AA	1311	A	O4'-C1'-N9	5.26	112.41	108.20
27	B8	225	C	N3-C4-N4	5.26	121.68	118.00
27	B8	241	A	C5-C6-N1	-5.26	115.07	117.70
1	AA	545	C	N3-C4-C5	-5.26	119.80	121.90
1	AA	560	A	C5-C6-N1	-5.26	115.07	117.70
1	AA	1383	C	N3-C4-C5	-5.26	119.80	121.90
1	AA	1411	C	N3-C4-C5	-5.26	119.80	121.90
26	B7	29	A	C5-C6-N1	-5.26	115.07	117.70
27	B8	386	G	O4'-C1'-N9	5.26	112.41	108.20
27	B8	631	A	C5-C6-N1	-5.26	115.07	117.70
27	B8	785	G	O4'-C1'-N9	5.26	112.41	108.20
27	B8	885	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	2050	C	N3-C4-N4	5.26	121.68	118.00
27	B8	2866	U	O4'-C1'-N1	5.26	112.41	108.20
1	AA	71	A	C4-C5-C6	5.26	119.63	117.00
1	AA	1533	C	N3-C4-N4	5.26	121.68	118.00
27	B8	57	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	621	A	C5-C6-N6	-5.26	119.49	123.70
27	B8	1531	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	1894	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	2067	G	O4'-C1'-N9	5.26	112.41	108.20
27	B8	2254	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	2714	G	N3-C2-N2	5.26	123.58	119.90
1	AA	143	A	O4'-C1'-N9	5.26	112.41	108.20
1	AA	162	A	O4'-C1'-N9	5.26	112.41	108.20
1	AA	178	C	N3-C4-C5	-5.26	119.80	121.90
1	AA	274	A	C5-C6-N6	-5.26	119.50	123.70
1	AA	1196	A	C5-C6-N1	-5.26	115.07	117.70
1	AA	1429	A	C5-C6-N6	-5.26	119.49	123.70
26	B7	68	C	N3-C4-C5	-5.26	119.80	121.90
27	B8	1025	G	O4'-C1'-N9	5.26	112.41	108.20
27	B8	1276	A	C5-C6-N1	-5.26	115.07	117.70
27	B8	1669	A	C5-C6-N6	-5.26	119.50	123.70
27	B8	1678	A	C5-C6-N1	-5.26	115.07	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	126	A	C5-C6-N1	-5.25	115.07	117.70
27	B8	335	C	N3-C4-N4	5.25	121.68	118.00
1	AA	95	C	N3-C4-C5	-5.25	119.80	121.90
1	AA	1229	A	O4'-C1'-N9	5.25	112.40	108.20
1	AA	1250	A	C5-C6-N1	-5.25	115.07	117.70
26	B7	35	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	159	G	N3-C2-N2	5.25	123.58	119.90
27	B8	1525	A	O4'-C1'-N9	5.25	112.40	108.20
27	B8	1598	A	C5-C6-N1	-5.25	115.07	117.70
27	B8	2097	A	C5-C6-N1	-5.25	115.07	117.70
27	B8	2611	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	2726	A	C5-C6-N6	-5.25	119.50	123.70
27	B8	2813	A	C5-C6-N1	-5.25	115.07	117.70
27	B8	2850	A	C5-C6-N1	-5.25	115.07	117.70
1	AA	864	A	C5-C6-N6	-5.25	119.50	123.70
1	AA	1054	C	C6-N1-C1'	-5.25	114.50	120.80
1	AA	1067	A	C5-C6-N6	-5.25	119.50	123.70
1	AA	1392	G	O4'-C1'-N9	5.25	112.40	108.20
27	B8	146	A	C5-C6-N1	-5.25	115.07	117.70
27	B8	479	A	C5-C6-N6	-5.25	119.50	123.70
27	B8	687	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	844	A	C5-C6-N6	-5.25	119.50	123.70
27	B8	983	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	1321	A	C5-C6-N6	-5.25	119.50	123.70
27	B8	2176	A	C5-C6-N1	-5.25	115.07	117.70
27	B8	2471	A	C4-C5-C6	5.25	119.62	117.00
27	B8	2660	A	O4'-C1'-N9	5.25	112.40	108.20
27	B8	2820	A	C5-C6-N1	-5.25	115.07	117.70
1	AA	1	A	C5-C6-N1	-5.25	115.08	117.70
26	B7	45	A	C4-C5-C6	5.25	119.62	117.00
27	B8	1752	C	N3-C4-N4	5.25	121.67	118.00
1	AA	196	A	C5-C6-N1	-5.25	115.08	117.70
1	AA	345	C	O4'-C1'-N1	5.25	112.40	108.20
1	AA	554	A	C5-C6-N1	-5.25	115.08	117.70
1	AA	808	C	N3-C4-C5	-5.25	119.80	121.90
1	AA	1353	G	O4'-C1'-N9	5.25	112.40	108.20
3	AV	38	G	C5-C6-O6	-5.25	125.45	128.60
3	AV	60	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	86	G	O4'-C1'-N9	5.25	112.40	108.20
27	B8	673	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	793	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	851	C	N3-C4-C5	-5.25	119.80	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	895	U	O4'-C1'-N1	5.25	112.40	108.20
27	B8	994	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	1265	A	C5-C6-N6	-5.25	119.50	123.70
27	B8	1323	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	1477	A	C5-C6-N6	-5.25	119.50	123.70
27	B8	1700	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	1910	G	O4'-C1'-N9	5.25	112.40	108.20
27	B8	2103	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	2248	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	2345	G	O4'-C1'-N9	5.25	112.40	108.20
27	B8	2416	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	2556	C	N3-C4-C5	-5.25	119.80	121.90
1	AA	1284	C	O4'-C1'-N1	5.25	112.40	108.20
1	AA	1331	G	O4'-C1'-N9	5.25	112.40	108.20
1	AA	1533	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	99	U	C6-N1-C1'	-5.25	113.86	121.20
27	B8	704	G	N3-C2-N2	5.25	123.57	119.90
27	B8	1324	G	C5'-C4'-C3'	-5.25	107.61	116.00
27	B8	1630	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	1632	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	2590	A	O4'-C1'-N9	5.25	112.40	108.20
27	B8	2721	A	C5-C6-N1	-5.25	115.08	117.70
1	AA	53	A	C5-C6-N1	-5.25	115.08	117.70
1	AA	328	C	C6-N1-C1'	-5.25	114.51	120.80
1	AA	1267	C	N3-C4-N4	5.25	121.67	118.00
27	B8	1555	G	O4'-C1'-N9	5.25	112.40	108.20
27	B8	1580	A	C5-C6-N1	-5.25	115.08	117.70
27	B8	2515	C	N3-C4-C5	-5.25	119.80	121.90
27	B8	2587	A	C5-C6-N1	-5.25	115.08	117.70
1	AA	195	A	C5-C6-N6	-5.24	119.50	123.70
1	AA	708	C	N3-C4-C5	-5.24	119.80	121.90
1	AA	767	A	C5-C6-N1	-5.24	115.08	117.70
1	AA	918	A	O4'-C1'-N9	5.24	112.39	108.20
2	AX	14	G	O4'-C1'-N9	5.24	112.39	108.20
27	B8	418	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	609	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	610	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	1821	A	C5-C6-N6	-5.24	119.51	123.70
1	AA	322	C	N3-C4-C5	-5.24	119.80	121.90
1	AA	574	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	472	A	O4'-C1'-N9	5.24	112.39	108.20
27	B8	743	A	C5-C6-N1	-5.24	115.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1327	A	O4'-C1'-N9	5.24	112.39	108.20
27	B8	2175	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	2321	U	O4'-C1'-N1	5.24	112.39	108.20
1	AA	852	G	O4'-C1'-N9	5.24	112.39	108.20
1	AA	1320	C	N3-C4-N4	5.24	121.67	118.00
27	B8	47	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	149	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	444	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	1256	G	O4'-C1'-N9	5.24	112.39	108.20
27	B8	1384	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	1908	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	2674	G	O4'-C1'-N9	5.24	112.39	108.20
27	B8	2837	A	C5-C6-N1	-5.24	115.08	117.70
1	AA	535	A	C5-C6-N6	-5.24	119.51	123.70
1	AA	680	C	N3-C4-C5	-5.24	119.81	121.90
1	AA	770	C	N3-C4-C5	-5.24	119.81	121.90
1	AA	1019	A	C5-C6-N1	-5.24	115.08	117.70
1	AA	1033	G	O4'-C1'-N9	5.24	112.39	108.20
1	AA	1105	A	C5-C6-N1	-5.24	115.08	117.70
1	AA	1257	A	C5-C6-N1	-5.24	115.08	117.70
2	AX	17	C	N3-C4-N4	5.24	121.67	118.00
27	B8	31	C	N3-C4-C5	-5.24	119.80	121.90
27	B8	1029	A	C5-C6-N6	-5.24	119.51	123.70
27	B8	1068	G	O4'-C1'-N9	5.24	112.39	108.20
27	B8	1189	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	2020	A	O4'-C1'-N9	5.24	112.39	108.20
27	B8	2060	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	2333	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	165	A	O4'-C1'-N9	5.24	112.39	108.20
27	B8	1547	C	N3-C4-C5	-5.24	119.81	121.90
27	B8	2616	C	N3-C4-C5	-5.24	119.81	121.90
27	B8	2693	G	O4'-C1'-N9	5.24	112.39	108.20
1	AA	587	G	P-O3'-C3'	5.24	125.98	119.70
1	AA	873	A	C5-C6-N6	-5.24	119.51	123.70
1	AA	1118	U	C2-N1-C1'	5.24	123.98	117.70
27	B8	640	C	N3-C4-C5	-5.24	119.81	121.90
27	B8	1337	G	O4'-C1'-N9	5.24	112.39	108.20
27	B8	1535	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	1609	A	O4'-C1'-N9	5.24	112.39	108.20
27	B8	1618	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	2062	A	C5-C6-N1	-5.24	115.08	117.70
27	B8	2397	G	O4'-C1'-N9	5.24	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	60	A	C5-C6-N6	-5.23	119.51	123.70
1	AA	1172	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	274	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	1499	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	1646	C	N3-C4-N4	5.23	121.66	118.00
28	BA	435	LYS	N-CA-CB	5.23	120.02	110.60
1	AA	415	A	O4'-C1'-N9	5.23	112.39	108.20
1	AA	622	A	C5-C6-N1	-5.23	115.08	117.70
1	AA	667	G	O4'-C1'-N9	5.23	112.39	108.20
1	AA	909	A	C5-C6-N1	-5.23	115.08	117.70
27	B8	1614	A	C5-C6-N1	-5.23	115.08	117.70
27	B8	1626	A	O4'-C1'-N9	5.23	112.39	108.20
27	B8	2114	A	C5-C6-N6	-5.23	119.51	123.70
27	B8	2153	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	2211	A	C5-C6-N1	-5.23	115.08	117.70
27	B8	2391	G	O4'-C1'-N9	5.23	112.39	108.20
1	AA	964	A	C5-C6-N1	-5.23	115.08	117.70
1	AA	1217	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	751	A	C5-C6-N1	-5.23	115.08	117.70
27	B8	1567	G	O4'-C1'-N9	5.23	112.38	108.20
27	B8	2418	A	C5-C6-N6	-5.23	119.52	123.70
1	AA	98	A	C5-C6-N1	-5.23	115.09	117.70
1	AA	1443	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	129	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	143	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	145	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	422	A	O4'-C1'-N9	5.23	112.38	108.20
27	B8	1152	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	1536	C	N3-C4-N4	5.23	121.66	118.00
27	B8	2738	A	C5-C6-N6	-5.23	119.52	123.70
27	B8	53	A	C5-C6-N1	-5.23	115.09	117.70
27	B8	199	A	C4-C5-C6	5.23	119.61	117.00
27	B8	1428	C	N3-C4-C5	-5.23	119.81	121.90
27	B8	2563	U	O4'-C1'-N1	5.23	112.38	108.20
27	B8	2639	A	C5-C6-N6	-5.23	119.52	123.70
1	AA	800	G	O4'-C1'-N9	5.22	112.38	108.20
1	AA	1254	A	C5-C6-N6	-5.22	119.52	123.70
3	AV	22	A	C5-C6-N1	-5.22	115.09	117.70
3	AV	28	C	N3-C4-C5	-5.22	119.81	121.90
3	AV	60	A	C5-C6-N6	-5.22	119.52	123.70
27	B8	655	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	896	A	C5-C6-N1	-5.22	115.09	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1021	A	C5-C6-N6	-5.22	119.52	123.70
27	B8	1463	C	N3-C4-C5	-5.22	119.81	121.90
27	B8	1788	C	N3-C4-C5	-5.22	119.81	121.90
1	AA	414	A	C5-C6-N1	-5.22	115.09	117.70
1	AA	918	A	C5-C6-N1	-5.22	115.09	117.70
1	AA	1082	A	C5-C6-N6	-5.22	119.52	123.70
1	AA	1150	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	241	A	O4'-C1'-N9	5.22	112.38	108.20
27	B8	518	G	O4'-C1'-N9	5.22	112.38	108.20
27	B8	2160	C	N3-C4-C5	-5.22	119.81	121.90
1	AA	7	A	C5-C6-N1	-5.22	115.09	117.70
1	AA	223	A	O4'-C1'-N9	5.22	112.38	108.20
1	AA	1012	A	C5-C6-N6	-5.22	119.52	123.70
1	AA	1154	G	O4'-C1'-N9	5.22	112.38	108.20
27	B8	706	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	1118	C	N3-C4-C5	-5.22	119.81	121.90
27	B8	1285	A	C5-C6-N1	-5.22	115.09	117.70
1	AA	132	C	N3-C4-C5	-5.22	119.81	121.90
1	AA	308	C	N3-C4-C5	-5.22	119.81	121.90
26	B7	90	C	N3-C4-C5	-5.22	119.81	121.90
27	B8	144	A	C5-C6-N6	-5.22	119.52	123.70
27	B8	344	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	1257	C	N3-C4-C5	-5.22	119.81	121.90
27	B8	1315	C	N3-C4-C5	-5.22	119.81	121.90
27	B8	1512	C	N3-C4-C5	-5.22	119.81	121.90
27	B8	2590	A	C5-C6-N6	-5.22	119.53	123.70
27	B8	2675	A	C5-C6-N6	-5.22	119.53	123.70
1	AA	1447	A	C5-C6-N6	-5.22	119.53	123.70
27	B8	320	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	1049	C	N3-C4-C5	-5.22	119.81	121.90
1	AA	349	A	C5-C6-N6	-5.22	119.53	123.70
1	AA	825	A	C5-C6-N6	-5.22	119.53	123.70
1	AA	1269	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	219	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	270	A	C5-C6-N1	-5.22	115.09	117.70
27	B8	278	A	C5-C6-N6	-5.22	119.53	123.70
27	B8	609	A	O4'-C1'-N9	5.22	112.37	108.20
27	B8	613	A	O4'-C1'-N9	5.22	112.37	108.20
27	B8	1460	U	C2-N1-C1'	5.22	123.96	117.70
27	B8	2060	A	C5-C6-N6	-5.22	119.53	123.70
1	AA	936	C	N3-C4-C5	-5.21	119.81	121.90
27	B8	156	A	C5-C6-N1	-5.21	115.09	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	590	A	C5-C6-N1	-5.21	115.09	117.70
27	B8	721	A	C5-C6-N6	-5.21	119.53	123.70
27	B8	854	C	N3-C4-C5	-5.21	119.81	121.90
27	B8	1401	G	O4'-C1'-N9	5.21	112.37	108.20
27	B8	1717	A	C5-C6-N6	-5.21	119.53	123.70
27	B8	1726	C	N3-C4-C5	-5.21	119.81	121.90
32	BD	156	PHE	CB-CG-CD1	5.21	124.45	120.80
1	AA	1409	C	N3-C4-N4	5.21	121.65	118.00
1	AA	215	C	N3-C4-N4	5.21	121.65	118.00
1	AA	498	A	C5-C6-N1	-5.21	115.09	117.70
1	AA	569	C	N3-C4-C5	-5.21	119.81	121.90
1	AA	702	A	C5-C6-N6	-5.21	119.53	123.70
1	AA	1132	C	N3-C4-N4	5.21	121.65	118.00
1	AA	1286	U	O4'-C1'-N1	5.21	112.37	108.20
1	AA	1350	A	O4'-C1'-N9	5.21	112.37	108.20
27	B8	275	C	N3-C4-N4	5.21	121.65	118.00
27	B8	547	A	C5-C6-N1	-5.21	115.09	117.70
27	B8	990	A	C5-C6-N6	-5.21	119.53	123.70
27	B8	1085	A	O4'-C1'-N9	5.21	112.37	108.20
27	B8	1544	A	C5-C6-N1	-5.21	115.09	117.70
27	B8	1609	A	C5-C6-N1	-5.21	115.09	117.70
27	B8	2198	A	C5-C6-N1	-5.21	115.09	117.70
1	AA	1344	C	N3-C4-C5	-5.21	119.82	121.90
26	B7	78	A	C4-C5-C6	5.21	119.61	117.00
27	B8	223	A	C5-C6-N1	-5.21	115.09	117.70
27	B8	497	A	O4'-C1'-N9	5.21	112.37	108.20
27	B8	917	A	C5-C6-N6	-5.21	119.53	123.70
1	AA	288	A	O4'-C1'-N9	5.21	112.37	108.20
1	AA	631	C	N3-C4-C5	-5.21	119.82	121.90
1	AA	998	C	N3-C4-N4	5.21	121.64	118.00
1	AA	1336	C	N3-C4-C5	-5.21	119.82	121.90
27	B8	1070	A	C5-C6-N1	-5.21	115.09	117.70
27	B8	1145	C	N3-C4-C5	-5.21	119.82	121.90
27	B8	1960	A	O4'-C1'-N9	5.21	112.37	108.20
1	AA	48	C	N3-C4-C5	-5.21	119.82	121.90
1	AA	1042	A	C5-C6-N1	-5.21	115.10	117.70
1	AA	1462	C	N3-C4-C5	-5.21	119.82	121.90
27	B8	879	G	O4'-C1'-N9	5.21	112.37	108.20
27	B8	913	U	O4'-C1'-N1	5.21	112.37	108.20
27	B8	945	A	C5-C6-N1	-5.21	115.10	117.70
27	B8	957	C	N3-C4-C5	-5.21	119.82	121.90
27	B8	1293	C	N3-C4-C5	-5.21	119.82	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1650	A	C5-C6-N1	-5.21	115.10	117.70
27	B8	2608	G	O4'-C1'-N9	5.21	112.36	108.20
27	B8	2892	G	O4'-C1'-N9	5.21	112.36	108.20
1	AA	858	G	O4'-C1'-N9	5.21	112.36	108.20
1	AA	1482	G	N3-C2-N2	5.21	123.54	119.90
27	B8	1912	A	C5-C6-N6	-5.21	119.54	123.70
27	B8	2503	A	O4'-C1'-N9	5.21	112.36	108.20
1	AA	33	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	787	A	C4-C5-C6	5.20	119.60	117.00
1	AA	792	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	1099	G	O4'-C1'-N9	5.20	112.36	108.20
1	AA	1253	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	440	C	N3-C4-C5	-5.20	119.82	121.90
27	B8	730	A	C5-C6-N1	-5.20	115.10	117.70
27	B8	1729	U	O4'-C1'-N1	5.20	112.36	108.20
1	AA	728	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	878	A	O4'-C1'-N9	5.20	112.36	108.20
3	AV	72	C	N3-C4-C5	-5.20	119.82	121.90
26	B7	43	C	N3-C4-C5	-5.20	119.82	121.90
27	B8	165	A	C5-C6-N6	-5.20	119.54	123.70
27	B8	332	A	P-O3'-C3'	5.20	125.94	119.70
27	B8	347	A	C5-C6-N1	-5.20	115.10	117.70
27	B8	976	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	1189	A	C5-C6-N6	-5.20	119.54	123.70
27	B8	1850	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	2532	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	2856	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	553	A	O4'-C1'-N9	5.20	112.36	108.20
1	AA	864	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	1158	C	N3-C4-N4	5.20	121.64	118.00
1	AA	1338	G	C4-N9-C1'	5.20	133.26	126.50
27	B8	1362	C	N3-C4-C5	-5.20	119.82	121.90
27	B8	1569	A	C5-C6-N1	-5.20	115.10	117.70
27	B8	2480	C	N3-C4-C5	-5.20	119.82	121.90
1	AA	1314	C	N3-C4-C5	-5.20	119.82	121.90
26	B7	23	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	331	C	N3-C4-C5	-5.20	119.82	121.90
27	B8	600	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	1244	A	C5-C6-N1	-5.20	115.10	117.70
27	B8	2163	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	320	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	643	C	N3-C4-C5	-5.20	119.82	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	860	A	C5-C6-N1	-5.20	115.10	117.70
27	B8	1652	A	O4'-C1'-N9	5.20	112.36	108.20
27	B8	1854	A	C5-C6-N1	-5.20	115.10	117.70
1	AA	520	A	O4'-C1'-N9	5.20	112.36	108.20
1	AA	521	G	O4'-C1'-N9	5.20	112.36	108.20
1	AA	1375	A	C5-C6-N6	-5.20	119.54	123.70
3	AV	32	C	N3-C4-N4	5.20	121.64	118.00
27	B8	131	A	C5-C6-N6	-5.20	119.54	123.70
27	B8	531	C	N3-C4-C5	-5.20	119.82	121.90
27	B8	705	A	C5-C6-N1	-5.20	115.10	117.70
27	B8	2414	G	O4'-C1'-N9	5.20	112.36	108.20
27	B8	2639	A	C4-C5-C6	5.20	119.60	117.00
27	B8	2755	C	N3-C4-C5	-5.20	119.82	121.90
32	BD	156	PHE	CB-CG-CD2	-5.20	117.16	120.80
27	B8	401	A	C5-C6-N1	-5.19	115.10	117.70
27	B8	1034	G	O4'-C1'-N9	5.19	112.36	108.20
1	AA	687	A	P-O3'-C3'	5.19	125.93	119.70
1	AA	819	A	C5-C6-N1	-5.19	115.10	117.70
1	AA	1378	C	N3-C4-C5	-5.19	119.82	121.90
3	AV	76	C	P-O5'-C5'	5.19	129.21	120.90
27	B8	457	A	C5-C6-N1	-5.19	115.10	117.70
27	B8	661	A	C5-C6-N1	-5.19	115.10	117.70
27	B8	1147	A	C5-C6-N1	-5.19	115.10	117.70
27	B8	2350	C	N3-C4-C5	-5.19	119.82	121.90
27	B8	2815	C	N3-C4-C5	-5.19	119.82	121.90
1	AA	272	C	N3-C4-C5	-5.19	119.82	121.90
1	AA	608	A	C5-C6-N6	-5.19	119.55	123.70
1	AA	884	U	O4'-C1'-N1	5.19	112.35	108.20
27	B8	32	C	N3-C4-N4	5.19	121.63	118.00
27	B8	527	C	N3-C4-C5	-5.19	119.82	121.90
27	B8	980	A	C5-C6-N1	-5.19	115.10	117.70
27	B8	1749	A	O4'-C1'-N9	5.19	112.35	108.20
27	B8	1865	U	P-O3'-C3'	5.19	125.93	119.70
27	B8	2071	A	C5-C6-N1	-5.19	115.11	117.70
27	B8	2456	C	N3-C4-C5	-5.19	119.82	121.90
27	B8	2510	C	N3-C4-C5	-5.19	119.82	121.90
1	AA	990	C	N3-C4-C5	-5.19	119.82	121.90
27	B8	613	A	C5-C6-N1	-5.19	115.11	117.70
27	B8	1070	A	C5-C6-N6	-5.19	119.55	123.70
27	B8	1732	C	O4'-C1'-N1	5.19	112.35	108.20
27	B8	338	G	N3-C2-N2	5.19	123.53	119.90
27	B8	432	A	C5-C6-N1	-5.19	115.11	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	595	C	N3-C4-C5	-5.19	119.83	121.90
27	B8	640	C	N3-C4-N4	5.19	121.63	118.00
27	B8	935	C	N3-C4-C5	-5.19	119.83	121.90
27	B8	1295	C	N3-C4-C5	-5.19	119.83	121.90
27	B8	1385	A	C5-C6-N6	-5.19	119.55	123.70
27	B8	2498	C	N3-C4-C5	-5.19	119.83	121.90
27	B8	2856	A	C5-C6-N6	-5.19	119.55	123.70
1	AA	84	U	C2-N1-C1'	5.19	123.92	117.70
1	AA	1100	C	N3-C4-C5	-5.19	119.83	121.90
1	AA	1193	G	O4'-C1'-N9	5.19	112.35	108.20
27	B8	1718	G	O4'-C1'-N9	5.19	112.35	108.20
27	B8	1892	C	N3-C4-C5	-5.19	119.83	121.90
27	B8	2750	A	C5-C6-N6	-5.19	119.55	123.70
1	AA	253	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	20	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	1155	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	2030	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	2179	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	2558	C	N3-C4-C5	-5.18	119.83	121.90
1	AA	315	A	C5-C6-N6	-5.18	119.56	123.70
1	AA	431	A	C5-C6-N6	-5.18	119.55	123.70
1	AA	913	A	C5-C6-N6	-5.18	119.56	123.70
1	AA	1016	A	C5-C6-N6	-5.18	119.55	123.70
1	AA	1346	A	C5-C6-N6	-5.18	119.55	123.70
1	AA	1486	G	O4'-C1'-N9	5.18	112.35	108.20
1	AA	1508	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	453	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	775	G	P-O3'-C3'	5.18	125.92	119.70
27	B8	796	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	972	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	1580	A	C5-C6-N6	-5.18	119.56	123.70
27	B8	1962	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	2044	C	N3-C4-C5	-5.18	119.83	121.90
1	AA	1394	A	O4'-C1'-N9	5.18	112.34	108.20
27	B8	821	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	1393	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	1803	A	C5-C6-N1	-5.18	115.11	117.70
27	B8	2301	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	162	U	O4'-C1'-N1	5.18	112.34	108.20
27	B8	1489	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	1768	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	1891	G	O4'-C1'-N9	5.18	112.34	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1916	A	C5-C6-N6	-5.18	119.56	123.70
27	B8	2326	C	N3-C4-C5	-5.18	119.83	121.90
1	AA	759	A	N1-C6-N6	5.18	121.71	118.60
1	AA	1534	A	C5-C6-N6	-5.18	119.56	123.70
27	B8	366	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	2359	C	N3-C4-C5	-5.18	119.83	121.90
3	AV	45	G	O4'-C1'-N9	5.18	112.34	108.20
27	B8	37	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	276	U	C6-N1-C1'	-5.18	113.95	121.20
27	B8	990	A	O4'-C1'-N9	5.18	112.34	108.20
27	B8	1164	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	1195	G	O4'-C1'-N9	5.18	112.34	108.20
27	B8	1297	C	N3-C4-C5	-5.18	119.83	121.90
27	B8	1858	A	O4'-C1'-N9	5.18	112.34	108.20
27	B8	2083	G	O4'-C1'-N9	5.18	112.34	108.20
1	AA	188	C	N3-C4-C5	-5.17	119.83	121.90
1	AA	406	G	O4'-C1'-N9	5.17	112.34	108.20
1	AA	1279	G	C4-N9-C1'	5.17	133.23	126.50
26	B7	119	A	C5-C6-N1	-5.17	115.11	117.70
27	B8	181	A	C5-C6-N1	-5.17	115.11	117.70
27	B8	239	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	897	C	N3-C4-N4	5.17	121.62	118.00
27	B8	995	C	C6-N1-C1'	-5.17	114.59	120.80
27	B8	1488	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	2135	A	C5-C6-N6	-5.17	119.56	123.70
27	B8	2227	A	C5-C6-N1	-5.17	115.11	117.70
27	B8	2433	A	C5-C6-N1	-5.17	115.11	117.70
27	B8	2443	C	N3-C4-C5	-5.17	119.83	121.90
1	AA	298	A	C5-C6-N1	-5.17	115.11	117.70
1	AA	1521	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	1289	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	2512	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	2636	C	N3-C4-C5	-5.17	119.83	121.90
1	AA	1101	A	C5-C6-N6	-5.17	119.56	123.70
27	B8	61	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	648	G	O4'-C1'-N9	5.17	112.34	108.20
27	B8	910	A	O4'-C1'-N9	5.17	112.34	108.20
27	B8	1345	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	1527	G	O4'-C1'-N9	5.17	112.34	108.20
27	B8	1652	A	C5-C6-N1	-5.17	115.11	117.70
27	B8	2141	G	O4'-C1'-N9	5.17	112.34	108.20
27	B8	2310	C	N3-C4-N4	5.17	121.62	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1234	C	N3-C4-C5	-5.17	119.83	121.90
26	B7	60	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	42	A	C5-C6-N6	-5.17	119.56	123.70
27	B8	66	C	N3-C4-N4	5.17	121.62	118.00
27	B8	106	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	2809	A	C5-C6-N1	-5.17	115.11	117.70
1	AA	201	G	O4'-C1'-N9	5.17	112.33	108.20
1	AA	203	G	N3-C2-N2	5.17	123.52	119.90
1	AA	450	G	O4'-C1'-N9	5.17	112.33	108.20
1	AA	715	A	O4'-C1'-N9	5.17	112.33	108.20
1	AA	805	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	691	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	1596	A	C5-C6-N6	-5.17	119.56	123.70
27	B8	1617	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	2355	G	O4'-C1'-N9	5.17	112.33	108.20
1	AA	55	A	O4'-C1'-N9	5.17	112.33	108.20
1	AA	372	C	N3-C4-N4	5.17	121.62	118.00
1	AA	547	A	C5-C6-N6	-5.17	119.57	123.70
1	AA	606	G	O4'-C1'-N9	5.17	112.33	108.20
1	AA	614	C	N3-C4-C5	-5.17	119.83	121.90
1	AA	676	A	O4'-C1'-N9	5.17	112.33	108.20
1	AA	831	A	C5-C6-N1	-5.17	115.12	117.70
1	AA	836	G	O4'-C1'-N9	5.17	112.33	108.20
1	AA	1225	A	O4'-C1'-N9	5.17	112.33	108.20
1	AA	1405	G	O4'-C1'-N9	5.17	112.33	108.20
27	B8	715	A	O4'-C1'-N9	5.17	112.33	108.20
27	B8	765	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	898	C	N3-C4-N4	5.17	121.62	118.00
27	B8	973	A	C5-C6-N1	-5.17	115.12	117.70
27	B8	1046	A	C5-C6-N1	-5.17	115.12	117.70
27	B8	1366	A	O4'-C1'-N9	5.17	112.33	108.20
27	B8	2150	C	N3-C4-C5	-5.17	119.83	121.90
27	B8	2774	C	N3-C4-C5	-5.17	119.83	121.90
1	AA	933	G	O4'-C1'-N9	5.17	112.33	108.20
1	AA	1005	A	O4'-C1'-N9	5.17	112.33	108.20
1	AA	1035	A	C5-C6-N1	-5.17	115.12	117.70
1	AA	1449	C	N3-C4-C5	-5.17	119.83	121.90
26	B7	14	U	O4'-C1'-N1	5.17	112.33	108.20
27	B8	101	A	C5-C6-N1	-5.17	115.12	117.70
27	B8	340	A	C5-C6-N1	-5.17	115.12	117.70
27	B8	856	G	O4'-C1'-N9	5.17	112.33	108.20
27	B8	1881	C	N3-C4-C5	-5.17	119.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2015	A	C5-C6-N6	-5.17	119.57	123.70
1	AA	79	G	O4'-C1'-N9	5.16	112.33	108.20
1	AA	998	C	N3-C4-C5	-5.16	119.83	121.90
1	AA	1400	C	N3-C4-N4	5.16	121.61	118.00
27	B8	21	A	C5-C6-N1	-5.16	115.12	117.70
27	B8	701	G	O4'-C1'-N9	5.16	112.33	108.20
27	B8	1974	C	N3-C4-C5	-5.16	119.83	121.90
1	AA	50	A	C5-C6-N1	-5.16	115.12	117.70
1	AA	199	A	O4'-C1'-N9	5.16	112.33	108.20
1	AA	888	G	N3-C2-N2	5.16	123.51	119.90
3	AV	27	A	C5-C6-N1	-5.16	115.12	117.70
27	B8	555	G	O4'-C1'-N9	5.16	112.33	108.20
27	B8	611	C	N3-C4-C5	-5.16	119.83	121.90
27	B8	1304	A	C5-C6-N6	-5.16	119.57	123.70
37	BI	87	SER	N-CA-CB	5.16	118.24	110.50
1	AA	364	A	O4'-C1'-N9	5.16	112.33	108.20
27	B8	479	A	C5-C6-N1	-5.16	115.12	117.70
27	B8	507	A	C5-C6-N1	-5.16	115.12	117.70
27	B8	900	A	C5-C6-N6	-5.16	119.57	123.70
27	B8	1085	A	C4-C5-C6	5.16	119.58	117.00
27	B8	1644	C	N3-C4-C5	-5.16	119.84	121.90
27	B8	1836	C	N3-C4-C5	-5.16	119.84	121.90
27	B8	2336	A	C5-C6-N1	-5.16	115.12	117.70
27	B8	2649	C	N3-C4-C5	-5.16	119.83	121.90
1	AA	1150	A	C5-C6-N6	-5.16	119.57	123.70
3	AV	17	C	N3-C4-N4	5.16	121.61	118.00
26	B7	70	C	N3-C4-C5	-5.16	119.84	121.90
27	B8	305	C	N3-C4-C5	-5.16	119.84	121.90
27	B8	1527	G	N3-C2-N2	5.16	123.51	119.90
27	B8	1600	C	N3-C4-C5	-5.16	119.84	121.90
27	B8	1638	C	N3-C4-C5	-5.16	119.84	121.90
26	B7	61	G	O4'-C1'-N9	5.16	112.33	108.20
27	B8	643	A	C5-C6-N1	-5.16	115.12	117.70
27	B8	1078	U	C2-N1-C1'	5.16	123.89	117.70
27	B8	1296	G	O4'-C1'-N9	5.16	112.33	108.20
1	AA	160	A	O4'-C1'-N9	5.16	112.32	108.20
1	AA	383	A	O4'-C1'-N9	5.16	112.33	108.20
27	B8	85	G	O4'-C1'-N9	5.16	112.32	108.20
27	B8	1872	A	C5-C6-N6	-5.16	119.58	123.70
1	AA	177	G	C5-C6-O6	-5.15	125.51	128.60
1	AA	1431	A	C5-C6-N1	-5.15	115.12	117.70
1	AA	695	A	C5-C6-N1	-5.15	115.12	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1287	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	127	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	670	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	911	A	O4'-C1'-N9	5.15	112.32	108.20
27	B8	2012	G	N3-C2-N2	5.15	123.51	119.90
27	B8	2145	C	C2-N1-C1'	5.15	124.47	118.80
1	AA	369	G	O4'-C1'-N9	5.15	112.32	108.20
1	AA	558	G	O4'-C1'-N9	5.15	112.32	108.20
1	AA	613	C	N3-C4-C5	-5.15	119.84	121.90
1	AA	969	A	C5-C6-N1	-5.15	115.12	117.70
1	AA	1285	A	C5-C6-N1	-5.15	115.12	117.70
1	AA	1318	A	C5-C6-N1	-5.15	115.12	117.70
1	AA	1332	A	C5-C6-N1	-5.15	115.12	117.70
1	AA	1352	C	N3-C4-C5	-5.15	119.84	121.90
27	B8	6	A	O4'-C1'-N9	5.15	112.32	108.20
27	B8	1496	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	2082	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	2430	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	2598	A	C5-C6-N1	-5.15	115.12	117.70
27	B8	121	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	1495	A	O4'-C1'-N9	5.15	112.32	108.20
27	B8	1628	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	2673	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	2682	A	O4'-C1'-N9	5.15	112.32	108.20
1	AA	59	A	C5-C6-N1	-5.15	115.13	117.70
1	AA	630	A	O4'-C1'-N9	5.15	112.32	108.20
1	AA	833	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	314	C	N3-C4-C5	-5.15	119.84	121.90
27	B8	477	A	C5-C6-N6	-5.15	119.58	123.70
27	B8	570	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	789	A	C5-C6-N1	-5.15	115.13	117.70
27	B8	1741	C	N3-C4-C5	-5.15	119.84	121.90
27	B8	1893	C	N3-C4-C5	-5.15	119.84	121.90
27	B8	2664	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	2765	A	C5-C6-N6	-5.15	119.58	123.70
1	AA	1142	G	O4'-C1'-N9	5.15	112.32	108.20
2	AX	17	C	N3-C4-C5	-5.15	119.84	121.90
3	AV	44	G	O4'-C1'-N9	5.15	112.32	108.20
27	B8	2595	G	O4'-C1'-N9	5.15	112.32	108.20
1	AA	489	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	999	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	1022	A	C5-C6-N6	-5.14	119.58	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1107	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	1111	A	O4'-C1'-N9	5.14	112.32	108.20
27	B8	844	A	O4'-C1'-N9	5.14	112.32	108.20
27	B8	2530	A	C5-C6-N1	-5.14	115.13	117.70
1	AA	331	G	O4'-C1'-N9	5.14	112.31	108.20
1	AA	750	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	857	C	N3-C4-N4	5.14	121.60	118.00
1	AA	1044	A	O4'-C1'-N9	5.14	112.31	108.20
1	AA	1492	A	C5-C6-N1	-5.14	115.13	117.70
27	B8	505	A	C5-C6-N1	-5.14	115.13	117.70
27	B8	1587	G	O4'-C1'-N9	5.14	112.31	108.20
27	B8	1753	G	O4'-C1'-N9	5.14	112.31	108.20
27	B8	2750	A	C5-C6-N1	-5.14	115.13	117.70
41	BM	122	ALA	N-CA-CB	5.14	117.30	110.10
1	AA	1214	C	C6-N1-C1'	-5.14	114.63	120.80
1	AA	1281	C	N3-C4-C5	-5.14	119.84	121.90
3	AV	27	A	O4'-C1'-N9	5.14	112.31	108.20
27	B8	616	A	C5-C6-N1	-5.14	115.13	117.70
27	B8	873	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	236	A	O4'-C1'-N9	5.14	112.31	108.20
1	AA	914	A	O4'-C1'-N9	5.14	112.31	108.20
1	AA	1418	A	C5-C6-N1	-5.14	115.13	117.70
27	B8	1048	A	O4'-C1'-N9	5.14	112.31	108.20
27	B8	1722	A	C5-C6-N6	-5.14	119.59	123.70
27	B8	2762	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	435	A	C5-C6-N1	-5.14	115.13	117.70
1	AA	608	A	C5-C6-N1	-5.14	115.13	117.70
1	AA	880	C	N3-C4-N4	5.14	121.60	118.00
27	B8	216	A	C5-C6-N6	-5.14	119.59	123.70
27	B8	719	C	N3-C4-C5	-5.14	119.84	121.90
27	B8	2455	G	O4'-C1'-N9	5.14	112.31	108.20
27	B8	2503	A	C5-C6-N1	-5.14	115.13	117.70
1	AA	980	C	N3-C4-C5	-5.14	119.84	121.90
1	AA	1368	A	C5-C6-N6	-5.14	119.59	123.70
1	AA	1468	A	C5-C6-N6	-5.14	119.59	123.70
26	B7	34	A	C5-C6-N6	-5.14	119.59	123.70
27	B8	94	A	C5-C6-N6	-5.14	119.59	123.70
27	B8	644	A	C5-C6-N1	-5.14	115.13	117.70
27	B8	905	A	C5-C6-N1	-5.14	115.13	117.70
27	B8	2208	C	N3-C4-C5	-5.14	119.85	121.90
1	AA	116	A	C5-C6-N6	-5.13	119.59	123.70
1	AA	1120	C	N3-C4-C5	-5.13	119.85	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	316	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	516	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	1454	C	N3-C4-N4	5.13	121.59	118.00
27	B8	2620	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	2875	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	1879	C	N3-C4-C5	-5.13	119.85	121.90
1	AA	727	G	N3-C2-N2	5.13	123.49	119.90
1	AA	1285	A	C5-C6-N6	-5.13	119.59	123.70
1	AA	1447	A	C4-C5-C6	5.13	119.56	117.00
27	B8	142	A	C5-C6-N6	-5.13	119.59	123.70
27	B8	385	C	N3-C4-N4	5.13	121.59	118.00
27	B8	1075	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	1302	A	C5-C6-N6	-5.13	119.59	123.70
27	B8	1909	C	N3-C4-C5	-5.13	119.85	121.90
1	AA	60	A	C5-C6-N1	-5.13	115.14	117.70
1	AA	452	A	C5-C6-N1	-5.13	115.14	117.70
1	AA	959	A	O4'-C1'-N9	5.13	112.30	108.20
27	B8	1383	A	C5-C6-N1	-5.13	115.14	117.70
27	B8	2509	G	O4'-C1'-N9	5.13	112.30	108.20
27	B8	2832	U	O4'-C1'-N1	5.13	112.30	108.20
1	AA	712	A	C5-C6-N1	-5.13	115.14	117.70
26	B7	17	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	195	A	C5-C6-N1	-5.13	115.14	117.70
27	B8	457	A	C4-C5-C6	5.13	119.56	117.00
27	B8	1298	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	2134	A	C5-C6-N6	-5.13	119.60	123.70
27	B8	2427	C	N3-C4-C5	-5.13	119.85	121.90
27	B8	2833	U	O4'-C1'-N1	5.13	112.30	108.20
27	B8	2883	A	C5-C6-N1	-5.13	115.14	117.70
1	AA	1027	C	C5-C4-N4	-5.13	116.61	120.20
1	AA	1188	A	O4'-C1'-N9	5.13	112.30	108.20
27	B8	251	A	O4'-C1'-N9	5.13	112.30	108.20
27	B8	849	A	C5-C6-N1	-5.13	115.14	117.70
27	B8	2499	C	N3-C4-C5	-5.13	119.85	121.90
1	AA	648	A	O4'-C1'-N9	5.12	112.30	108.20
1	AA	139	A	C5-C6-N1	-5.12	115.14	117.70
1	AA	507	C	N3-C4-C5	-5.12	119.85	121.90
1	AA	1269	A	C4-C5-C6	5.12	119.56	117.00
1	AA	1350	A	C5-C6-N1	-5.12	115.14	117.70
26	B7	26	C	N3-C4-N4	5.12	121.59	118.00
27	B8	34	U	C2-N1-C1'	5.12	123.85	117.70
27	B8	56	A	C5-C6-N1	-5.12	115.14	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	513	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	599	A	O4'-C1'-N9	5.12	112.30	108.20
27	B8	1264	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	1529	G	O4'-C1'-N9	5.12	112.30	108.20
27	B8	1572	A	O4'-C1'-N9	5.12	112.30	108.20
27	B8	1668	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	2761	A	O4'-C1'-N9	5.12	112.30	108.20
1	AA	54	C	N3-C4-C5	-5.12	119.85	121.90
26	B7	107	G	N3-C2-N2	5.12	123.49	119.90
27	B8	737	C	N3-C4-C5	-5.12	119.85	121.90
27	B8	878	A	O4'-C1'-N9	5.12	112.30	108.20
27	B8	1996	C	O4'-C1'-N1	5.12	112.30	108.20
27	B8	2706	A	C5-C6-N1	-5.12	115.14	117.70
1	AA	177	G	O4'-C1'-N9	5.12	112.30	108.20
27	B8	1	G	O4'-C1'-N9	5.12	112.30	108.20
27	B8	218	A	O4'-C1'-N9	5.12	112.30	108.20
27	B8	250	G	O4'-C1'-N9	5.12	112.30	108.20
27	B8	387	U	O4'-C1'-N1	5.12	112.30	108.20
27	B8	899	A	C5-C6-N1	-5.12	115.14	117.70
1	AA	699	C	N3-C4-C5	-5.12	119.85	121.90
1	AA	888	G	O4'-C1'-N9	5.12	112.30	108.20
27	B8	38	A	O4'-C1'-N9	5.12	112.30	108.20
27	B8	231	A	C5-C6-N6	-5.12	119.60	123.70
27	B8	1117	C	N3-C4-C5	-5.12	119.85	121.90
27	B8	1367	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	2274	A	O4'-C1'-N9	5.12	112.30	108.20
1	AA	560	A	O4'-C1'-N9	5.12	112.29	108.20
1	AA	1014	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	120	U	O4'-C1'-N1	5.12	112.29	108.20
27	B8	621	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	2020	A	C5-C6-N6	-5.12	119.61	123.70
27	B8	2467	C	N3-C4-N4	5.12	121.58	118.00
27	B8	2666	C	N3-C4-N4	5.12	121.58	118.00
1	AA	342	C	N3-C4-C5	-5.12	119.85	121.90
1	AA	579	A	C5-C6-N1	-5.12	115.14	117.70
1	AA	938	A	C5-C6-N1	-5.12	115.14	117.70
1	AA	1266	G	O4'-C1'-N9	5.12	112.29	108.20
1	AA	1340	A	C5-C6-N6	-5.12	119.61	123.70
1	AA	1434	A	C5-C6-N1	-5.12	115.14	117.70
27	B8	70	G	O4'-C1'-N9	5.12	112.29	108.20
27	B8	1074	G	O4'-C1'-N9	5.12	112.29	108.20
27	B8	2365	G	N3-C2-N2	5.12	123.48	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2440	C	N3-C4-C5	-5.12	119.85	121.90
1	AA	190	A	C5-C6-N6	-5.11	119.61	123.70
1	AA	1047	G	O4'-C1'-N9	5.11	112.29	108.20
1	AA	1096	C	N3-C4-C5	-5.11	119.86	121.90
6	AB	212	TYR	CB-CG-CD2	-5.11	117.93	121.00
27	B8	330	A	O4'-C1'-N9	5.11	112.29	108.20
27	B8	398	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	1308	A	O4'-C1'-N9	5.11	112.29	108.20
27	B8	1428	C	P-O3'-C3'	5.11	125.84	119.70
27	B8	1674	G	O4'-C1'-N9	5.11	112.29	108.20
27	B8	1978	A	C5-C6-N1	-5.11	115.14	117.70
27	B8	2164	C	C6-N1-C1'	-5.11	114.67	120.80
28	BA	200	PRO	CA-C-N	5.11	131.42	117.10
1	AA	1245	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	91	A	O4'-C1'-N9	5.11	112.29	108.20
47	BS	89	ALA	N-CA-CB	5.11	117.26	110.10
1	AA	530	G	O4'-C1'-N9	5.11	112.29	108.20
1	AA	1113	C	P-O5'-C5'	5.11	129.08	120.90
1	AA	1252	A	C5-C6-N1	-5.11	115.14	117.70
27	B8	52	A	C5-C6-N6	-5.11	119.61	123.70
27	B8	2258	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	2531	A	C5-C6-N6	-5.11	119.61	123.70
27	B8	2711	A	C5-C6-N1	-5.11	115.14	117.70
1	AA	810	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	1208	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	1711	A	C5-C6-N6	-5.11	119.61	123.70
27	B8	910	A	C5-C6-N6	-5.11	119.61	123.70
1	AA	285	C	N3-C4-C5	-5.11	119.86	121.90
1	AA	475	C	N3-C4-C5	-5.11	119.86	121.90
1	AA	639	G	O4'-C1'-N9	5.11	112.28	108.20
27	B8	124	G	O4'-C1'-N9	5.11	112.28	108.20
27	B8	1454	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	1494	A	O4'-C1'-N9	5.11	112.28	108.20
27	B8	1553	A	C5-C6-N1	-5.11	115.15	117.70
27	B8	2321	U	C2-N1-C1'	5.11	123.83	117.70
27	B8	2704	C	N3-C4-C5	-5.11	119.86	121.90
27	B8	2787	C	N3-C4-C5	-5.11	119.86	121.90
1	AA	1469	C	N3-C4-C5	-5.10	119.86	121.90
27	B8	2810	A	C5-C6-N1	-5.10	115.15	117.70
42	BN	21	PHE	CB-CG-CD2	5.10	124.37	120.80
1	AA	528	C	N3-C4-N4	5.10	121.57	118.00
1	AA	966	G	O4'-C1'-N9	5.10	112.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1502	A	C5-C6-N6	-5.10	119.62	123.70
3	AV	54	G	O4'-C1'-N9	5.10	112.28	108.20
27	B8	529	A	C5-C6-N6	-5.10	119.62	123.70
27	B8	633	A	C5-C6-N6	-5.10	119.62	123.70
27	B8	2214	C	N3-C4-C5	-5.10	119.86	121.90
1	AA	134	G	O4'-C1'-N9	5.10	112.28	108.20
27	B8	867	C	N3-C4-N4	5.10	121.57	118.00
27	B8	1414	C	N3-C4-C5	-5.10	119.86	121.90
27	B8	1789	A	O4'-C1'-N9	5.10	112.28	108.20
1	AA	326	G	O4'-C1'-N9	5.10	112.28	108.20
27	B8	343	C	N3-C4-C5	-5.10	119.86	121.90
27	B8	1403	A	O4'-C1'-N9	5.10	112.28	108.20
27	B8	1866	A	C5-C6-N1	-5.10	115.15	117.70
27	B8	2035	G	O4'-C1'-N9	5.10	112.28	108.20
27	B8	2678	C	N3-C4-C5	-5.10	119.86	121.90
27	B8	2785	C	N3-C4-C5	-5.10	119.86	121.90
1	AA	364	A	C5-C6-N1	-5.10	115.15	117.70
1	AA	865	A	C5-C6-N1	-5.10	115.15	117.70
27	B8	63	A	C5-C6-N1	-5.10	115.15	117.70
27	B8	167	A	C5-C6-N1	-5.10	115.15	117.70
27	B8	1695	G	O4'-C1'-N9	5.10	112.28	108.20
1	AA	1325	C	N3-C4-C5	-5.10	119.86	121.90
27	B8	5	A	O4'-C1'-N9	5.10	112.28	108.20
1	AA	282	A	C5-C6-N1	-5.09	115.15	117.70
1	AA	647	C	N3-C4-C5	-5.09	119.86	121.90
1	AA	743	A	O4'-C1'-N9	5.09	112.28	108.20
1	AA	1113	C	N3-C4-C5	-5.09	119.86	121.90
1	AA	1397	C	N3-C4-C5	-5.09	119.86	121.90
26	B7	37	C	N3-C4-N4	5.09	121.57	118.00
27	B8	109	C	N3-C4-C5	-5.09	119.86	121.90
27	B8	469	G	N3-C2-N2	5.09	123.47	119.90
27	B8	668	A	O4'-C1'-N9	5.09	112.28	108.20
27	B8	874	G	O4'-C1'-N9	5.09	112.28	108.20
27	B8	1387	A	C5-C6-N1	-5.09	115.15	117.70
27	B8	1630	A	C5-C6-N6	-5.09	119.62	123.70
27	B8	2368	C	N3-C4-C5	-5.09	119.86	121.90
27	B8	2620	C	N3-C4-N4	5.09	121.57	118.00
27	B8	2793	C	N3-C4-C5	-5.09	119.86	121.90
27	B8	2857	G	O4'-C1'-N9	5.09	112.28	108.20
27	B8	2879	A	C5-C6-N1	-5.09	115.15	117.70
1	AA	910	C	N3-C4-C5	-5.09	119.86	121.90
27	B8	626	A	O4'-C1'-N9	5.09	112.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	973	A	C5'-C4'-O4'	5.09	115.21	109.10
27	B8	1640	A	C5-C6-N1	-5.09	115.15	117.70
1	AA	52	C	N3-C4-C5	-5.09	119.86	121.90
1	AA	411	A	C5-C6-N1	-5.09	115.15	117.70
1	AA	1446	A	C5-C6-N1	-5.09	115.16	117.70
27	B8	39	G	O4'-C1'-N9	5.09	112.27	108.20
27	B8	1287	A	C5-C6-N6	-5.09	119.63	123.70
27	B8	1533	C	N3-C4-C5	-5.09	119.86	121.90
27	B8	1902	C	N3-C4-N4	5.09	121.56	118.00
27	B8	2077	A	C5-C6-N6	-5.09	119.63	123.70
27	B8	2306	C	N3-C4-C5	-5.09	119.86	121.90
1	AA	71	A	C5-C6-N1	-5.09	115.16	117.70
1	AA	280	C	O4'-C1'-N1	5.09	112.27	108.20
1	AA	876	C	N3-C4-C5	-5.09	119.86	121.90
3	AV	11	C	N3-C4-N4	5.09	121.56	118.00
27	B8	1111	A	C5-C6-N6	-5.09	119.63	123.70
27	B8	2386	A	C5-C6-N1	-5.09	115.16	117.70
27	B8	2520	C	N3-C4-C5	-5.09	119.86	121.90
27	B8	2654	A	C5-C6-N1	-5.09	115.16	117.70
1	AA	539	A	C5-C6-N1	-5.09	115.16	117.70
27	B8	1050	A	C5-C6-N1	-5.09	115.16	117.70
27	B8	1522	A	C4-C5-C6	5.09	119.54	117.00
27	B8	1679	A	C5-C6-N6	-5.09	119.63	123.70
1	AA	109	A	C5-C6-N6	-5.09	119.63	123.70
1	AA	234	C	N3-C4-C5	-5.09	119.87	121.90
1	AA	896	C	N3-C4-C5	-5.09	119.87	121.90
27	B8	1233	C	N3-C4-C5	-5.09	119.87	121.90
27	B8	2091	C	N3-C4-C5	-5.09	119.87	121.90
27	B8	2679	A	C5-C6-N1	-5.09	115.16	117.70
1	AA	1261	A	O4'-C1'-N9	5.08	112.27	108.20
27	B8	794	A	O4'-C1'-N9	5.08	112.27	108.20
27	B8	2486	C	N3-C4-C5	-5.08	119.87	121.90
1	AA	1236	A	O4'-C1'-N9	5.08	112.27	108.20
2	AX	19	U	O4'-C1'-N1	5.08	112.27	108.20
27	B8	1565	C	P-O3'-C3'	5.08	125.80	119.70
27	B8	1854	A	C5-C6-N6	-5.08	119.63	123.70
27	B8	1961	C	N3-C4-C5	-5.08	119.87	121.90
27	B8	2366	A	O4'-C1'-N9	5.08	112.27	108.20
27	B8	2487	G	O4'-C1'-N9	5.08	112.27	108.20
1	AA	432	A	C5-C6-N1	-5.08	115.16	117.70
1	AA	766	A	C5-C6-N1	-5.08	115.16	117.70
1	AA	1265	C	N3-C4-C5	-5.08	119.87	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	104	A	O4'-C1'-N9	5.08	112.27	108.20
27	B8	586	A	O4'-C1'-N9	5.08	112.27	108.20
27	B8	1044	C	N3-C4-C5	-5.08	119.87	121.90
27	B8	2542	A	C5-C6-N1	-5.08	115.16	117.70
1	AA	393	A	C5-C6-N6	-5.08	119.64	123.70
1	AA	1178	G	N3-C2-N2	5.08	123.46	119.90
27	B8	74	A	O4'-C1'-N9	5.08	112.26	108.20
1	AA	115	G	N3-C2-N2	5.08	123.46	119.90
1	AA	954	G	O4'-C1'-N9	5.08	112.26	108.20
27	B8	71	A	C5-C6-N6	-5.08	119.64	123.70
27	B8	1607	C	N3-C4-N4	5.08	121.55	118.00
27	B8	1977	A	O4'-C1'-N9	5.08	112.26	108.20
27	B8	2626	C	N3-C4-C5	-5.08	119.87	121.90
1	AA	729	A	C5-C6-N1	-5.08	115.16	117.70
1	AA	790	A	O4'-C1'-N9	5.08	112.26	108.20
1	AA	1417	G	N3-C2-N2	5.08	123.45	119.90
27	B8	792	A	O4'-C1'-N9	5.08	112.26	108.20
27	B8	1574	C	N3-C4-C5	-5.08	119.87	121.90
1	AA	660	C	N3-C4-C5	-5.08	119.87	121.90
1	AA	1208	C	N3-C4-C5	-5.08	119.87	121.90
1	AA	1275	A	C5-C6-N6	-5.08	119.64	123.70
3	AV	59	A	C5-C6-N1	-5.08	115.16	117.70
27	B8	242	G	P-O3'-C3'	5.08	125.79	119.70
27	B8	958	U	O4'-C1'-N1	5.08	112.26	108.20
27	B8	2366	A	C5-C6-N6	-5.08	119.64	123.70
27	B8	2822	G	O4'-C1'-N9	5.08	112.26	108.20
1	AA	744	C	N3-C4-C5	-5.07	119.87	121.90
1	AA	802	A	C5-C6-N1	-5.07	115.16	117.70
1	AA	878	A	C5-C6-N1	-5.07	115.16	117.70
1	AA	1218	C	N3-C4-C5	-5.07	119.87	121.90
27	B8	581	C	N3-C4-C5	-5.07	119.87	121.90
27	B8	1395	A	C5-C6-N6	-5.07	119.64	123.70
27	B8	2795	C	N3-C4-C5	-5.07	119.87	121.90
1	AA	704	A	C5-C6-N1	-5.07	115.16	117.70
1	AA	864	A	O4'-C1'-N9	5.07	112.26	108.20
1	AA	1112	C	N3-C4-C5	-5.07	119.87	121.90
27	B8	1515	A	C4-C5-C6	5.07	119.54	117.00
27	B8	2003	A	C5-C6-N1	-5.07	115.16	117.70
27	B8	2015	A	C5-C6-N1	-5.07	115.16	117.70
27	B8	2705	A	C5-C6-N1	-5.07	115.16	117.70
1	AA	389	A	C5-C6-N1	-5.07	115.17	117.70
1	AA	685	G	N3-C2-N2	5.07	123.45	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	799	G	O4'-C1'-N9	5.07	112.26	108.20
26	B7	24	G	N3-C2-N2	5.07	123.45	119.90
27	B8	675	A	C5-C6-N6	-5.07	119.64	123.70
27	B8	676	A	C5-C6-N1	-5.07	115.17	117.70
27	B8	1749	A	C5-C6-N6	-5.07	119.64	123.70
27	B8	1791	A	C5-C6-N1	-5.07	115.17	117.70
27	B8	2392	A	C5-C6-N1	-5.07	115.17	117.70
1	AA	181	A	C5-C6-N1	-5.07	115.17	117.70
27	B8	2115	G	N3-C2-N2	5.07	123.45	119.90
1	AA	353	A	C5-C6-N1	-5.07	115.17	117.70
1	AA	890	G	O4'-C1'-N9	5.07	112.25	108.20
1	AA	1476	A	C5-C6-N6	-5.07	119.65	123.70
27	B8	204	A	C4-C5-C6	5.07	119.53	117.00
27	B8	916	G	O4'-C1'-N9	5.07	112.25	108.20
27	B8	2080	A	O4'-C1'-N9	5.07	112.25	108.20
1	AA	746	A	C5-C6-N1	-5.07	115.17	117.70
26	B7	28	C	N3-C4-C5	-5.07	119.87	121.90
27	B8	353	C	N3-C4-C5	-5.07	119.87	121.90
27	B8	374	A	C5-C6-N6	-5.07	119.65	123.70
27	B8	893	C	N3-C4-N4	5.07	121.55	118.00
27	B8	1545	A	O4'-C1'-N9	5.07	112.25	108.20
27	B8	2090	A	O4'-C1'-N9	5.07	112.25	108.20
27	B8	2224	G	N3-C2-N2	5.07	123.45	119.90
1	AA	523	A	O4'-C1'-N9	5.06	112.25	108.20
1	AA	595	A	O4'-C1'-N9	5.06	112.25	108.20
3	AV	25	G	O4'-C1'-N9	5.06	112.25	108.20
27	B8	721	A	O4'-C1'-N9	5.06	112.25	108.20
27	B8	735	A	O4'-C1'-N9	5.06	112.25	108.20
1	AA	187	G	O4'-C1'-N9	5.06	112.25	108.20
1	AA	561	U	P-O3'-C3'	5.06	125.78	119.70
1	AA	1037	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	267	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	310	A	C5-C6-N6	-5.06	119.65	123.70
27	B8	745	G	O4'-C1'-N9	5.06	112.25	108.20
27	B8	1502	A	O4'-C1'-N9	5.06	112.25	108.20
27	B8	1635	A	C5-C6-N1	-5.06	115.17	117.70
27	B8	2004	G	O4'-C1'-N9	5.06	112.25	108.20
27	B8	2733	A	C5-C6-N6	-5.06	119.65	123.70
1	AA	553	A	C5-C6-N1	-5.06	115.17	117.70
1	AA	1388	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	644	A	O4'-C1'-N9	5.06	112.25	108.20
27	B8	679	C	N3-C4-C5	-5.06	119.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	1241	A	C5-C6-N1	-5.06	115.17	117.70
27	B8	1462	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	2354	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	2446	G	O4'-C1'-N9	5.06	112.25	108.20
1	AA	334	C	N3-C4-C5	-5.06	119.88	121.90
1	AA	525	C	N3-C4-C5	-5.06	119.88	121.90
1	AA	1268	G	N3-C2-N2	5.06	123.44	119.90
27	B8	117	G	N3-C2-N2	5.06	123.44	119.90
27	B8	687	C	N3-C4-N4	5.06	121.54	118.00
27	B8	723	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	880	G	O4'-C1'-N9	5.06	112.25	108.20
27	B8	1196	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	2169	A	C5-C6-N1	-5.06	115.17	117.70
27	B8	2729	G	C5'-C4'-O4'	5.06	115.17	109.10
1	AA	698	G	O4'-C1'-N9	5.06	112.25	108.20
1	AA	841	C	N3-C4-C5	-5.06	119.88	121.90
26	B7	109	A	C5-C6-N1	-5.06	115.17	117.70
27	B8	517	C	N3-C4-C5	-5.06	119.88	121.90
27	B8	1336	A	C5'-C4'-O4'	5.06	115.17	109.10
1	AA	1304	G	N3-C2-N2	5.06	123.44	119.90
27	B8	139	U	O4'-C1'-N1	5.06	112.25	108.20
27	B8	439	A	C5-C6-N6	-5.06	119.66	123.70
27	B8	478	A	C5-C6-N1	-5.06	115.17	117.70
27	B8	1668	A	C5-C6-N6	-5.06	119.66	123.70
1	AA	207	C	N3-C4-C5	-5.05	119.88	121.90
1	AA	300	A	C5-C6-N1	-5.05	115.17	117.70
1	AA	617	G	O4'-C1'-N9	5.05	112.24	108.20
1	AA	795	C	N3-C4-N4	5.05	121.54	118.00
1	AA	816	A	C5-C6-N1	-5.05	115.17	117.70
1	AA	1102	A	C5-C6-N6	-5.05	119.66	123.70
1	AA	1124	G	N3-C2-N2	5.05	123.44	119.90
1	AA	1300	G	O4'-C1'-N9	5.05	112.24	108.20
27	B8	791	C	N3-C4-N4	5.05	121.54	118.00
27	B8	1047	G	N3-C2-N2	5.05	123.44	119.90
27	B8	2880	C	N3-C4-C5	-5.05	119.88	121.90
27	B8	556	A	C5-C6-N1	-5.05	115.17	117.70
27	B8	892	A	C5-C6-N1	-5.05	115.17	117.70
27	B8	1814	G	N3-C2-N2	5.05	123.44	119.90
27	B8	2452	C	N3-C4-C5	-5.05	119.88	121.90
27	B8	1021	A	C5-C6-N1	-5.05	115.17	117.70
27	B8	1508	A	C5-C6-N1	-5.05	115.17	117.70
27	B8	1848	A	C5-C6-N6	-5.05	119.66	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	2379	G	O4'-C1'-N9	5.05	112.24	108.20
1	AA	329	A	C5-C6-N6	-5.05	119.66	123.70
1	AA	1447	A	O4'-C1'-N9	5.05	112.24	108.20
27	B8	1030	C	N3-C4-C5	-5.05	119.88	121.90
27	B8	2197	U	P-O3'-C3'	5.05	125.76	119.70
27	B8	2676	C	N3-C4-C5	-5.05	119.88	121.90
1	AA	120	A	C5-C6-N1	-5.05	115.18	117.70
27	B8	654	A	C5-C6-N1	-5.05	115.18	117.70
27	B8	1266	G	P-O3'-C3'	5.05	125.76	119.70
27	B8	1575	C	N3-C4-C5	-5.05	119.88	121.90
27	B8	1654	A	O4'-C1'-N9	5.05	112.24	108.20
27	B8	2154	A	O4'-C1'-N9	5.05	112.24	108.20
27	B8	2559	C	N3-C4-C5	-5.05	119.88	121.90
1	AA	26	A	O4'-C1'-N9	5.05	112.24	108.20
1	AA	43	C	N3-C4-C5	-5.05	119.88	121.90
1	AA	169	C	N3-C4-N4	5.05	121.53	118.00
1	AA	345	C	N3-C4-N4	5.05	121.53	118.00
1	AA	554	A	C5-C6-N6	-5.05	119.66	123.70
1	AA	738	C	N3-C4-C5	-5.05	119.88	121.90
1	AA	1125	U	O4'-C1'-N1	5.05	112.24	108.20
27	B8	127	A	O4'-C1'-N9	5.05	112.24	108.20
27	B8	345	A	C5-C6-N1	-5.05	115.18	117.70
27	B8	1612	C	N3-C4-C5	-5.05	119.88	121.90
27	B8	2567	G	O4'-C1'-N9	5.05	112.24	108.20
27	B8	2589	A	O4'-C1'-N9	5.05	112.24	108.20
27	B8	1282	U	P-O3'-C3'	5.04	125.75	119.70
27	B8	1919	A	O4'-C1'-N9	5.04	112.24	108.20
27	B8	2199	A	O4'-C1'-N9	5.04	112.24	108.20
1	AA	1012	A	O4'-C1'-N9	5.04	112.23	108.20
1	AA	1289	A	C5-C6-N1	-5.04	115.18	117.70
27	B8	933	A	C5-C6-N6	-5.04	119.67	123.70
1	AA	1263	C	N3-C4-C5	-5.04	119.88	121.90
27	B8	103	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	927	A	C5-C6-N1	-5.04	115.18	117.70
27	B8	1393	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	1494	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	1656	C	N3-C4-C5	-5.04	119.88	121.90
27	B8	1919	A	C5-C6-N1	-5.04	115.18	117.70
27	B8	2054	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	2283	C	N3-C4-C5	-5.04	119.88	121.90
27	B8	2433	A	O4'-C1'-N9	5.04	112.23	108.20
27	B8	2886	A	C5-C6-N1	-5.04	115.18	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	251	G	O4'-C1'-N9	5.04	112.23	108.20
1	AA	1124	G	O4'-C1'-N9	5.04	112.23	108.20
1	AA	1166	G	O4'-C1'-N9	5.04	112.23	108.20
27	B8	1177	G	O4'-C1'-N9	5.04	112.23	108.20
27	B8	2366	A	C5-C6-N1	-5.04	115.18	117.70
1	AA	129	A	C5-C6-N6	-5.04	119.67	123.70
1	AA	690	G	N3-C2-N2	5.04	123.43	119.90
1	AA	1357	A	C5-C6-N1	-5.04	115.18	117.70
27	B8	181	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	787	C	N3-C4-C5	-5.04	119.89	121.90
27	B8	1691	C	N3-C4-C5	-5.04	119.89	121.90
27	B8	2006	C	N3-C4-C5	-5.04	119.89	121.90
27	B8	2014	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	2767	C	N3-C4-C5	-5.04	119.89	121.90
27	B8	2879	A	O4'-C1'-N9	5.04	112.23	108.20
40	BL	113	ALA	N-CA-CB	5.04	117.15	110.10
1	AA	687	A	C5-C6-N1	-5.04	115.18	117.70
1	AA	766	A	C5-C6-N6	-5.04	119.67	123.70
1	AA	1256	A	C5-C6-N1	-5.04	115.18	117.70
27	B8	972	A	O4'-C1'-N9	5.04	112.23	108.20
27	B8	1652	A	C5-C6-N6	-5.04	119.67	123.70
1	AA	183	C	C6-N1-C1'	-5.04	114.76	120.80
1	AA	784	A	O4'-C1'-N9	5.04	112.23	108.20
26	B7	71	C	N3-C4-C5	-5.04	119.89	121.90
27	B8	279	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	975	A	C5-C6-N6	-5.04	119.67	123.70
27	B8	2052	A	C5-C6-N6	-5.04	119.67	123.70
1	AA	77	A	C5-C6-N1	-5.03	115.18	117.70
1	AA	130	A	C5-C6-N1	-5.03	115.18	117.70
1	AA	281	G	N3-C2-N2	5.03	123.42	119.90
1	AA	483	C	O4'-C1'-N1	5.03	112.23	108.20
1	AA	883	C	N3-C4-C5	-5.03	119.89	121.90
27	B8	886	A	C5-C6-N6	-5.03	119.67	123.70
1	AA	1292	G	O4'-C1'-N9	5.03	112.22	108.20
27	B8	791	C	N3-C4-C5	-5.03	119.89	121.90
1	AA	194	C	N3-C4-C5	-5.03	119.89	121.90
1	AA	370	C	N3-C4-N4	5.03	121.52	118.00
1	AA	400	C	N3-C4-C5	-5.03	119.89	121.90
1	AA	511	C	N3-C4-C5	-5.03	119.89	121.90
1	AA	914	A	C5-C6-N1	-5.03	115.19	117.70
1	AA	1219	A	C5-C6-N1	-5.03	115.18	117.70
26	B7	59	A	C5-C6-N1	-5.03	115.19	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	394	C	N3-C4-C5	-5.03	119.89	121.90
27	B8	1492	G	O4'-C1'-N9	5.03	112.22	108.20
27	B8	1785	A	C5-C6-N1	-5.03	115.19	117.70
1	AA	495	A	P-O3'-C3'	5.03	125.73	119.70
1	AA	860	A	C5-C6-N6	-5.03	119.68	123.70
1	AA	914	A	C5-C6-N6	-5.03	119.68	123.70
27	B8	478	A	O4'-C1'-N9	5.03	112.22	108.20
27	B8	2250	G	O4'-C1'-N9	5.03	112.22	108.20
1	AA	618	C	N3-C4-N4	5.03	121.52	118.00
26	B7	26	C	N3-C4-C5	-5.03	119.89	121.90
26	B7	72	G	O4'-C1'-N9	5.03	112.22	108.20
27	B8	5	A	C5-C6-N1	-5.03	115.19	117.70
27	B8	1093	G	N3-C2-N2	5.03	123.42	119.90
27	B8	1728	C	N3-C4-C5	-5.03	119.89	121.90
27	B8	1771	C	N3-C4-C5	-5.03	119.89	121.90
27	B8	1802	A	C5-C6-N6	-5.03	119.68	123.70
27	B8	2304	G	O4'-C1'-N9	5.03	112.22	108.20
26	B7	107	G	C5'-C4'-O4'	5.03	115.13	109.10
27	B8	422	A	C5-C6-N1	-5.03	115.19	117.70
27	B8	858	G	N3-C2-N2	5.03	123.42	119.90
27	B8	1032	A	C5-C6-N6	-5.03	119.68	123.70
27	B8	2140	G	O4'-C1'-N9	5.03	112.22	108.20
27	B8	2700	A	C5-C6-N1	-5.03	115.19	117.70
1	AA	370	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	486	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	911	A	C5-C6-N1	-5.02	115.19	117.70
27	B8	1230	A	C5-C6-N1	-5.02	115.19	117.70
27	B8	2108	A	C5-C6-N6	-5.02	119.68	123.70
1	AA	65	A	O4'-C1'-N9	5.02	112.22	108.20
1	AA	393	A	O4'-C1'-N9	5.02	112.22	108.20
1	AA	1225	A	C5-C6-N6	-5.02	119.68	123.70
27	B8	335	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	602	A	C5-C6-N1	-5.02	115.19	117.70
27	B8	1830	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	2278	A	O4'-C1'-N9	5.02	112.22	108.20
27	B8	2538	C	N3-C4-C5	-5.02	119.89	121.90
1	AA	274	A	C5-C6-N1	-5.02	115.19	117.70
1	AA	1246	A	C5-C6-N6	-5.02	119.68	123.70
27	B8	157	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	247	G	N3-C2-N2	5.02	123.42	119.90
27	B8	2032	G	O4'-C1'-N9	5.02	112.22	108.20
3	AV	23	G	O4'-C1'-N9	5.02	112.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AV	33	A	C5-C6-N1	-5.02	115.19	117.70
26	B7	97	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	244	A	C5-C6-N6	-5.02	119.68	123.70
27	B8	435	C	N3-C4-N4	5.02	121.51	118.00
27	B8	781	A	C5-C6-N6	-5.02	119.69	123.70
27	B8	816	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	1284	A	C5-C6-N1	-5.02	115.19	117.70
27	B8	1635	A	O4'-C1'-N9	5.02	112.22	108.20
27	B8	2645	G	O4'-C1'-N9	5.02	112.22	108.20
27	B8	228	C	N3-C4-C5	-5.02	119.89	121.90
1	AA	586	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	654	A	C5-C6-N6	-5.02	119.69	123.70
27	B8	1565	C	N3-C4-C5	-5.02	119.89	121.90
27	B8	2349	G	C5-C6-O6	-5.02	125.59	128.60
1	AA	221	C	N3-C4-C5	-5.01	119.89	121.90
1	AA	316	C	N3-C4-C5	-5.01	119.89	121.90
1	AA	583	A	C5-C6-N1	-5.01	115.19	117.70
1	AA	1170	A	C5-C6-N1	-5.01	115.19	117.70
27	B8	301	G	P-O3'-C3'	5.01	125.72	119.70
27	B8	548	G	O4'-C1'-N9	5.01	112.21	108.20
27	B8	800	A	C5-C6-N6	-5.01	119.69	123.70
27	B8	936	A	O4'-C1'-N9	5.01	112.21	108.20
27	B8	1029	A	O4'-C1'-N9	5.01	112.21	108.20
27	B8	1335	C	N3-C4-C5	-5.01	119.89	121.90
27	B8	2050	C	N3-C4-C5	-5.01	119.89	121.90
1	AA	939	G	O4'-C1'-N9	5.01	112.21	108.20
27	B8	2501	C	N3-C4-C5	-5.01	119.89	121.90
1	AA	83	C	N3-C4-C5	-5.01	119.89	121.90
1	AA	152	A	O4'-C1'-N9	5.01	112.21	108.20
1	AA	1329	A	C5-C6-N6	-5.01	119.69	123.70
27	B8	1526	C	N3-C4-C5	-5.01	119.89	121.90
27	B8	1972	G	O4'-C1'-N9	5.01	112.21	108.20
27	B8	240	C	N3-C4-C5	-5.01	119.90	121.90
27	B8	722	A	C5-C6-N1	-5.01	115.19	117.70
27	B8	1329	U	O4'-C1'-N1	5.01	112.21	108.20
27	B8	2657	A	O4'-C1'-N9	5.01	112.21	108.20
1	AA	232	G	N3-C2-N2	5.01	123.41	119.90
27	B8	1027	A	O4'-C1'-N9	5.01	112.21	108.20
27	B8	1469	A	C5-C6-N6	-5.01	119.69	123.70
27	B8	1828	G	O4'-C1'-N9	5.01	112.21	108.20
27	B8	2740	A	C5-C6-N1	-5.01	115.20	117.70
27	B8	116	C	N3-C4-N4	5.01	121.50	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B8	249	C	N3-C4-N4	5.01	121.50	118.00
27	B8	582	A	C5-C6-N1	-5.01	115.20	117.70
27	B8	883	G	O4'-C1'-N9	5.01	112.20	108.20
27	B8	912	C	N3-C4-C5	-5.01	119.90	121.90
27	B8	1997	C	N3-C4-C5	-5.01	119.90	121.90
27	B8	2232	C	N3-C4-C5	-5.01	119.90	121.90
27	B8	2782	G	O4'-C1'-N9	5.01	112.21	108.20
27	B8	2860	A	O4'-C1'-N9	5.01	112.20	108.20
1	AA	349	A	O4'-C1'-N9	5.00	112.20	108.20
1	AA	1249	C	N3-C4-C5	-5.00	119.90	121.90
27	B8	532	A	C5-C6-N1	-5.00	115.20	117.70
27	B8	2338	C	N3-C4-C5	-5.00	119.90	121.90
27	B8	2614	A	C5-C6-N1	-5.00	115.20	117.70
27	B8	2750	A	O4'-C1'-N9	5.00	112.20	108.20
1	AA	782	A	C5-C6-N1	-5.00	115.20	117.70
27	B8	299	A	O4'-C1'-N9	5.00	112.20	108.20
27	B8	1155	A	O4'-C1'-N9	5.00	112.20	108.20
27	B8	1743	G	O4'-C1'-N9	5.00	112.20	108.20
27	B8	2474	U	C2-N1-C1'	5.00	123.70	117.70
27	B8	2901	C	N3-C4-C5	-5.00	119.90	121.90
1	AA	386	C	N3-C4-C5	-5.00	119.90	121.90
1	AA	578	C	N3-C4-C5	-5.00	119.90	121.90
1	AA	1142	G	N1-C6-O6	5.00	122.90	119.90
27	B8	423	A	C5-C6-N1	-5.00	115.20	117.70
27	B8	758	C	N3-C4-C5	-5.00	119.90	121.90
27	B8	2263	C	N3-C4-C5	-5.00	119.90	121.90
27	B8	2298	A	C5-C6-N6	-5.00	119.70	123.70
27	B8	2319	G	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (189) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A1	237	THR	Peptide
1	AA	102	G	Sidechain
1	AA	1024	G	Sidechain
1	AA	1027	C	Sidechain
1	AA	1044	A	Sidechain
1	AA	1094	G	Sidechain
1	AA	1095	U	Sidechain
1	AA	1101	A	Sidechain
1	AA	1125	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1129	C	Sidechain
1	AA	1131	G	Sidechain
1	AA	1139	G	Sidechain
1	AA	1144	G	Sidechain
1	AA	115	G	Sidechain
1	AA	1179	A	Sidechain
1	AA	1226	C	Sidechain
1	AA	1268	G	Sidechain
1	AA	1269	A	Sidechain
1	AA	1289	A	Sidechain
1	AA	1299	A	Sidechain
1	AA	13	U	Sidechain
1	AA	130	A	Sidechain
1	AA	1323	G	Sidechain
1	AA	1346	A	Sidechain
1	AA	1347	G	Sidechain
1	AA	1417	G	Sidechain
1	AA	1418	A	Sidechain
1	AA	1465	A	Sidechain
1	AA	1502	A	Sidechain
1	AA	1516	G	Sidechain
1	AA	152	A	Sidechain
1	AA	1526	G	Sidechain
1	AA	1529	G	Sidechain
1	AA	173	U	Sidechain
1	AA	180	U	Sidechain
1	AA	181	A	Sidechain
1	AA	184	G	Sidechain
1	AA	185	U	Sidechain
1	AA	202	G	Sidechain
1	AA	204	G	Sidechain
1	AA	244	U	Sidechain
1	AA	262	A	Sidechain
1	AA	265	G	Sidechain
1	AA	298	A	Sidechain
1	AA	315	A	Sidechain
1	AA	353	A	Sidechain
1	AA	378	G	Sidechain
1	AA	380	G	Sidechain
1	AA	439	U	Sidechain
1	AA	450	G	Sidechain
1	AA	454	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	496	A	Sidechain
1	AA	527	G	Sidechain
1	AA	557	G	Sidechain
1	AA	565	U	Sidechain
1	AA	566	G	Sidechain
1	AA	581	G	Sidechain
1	AA	587	G	Sidechain
1	AA	588	G	Sidechain
1	AA	620	C	Sidechain
1	AA	622	A	Sidechain
1	AA	69	G	Sidechain
1	AA	718	A	Sidechain
1	AA	728	A	Sidechain
1	AA	752	G	Sidechain
1	AA	874	G	Sidechain
1	AA	883	C	Sidechain
1	AA	884	U	Sidechain
1	AA	927	G	Sidechain
1	AA	95	C	Sidechain
1	AA	960	U	Sidechain
1	AA	974	A	Sidechain
1	AA	978	A	Sidechain
7	AC	218	LYS	Peptide
12	AH	14	ARG	Sidechain
13	AI	6	TYR	Sidechain
3	AV	53	G	Sidechain
3	AV	7	G	Sidechain
57	B2	12	ARG	Sidechain
26	B7	111	U	Sidechain
26	B7	5	U	Sidechain
27	B8	1025	G	Sidechain
27	B8	1027	A	Sidechain
27	B8	1070	A	Sidechain
27	B8	1084	A	Sidechain
27	B8	1095	A	Sidechain
27	B8	1099	G	Sidechain
27	B8	1130	U	Sidechain
27	B8	1138	G	Sidechain
27	B8	120	U	Sidechain
27	B8	1204	A	Sidechain
27	B8	1224	U	Sidechain
27	B8	1235	G	Sidechain

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Mol	Chain	Res	Type	Group
27	B8	1236	G	Sidechain
27	B8	1296	G	Sidechain
27	B8	1327	A	Sidechain
27	B8	1334	G	Sidechain
27	B8	1360	G	Sidechain
27	B8	1383	A	Sidechain
27	B8	1394	U	Sidechain
27	B8	1427	A	Sidechain
27	B8	1515	A	Sidechain
27	B8	1517	G	Sidechain
27	B8	1530	G	Sidechain
27	B8	1573	G	Sidechain
27	B8	161	A	Sidechain
27	B8	1672	A	Sidechain
27	B8	1680	U	Sidechain
27	B8	1682	G	Sidechain
27	B8	1699	G	Sidechain
27	B8	1738	G	Sidechain
27	B8	1743	G	Sidechain
27	B8	1784	A	Sidechain
27	B8	1813	G	Sidechain
27	B8	1846	G	Sidechain
27	B8	1904	G	Sidechain
27	B8	1920	C	Sidechain
27	B8	1927	A	Sidechain
27	B8	1952	A	Sidechain
27	B8	1954	G	Sidechain
27	B8	2005	A	Sidechain
27	B8	205	G	Sidechain
27	B8	2125	G	Sidechain
27	B8	2143	C	Sidechain
27	B8	2148	G	Sidechain
27	B8	2155	U	Sidechain
27	B8	2272	U	Sidechain
27	B8	2345	G	Sidechain
27	B8	2365	G	Sidechain
27	B8	2382	G	Sidechain
27	B8	2460	U	Sidechain
27	B8	2471	A	Sidechain
27	B8	250	G	Sidechain
27	B8	2517	C	Sidechain
27	B8	2580	U	Sidechain

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Mol	Chain	Res	Type	Group
27	B8	2596	U	Sidechain
27	B8	261	G	Sidechain
27	B8	2637	U	Sidechain
27	B8	265	A	Sidechain
27	B8	2689	U	Sidechain
27	B8	27	G	Sidechain
27	B8	2746	U	Sidechain
27	B8	2756	U	Sidechain
27	B8	2857	G	Sidechain
27	B8	2858	C	Sidechain
27	B8	2866	U	Sidechain
27	B8	2903	U	Sidechain
27	B8	303	G	Sidechain
27	B8	346	A	Sidechain
27	B8	362	A	Sidechain
27	B8	370	G	Sidechain
27	B8	395	U	Sidechain
27	B8	428	A	Sidechain
27	B8	445	C	Sidechain
27	B8	446	G	Sidechain
27	B8	457	A	Sidechain
27	B8	467	G	Sidechain
27	B8	480	A	Sidechain
27	B8	505	A	Sidechain
27	B8	507	A	Sidechain
27	B8	532	A	Sidechain
27	B8	569	U	Sidechain
27	B8	60	G	Sidechain
27	B8	630	G	Sidechain
27	B8	642	U	Sidechain
27	B8	674	G	Sidechain
27	B8	675	A	Sidechain
27	B8	676	A	Sidechain
27	B8	684	G	Sidechain
27	B8	705	A	Sidechain
27	B8	712	G	Sidechain
27	B8	72	U	Sidechain
27	B8	728	G	Sidechain
27	B8	738	G	Sidechain
27	B8	773	U	Sidechain
27	B8	821	A	Sidechain
27	B8	849	A	Sidechain

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Mol	Chain	Res	Type	Group
27	B8	858	G	Sidechain
27	B8	877	A	Sidechain
27	B8	899	A	Sidechain
27	B8	959	A	Sidechain
28	BA	181	ARG	Peptide
28	BA	198	GLY	Peptide
28	BA	293	TRP	Peptide
28	BA	314	GLN	Peptide
28	BA	72	LEU	Peptide
34	BF	137	PHE	Peptide
36	BH	31	VAL	Peptide
49	BU	48	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	33080	0	16649	21	0
2	AX	231	0	120	0	0
3	AV	1649	0	834	1	0
4	AZ	779	0	798	4	0
5	A0	1640	0	1641	0	0
5	A1	1640	0	1641	0	0
6	AB	1872	0	1885	3	0
7	AC	1822	0	1913	2	0
8	AD	1643	0	1710	1	0
9	AE	1225	0	1273	1	0
10	AF	1101	0	1050	1	0
11	AG	1400	0	1449	0	0
12	AH	979	0	1034	1	0
13	AI	1036	0	1084	0	0
14	AJ	825	0	865	2	0
15	AK	965	0	997	0	0
16	AL	955	0	1019	2	0
17	AM	910	0	981	0	0
18	AN	805	0	847	1	0
19	AO	716	0	742	0	0
20	AP	649	0	666	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	AQ	672	0	716	1	0
22	AR	626	0	651	0	0
23	AS	727	0	769	0	0
24	AT	670	0	722	2	0
25	AU	590	0	631	1	0
26	B7	2570	0	1301	0	0
27	B8	62341	0	31354	41	0
28	BA	3362	0	3511	38	0
29	BB	889	0	982	1	0
30	B5	1733	0	1824	1	0
31	B6	2092	0	2170	2	0
32	BD	1565	0	1616	1	0
33	BE	1552	0	1619	1	0
34	BF	1420	0	1460	1	0
35	BG	1323	0	1374	0	0
36	BH	1111	0	1148	2	0
37	BI	1032	0	1088	0	0
38	BJ	1129	0	1162	0	0
39	BK	947	0	1023	0	0
40	BL	1053	0	1129	1	0
41	BM	1074	0	1157	1	0
42	BN	1008	0	1045	1	0
43	BO	900	0	935	0	0
44	BP	917	0	965	0	0
45	BQ	947	0	1022	0	0
46	BR	816	0	839	1	0
47	BS	857	0	922	0	0
48	BT	787	0	846	0	0
49	BU	789	0	847	0	0
50	BV	753	0	780	0	0
51	BW	634	0	656	0	0
52	BX	625	0	655	0	0
53	BY	509	0	543	0	0
54	BZ	449	0	491	0	0
55	B0	444	0	461	0	0
56	B1	441	0	485	2	0
57	B2	377	0	418	1	0
58	B3	504	0	574	1	0
59	B4	302	0	343	0	0
60	A0	1078	0	1694	1	0
60	A1	1225	0	1925	4	0
60	AZ	245	0	385	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	B8	294	0	462	2	0
60	BA	1568	0	2464	34	0
60	BB	539	0	847	0	0
61	A0	510	0	760	0	0
61	A1	204	0	304	2	0
61	AZ	102	0	152	0	0
61	B8	51	0	76	0	0
61	BA	408	0	608	1	0
61	BB	357	0	532	0	0
All	All	163040	0	119641	141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BA:416:PHE:CE1	28:BA:416:PHE:CD1	1.92	1.58
28:BA:416:PHE:CD2	28:BA:416:PHE:CE2	1.95	1.54
28:BA:416:PHE:CZ	28:BA:416:PHE:CE2	1.95	1.53
28:BA:416:PHE:CE1	28:BA:416:PHE:CZ	1.95	1.51
28:BA:416:PHE:CD1	28:BA:416:PHE:CG	1.98	1.49
28:BA:416:PHE:CD2	28:BA:416:PHE:CG	2.01	1.46
28:BA:416:PHE:CG	60:BA:533:PEV:H401	1.82	1.13
28:BA:416:PHE:CD2	60:BA:533:PEV:C39	2.32	1.12
28:BA:416:PHE:CE2	60:BA:533:PEV:C39	2.33	1.12
28:BA:416:PHE:CD1	60:BA:533:PEV:C39	2.33	1.12
28:BA:416:PHE:CE2	60:BA:533:PEV:C40	2.33	1.12
28:BA:416:PHE:CD2	60:BA:533:PEV:H392	1.84	1.12
28:BA:416:PHE:CG	60:BA:533:PEV:C40	2.33	1.12
28:BA:416:PHE:CD1	60:BA:533:PEV:C40	2.33	1.11
28:BA:416:PHE:CD2	60:BA:533:PEV:H402	1.85	1.11
28:BA:416:PHE:CZ	60:BA:533:PEV:C40	2.33	1.11
28:BA:416:PHE:CE1	60:BA:533:PEV:C39	2.33	1.11
28:BA:416:PHE:CD2	60:BA:533:PEV:C40	2.32	1.11
28:BA:416:PHE:CZ	60:BA:533:PEV:C39	2.33	1.11
28:BA:416:PHE:CE1	60:BA:533:PEV:C40	2.34	1.11
28:BA:416:PHE:CG	60:BA:533:PEV:C39	2.33	1.10
28:BA:416:PHE:CG	60:BA:533:PEV:H391	1.86	1.10
28:BA:416:PHE:CE2	60:BA:533:PEV:H402	1.91	1.04
28:BA:416:PHE:CD1	60:BA:533:PEV:H391	1.94	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BA:416:PHE:CE2	60:BA:533:PEV:H392	1.96	1.01
28:BA:416:PHE:CD1	60:BA:533:PEV:H401	1.97	0.99
60:BA:533:PEV:C40	60:BA:533:PEV:C39	2.52	0.87
4:AZ:81:LEU:HD13	4:AZ:82:GLY:H	1.53	0.72
28:BA:324:ALA:HB2	60:BA:531:PEV:H402	1.73	0.70
28:BA:416:PHE:CZ	60:BA:533:PEV:C38	2.77	0.68
28:BA:416:PHE:CE1	60:BA:533:PEV:C38	2.79	0.65
28:BA:416:PHE:CZ	60:BA:533:PEV:H381	2.33	0.63
28:BA:416:PHE:CE1	60:BA:533:PEV:C41	2.82	0.62
28:BA:416:PHE:CZ	60:BA:533:PEV:C41	2.85	0.59
28:BA:416:PHE:CE1	60:BA:533:PEV:H381	2.39	0.57
27:B8:2091:C:H3'	27:B8:2092:U:H5''	1.87	0.56
27:B8:1021:A:H61	27:B8:1142:A:H61	1.53	0.56
3:AV:27:A:H61	3:AV:45:G:H1	1.52	0.55
27:B8:1024:G:H3'	27:B8:1025:G:H5''	1.88	0.55
1:AA:664:G:H22	1:AA:741:G:H1	1.54	0.55
27:B8:500:G:H21	27:B8:505:A:H62	1.55	0.55
27:B8:2792:A:H3'	27:B8:2793:C:H5''	1.90	0.53
27:B8:871:U:H3	27:B8:906:U:H3	1.56	0.53
27:B8:962:G:H21	27:B8:2250:G:H1	1.57	0.53
27:B8:870:U:H2'	27:B8:871:U:H5''	1.90	0.53
61:BA:512:PGV:H72	60:BA:513:PEV:H401	1.91	0.53
27:B8:1083:U:HO2'	27:B8:1084:A:H8	1.58	0.51
14:AJ:15:HIS:CD2	14:AJ:16:ARG:HE	2.29	0.51
1:AA:507:C:H3'	1:AA:508:U:H5''	1.92	0.50
4:AZ:39:LEU:HD13	28:BA:286:PHE:HB3	1.93	0.50
60:B8:3001:PEV:H401	60:B8:3002:PEV:H401	1.92	0.50
21:AQ:18:LYS:H	21:AQ:50:ASN:HD21	1.59	0.50
25:AU:33:ARG:HE	25:AU:34:ARG:H	1.59	0.50
1:AA:1239:A:H62	1:AA:1299:A:H62	1.60	0.50
27:B8:1065:U:H3	27:B8:1069:A:H2'	1.76	0.49
1:AA:1305:G:H21	1:AA:1332:A:H8	1.59	0.49
36:BH:126:GLY:H	36:BH:128:HIS:CE1	2.30	0.49
27:B8:713:G:H21	27:B8:718:A:H2	1.60	0.49
1:AA:82:G:H3'	1:AA:83:C:H4'	1.95	0.49
28:BA:416:PHE:CZ	60:BA:533:PEV:H411	2.48	0.49
1:AA:632:U:H3'	1:AA:633:G:H5'	1.95	0.49
27:B8:870:U:C2'	27:B8:871:U:H5''	2.43	0.48
1:AA:243:A:H4'	1:AA:244:U:H5'	1.94	0.48
27:B8:1551:A:H3'	27:B8:1552:A:H5''	1.95	0.48
9:AE:89:THR:HG22	9:AE:90:GLY:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:BA:503:PEV:H401	60:BA:503:PEV:H442	1.95	0.48
20:AP:54:LEU:H	20:AP:54:LEU:HD12	1.78	0.48
1:AA:1122:U:H5''	7:AC:222:GLN:H	1.78	0.48
28:BA:416:PHE:CE1	60:BA:533:PEV:H411	2.48	0.48
12:AH:60:LEU:H	12:AH:60:LEU:HD23	1.79	0.48
20:AP:78:VAL:HG23	20:AP:81:ALA:H	1.79	0.48
24:AT:67:HIS:CD2	24:AT:69:ASN:H	2.32	0.47
60:A1:301:PEV:H392	61:A1:303:PGV:H02	1.96	0.47
27:B8:82:U:H3	27:B8:104:A:H61	1.63	0.47
30:B5:165:ASN:HD21	30:B5:169:GLY:H	1.63	0.47
1:AA:1223:C:H3'	1:AA:1224:U:C5'	2.45	0.47
58:B3:36:ALA:H	58:B3:39:ARG:HE	1.62	0.47
60:A0:315:PEV:H391	60:A1:302:PEV:H401	1.96	0.47
27:B8:957:C:H42	27:B8:2494:G:H21	1.61	0.47
27:B8:2091:C:H3'	27:B8:2092:U:C5'	2.46	0.46
36:BH:101:ASP:H	36:BH:111:ALA:HB3	1.80	0.46
4:AZ:25:LEU:CB	28:BA:333:THR:HG23	2.46	0.46
27:B8:2371:G:H21	56:B1:45:HIS:HE1	1.63	0.46
27:B8:63:A:H2'	27:B8:64:A:C8	2.51	0.46
60:A1:323:PEV:H392	60:A1:323:PEV:H142	1.97	0.46
27:B8:2171:A:H1'	27:B8:2172:U:C6	2.50	0.45
27:B8:480:A:H3'	27:B8:481:G:H5''	1.98	0.45
1:AA:262:A:H4'	24:AT:67:HIS:CD2	2.52	0.44
60:A1:319:PEV:H392	60:A1:319:PEV:H361	1.91	0.44
27:B8:2371:G:H21	56:B1:45:HIS:CE1	2.35	0.44
27:B8:890:C:H3'	27:B8:891:G:H4'	2.00	0.44
6:AB:14:HIS:CE1	6:AB:200:PRO:HB3	2.53	0.44
1:AA:973:G:H3'	1:AA:974:A:H5''	1.99	0.44
27:B8:1203:U:H3'	27:B8:1204:A:H5''	1.99	0.44
10:AF:94:HIS:CG	10:AF:95:ALA:H	2.37	0.43
8:AD:96:ARG:HB2	8:AD:99:ASN:HD22	1.82	0.43
1:AA:404:G:H1	1:AA:499:A:H62	1.65	0.43
32:BD:33:ARG:HH11	32:BD:93:GLY:H	1.67	0.43
27:B8:1273:U:H3	27:B8:2002:G:H21	1.67	0.43
27:B8:2874:C:H4'	42:BN:4:ARG:HH21	1.84	0.43
27:B8:532:A:H4'	27:B8:533:G:C8	2.54	0.43
57:B2:24:THR:HG23	57:B2:27:GLY:H	1.84	0.43
27:B8:572:A:H5''	46:BR:80:ARG:HH21	1.84	0.43
27:B8:1567:G:H5'	31:B6:57:HIS:CD2	2.54	0.43
27:B8:2682:A:C2	27:B8:2683:C:C5	3.06	0.42
6:AB:103:TRP:HE1	6:AB:107:ARG:HH21	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B8:1205:A:C5	33:BE:165:HIS:HB3	2.54	0.42
27:B8:880:G:H2'	27:B8:881:G:C8	2.55	0.42
29:BB:123:THR:HA	29:BB:126:ARG:HH12	1.84	0.42
27:B8:877:A:C2	27:B8:901:C:C2	3.08	0.42
27:B8:1391:U:H2'	27:B8:1393:A:C2	2.53	0.42
34:BF:106:ALA:HA	34:BF:111:ARG:HH11	1.85	0.42
31:B6:264:LYS:H	31:B6:264:LYS:HD2	1.85	0.42
27:B8:962:G:N2	27:B8:2250:G:H1	2.17	0.42
1:AA:413:G:H4'	1:AA:414:A:H5''	2.02	0.42
6:AB:169:HIS:H	6:AB:169:HIS:CD2	2.37	0.42
27:B8:2233:U:H2'	27:B8:2234:G:C8	2.55	0.42
1:AA:995:C:H2'	1:AA:996:A:H5''	2.02	0.42
27:B8:900:A:H2'	27:B8:901:C:H5'	2.02	0.41
16:AL:41:PRO:HG2	16:AL:45:ASN:H	1.85	0.41
1:AA:537:G:H5''	16:AL:109:ARG:HH12	1.85	0.41
1:AA:1130:A:H61	1:AA:1144:G:H1'	1.86	0.41
1:AA:1144:G:N2	1:AA:1146:A:H62	2.19	0.41
27:B8:1082:U:N3	27:B8:1086:A:C2	2.88	0.41
1:AA:412:A:H3'	1:AA:413:G:C5'	2.51	0.41
60:BA:514:PEV:H391	60:BA:514:PEV:H362	1.94	0.41
27:B8:1283:G:H22	27:B8:1286:A:H5'	1.85	0.41
27:B8:251:A:H4'	40:BL:49:GLY:HA2	2.02	0.41
27:B8:2351:G:H2'	27:B8:2365:G:H22	1.84	0.41
4:AZ:25:LEU:HB3	28:BA:333:THR:HG23	2.03	0.41
61:A1:315:PGV:H132	61:A1:315:PGV:H102	1.98	0.41
1:AA:781:A:H2'	1:AA:782:A:H5'	2.02	0.41
60:B8:3002:PEV:H362	60:B8:3002:PEV:H392	1.94	0.41
27:B8:2645:G:H3'	27:B8:2646:C:H5'	2.02	0.41
1:AA:1118:U:H1'	1:AA:1179:A:C4	2.55	0.41
14:AJ:15:HIS:HA	14:AJ:18:ILE:HG22	2.01	0.40
60:BA:520:PEV:H402	60:BA:526:PEV:H441	2.04	0.40
7:AC:10:ARG:HH21	7:AC:175:HIS:HA	1.85	0.40
1:AA:483:C:H2'	1:AA:484:G:C8	2.57	0.40
18:AN:60:ARG:HE	18:AN:60:ARG:HA	1.86	0.40
41:BM:78:LEU:HD23	41:BM:78:LEU:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AZ	96/98 (98%)	74 (77%)	13 (14%)	9 (9%)	1	16
5	A0	198/200 (99%)	174 (88%)	20 (10%)	4 (2%)	9	51
5	A1	198/200 (99%)	169 (85%)	23 (12%)	6 (3%)	5	42
6	AB	238/240 (99%)	190 (80%)	42 (18%)	6 (2%)	7	46
7	AC	230/232 (99%)	184 (80%)	31 (14%)	15 (6%)	1	25
8	AD	203/205 (99%)	163 (80%)	28 (14%)	12 (6%)	2	27
9	AE	164/166 (99%)	137 (84%)	21 (13%)	6 (4%)	4	37
10	AF	133/135 (98%)	109 (82%)	22 (16%)	2 (2%)	13	57
11	AG	176/178 (99%)	142 (81%)	29 (16%)	5 (3%)	6	44
12	AH	127/129 (98%)	102 (80%)	23 (18%)	2 (2%)	12	56
13	AI	127/129 (98%)	108 (85%)	11 (9%)	8 (6%)	2	25
14	AJ	101/103 (98%)	85 (84%)	9 (9%)	7 (7%)	1	23
15	AK	126/128 (98%)	106 (84%)	15 (12%)	5 (4%)	4	35
16	AL	121/123 (98%)	108 (89%)	12 (10%)	1 (1%)	24	69
17	AM	115/117 (98%)	96 (84%)	13 (11%)	6 (5%)	2	30
18	AN	98/100 (98%)	81 (83%)	9 (9%)	8 (8%)	1	18
19	AO	86/88 (98%)	79 (92%)	5 (6%)	2 (2%)	8	48
20	AP	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	7	46
21	AQ	81/83 (98%)	67 (83%)	8 (10%)	6 (7%)	1	21
22	AR	72/74 (97%)	59 (82%)	9 (12%)	4 (6%)	2	28
23	AS	89/91 (98%)	73 (82%)	12 (14%)	4 (4%)	3	33
24	AT	84/86 (98%)	76 (90%)	7 (8%)	1 (1%)	16	61
25	AU	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
28	BA	433/435 (100%)	313 (72%)	66 (15%)	54 (12%)	0	8
29	BB	114/116 (98%)	96 (84%)	12 (10%)	6 (5%)	2	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	B5	232/234 (99%)	211 (91%)	15 (6%)	6 (3%)	7	45
31	B6	270/272 (99%)	227 (84%)	31 (12%)	12 (4%)	3	33
32	BD	207/209 (99%)	172 (83%)	24 (12%)	11 (5%)	2	29
33	BE	199/201 (99%)	169 (85%)	20 (10%)	10 (5%)	3	31
34	BF	176/178 (99%)	137 (78%)	27 (15%)	12 (7%)	1	23
35	BG	174/176 (99%)	137 (79%)	28 (16%)	9 (5%)	2	30
36	BH	147/149 (99%)	108 (74%)	31 (21%)	8 (5%)	2	29
37	BI	139/141 (99%)	125 (90%)	11 (8%)	3 (2%)	8	49
38	BJ	140/142 (99%)	117 (84%)	19 (14%)	4 (3%)	6	43
39	BK	121/123 (98%)	99 (82%)	16 (13%)	6 (5%)	3	31
40	BL	142/144 (99%)	129 (91%)	10 (7%)	3 (2%)	9	50
41	BM	134/136 (98%)	107 (80%)	17 (13%)	10 (8%)	1	21
42	BN	125/127 (98%)	104 (83%)	12 (10%)	9 (7%)	1	22
43	BO	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	7	45
44	BP	112/114 (98%)	94 (84%)	11 (10%)	7 (6%)	2	25
45	BQ	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	2	30
46	BR	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	3	31
47	BS	108/110 (98%)	81 (75%)	18 (17%)	9 (8%)	1	18
48	BT	98/100 (98%)	71 (72%)	20 (20%)	7 (7%)	1	22
49	BU	101/103 (98%)	84 (83%)	14 (14%)	3 (3%)	5	42
50	BV	92/94 (98%)	82 (89%)	9 (10%)	1 (1%)	17	63
51	BW	82/84 (98%)	59 (72%)	19 (23%)	4 (5%)	3	31
52	BX	75/77 (97%)	57 (76%)	12 (16%)	6 (8%)	1	19
53	BY	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	5	40
54	BZ	56/58 (97%)	49 (88%)	4 (7%)	3 (5%)	2	29
55	B0	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	10	52
56	B1	52/54 (96%)	46 (88%)	5 (10%)	1 (2%)	10	52
57	B2	44/46 (96%)	31 (70%)	10 (23%)	3 (7%)	1	23
58	B3	62/64 (97%)	52 (84%)	9 (14%)	1 (2%)	12	56
59	B4	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6	44
All	All	7128/7238 (98%)	5877 (82%)	904 (13%)	347 (5%)	5	31

All (347) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AZ	48	TRP
4	AZ	61	VAL
4	AZ	81	LEU
5	A1	177	ARG
7	AC	206	ILE
7	AC	219	PRO
9	AE	17	VAL
13	AI	127	SER
14	AJ	57	VAL
14	AJ	67	ILE
17	AM	3	ILE
18	AN	80	ARG
28	BA	48	VAL
28	BA	56	GLN
28	BA	68	SER
28	BA	72	LEU
28	BA	79	ALA
28	BA	148	LEU
28	BA	200	PRO
28	BA	237	VAL
28	BA	249	ALA
28	BA	275	ILE
28	BA	314	GLN
28	BA	319	LEU
28	BA	332	TYR
28	BA	353	VAL
28	BA	358	PRO
28	BA	373	LEU
29	BB	67	ALA
31	B6	132	ARG
31	B6	197	ALA
31	B6	231	HIS
31	B6	261	ARG
33	BE	4	VAL
34	BF	82	TYR
34	BF	136	ILE
35	BG	2	ARG
35	BG	94	ARG
36	BH	32	PRO
36	BH	115	VAL
38	BJ	40	HIS
39	BK	71	ARG

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Mol	Chain	Res	Type
41	BM	43	ALA
41	BM	56	ALA
41	BM	122	ALA
44	BP	25	VAL
45	BQ	71	ASN
46	BR	3	ALA
46	BR	48	LYS
46	BR	101	ILE
47	BS	76	VAL
48	BT	35	ALA
48	BT	36	LYS
48	BT	99	ALA
49	BU	49	PRO
4	AZ	49	MET
6	AB	95	TRP
6	AB	224	ARG
7	AC	190	THR
8	AD	7	LYS
10	AF	85	ILE
11	AG	77	ARG
12	AH	73	SER
14	AJ	85	ASP
15	AK	11	VAL
16	AL	54	VAL
17	AM	29	SER
17	AM	87	GLY
18	AN	21	ALA
21	AQ	12	VAL
21	AQ	13	SER
21	AQ	81	ALA
22	AR	24	ASP
23	AS	28	LYS
28	BA	235	VAL
28	BA	256	ARG
28	BA	267	LEU
28	BA	308	LEU
28	BA	320	LEU
28	BA	333	THR
28	BA	340	ARG
28	BA	351	ALA
28	BA	362	THR
28	BA	363	ALA

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Mol	Chain	Res	Type
28	BA	369	VAL
28	BA	371	THR
28	BA	401	PHE
28	BA	431	SER
29	BB	19	TRP
29	BB	71	PHE
31	B6	142	ASN
32	BD	31	ALA
32	BD	46	ARG
32	BD	107	VAL
33	BE	12	LEU
33	BE	30	GLN
34	BF	74	ALA
34	BF	84	ILE
34	BF	103	ILE
34	BF	138	PRO
37	BI	87	SER
40	BL	113	ALA
41	BM	55	ARG
41	BM	72	PRO
41	BM	73	ILE
41	BM	135	VAL
42	BN	63	ARG
44	BP	106	ALA
45	BQ	101	ASP
46	BR	65	ALA
47	BS	12	SER
47	BS	53	SER
47	BS	89	ALA
48	BT	72	GLN
53	BY	2	LYS
53	BY	37	LEU
4	AZ	109	ASP
5	A0	170	LEU
5	A1	228	SER
7	AC	53	ARG
7	AC	106	ARG
7	AC	116	ALA
8	AD	6	PRO
8	AD	21	LYS
8	AD	146	GLU
8	AD	176	LYS

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Mol	Chain	Res	Type
9	AE	120	HIS
11	AG	80	GLY
11	AG	138	GLU
12	AH	116	ARG
13	AI	35	GLU
13	AI	59	LYS
14	AJ	17	LEU
17	AM	105	ALA
19	AO	87	ARG
20	AP	54	LEU
23	AS	86	LYS
28	BA	57	ARG
28	BA	71	ALA
28	BA	78	PHE
28	BA	145	MET
28	BA	236	PHE
28	BA	254	GLY
28	BA	260	ALA
28	BA	278	ILE
28	BA	356	ILE
28	BA	391	MET
28	BA	432	ALA
29	BB	45	ALA
29	BB	69	VAL
30	B5	87	ALA
30	B5	159	GLY
31	B6	112	GLY
31	B6	152	GLN
31	B6	189	ALA
31	B6	205	GLY
32	BD	65	ALA
32	BD	140	HIS
32	BD	175	LEU
33	BE	16	GLU
33	BE	130	LYS
33	BE	154	ASP
34	BF	42	ALA
34	BF	77	LYS
34	BF	123	GLY
34	BF	124	ARG
35	BG	21	GLN
36	BH	14	SER

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Mol	Chain	Res	Type
36	BH	75	LEU
36	BH	84	ALA
38	BJ	111	LYS
39	BK	36	GLY
40	BL	53	GLY
42	BN	13	ASN
42	BN	122	ALA
43	BO	89	ASP
43	BO	113	ALA
44	BP	54	LEU
44	BP	113	LEU
48	BT	97	GLY
50	BV	44	HIS
51	BW	27	GLY
51	BW	41	GLY
51	BW	52	CYS
52	BX	27	ARG
52	BX	32	LEU
54	BZ	8	GLN
54	BZ	10	ARG
57	B2	23	ALA
57	B2	35	ARG
4	AZ	55	LEU
4	AZ	101	GLN
5	A0	154	ALA
5	A1	71	PHE
5	A1	164	ALA
6	AB	74	ALA
7	AC	82	ASP
8	AD	20	LEU
8	AD	28	ASP
8	AD	35	GLN
8	AD	36	ALA
8	AD	174	ALA
9	AE	9	GLU
10	AF	114	ASP
13	AI	121	ARG
14	AJ	78	GLU
15	AK	2	LYS
17	AM	16	ILE
18	AN	38	GLU
18	AN	68	ARG

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Mol	Chain	Res	Type
21	AQ	15	LYS
21	AQ	51	GLU
22	AR	2	ARG
22	AR	26	ALA
23	AS	55	GLN
23	AS	87	LYS
28	BA	39	ILE
28	BA	42	PRO
28	BA	151	ASN
28	BA	214	ASP
28	BA	346	LEU
28	BA	352	PHE
28	BA	435	LYS
30	B5	52	ALA
30	B5	82	ALA
30	B5	89	ALA
30	B5	147	PRO
31	B6	214	GLY
31	B6	240	GLY
32	BD	122	VAL
32	BD	203	VAL
33	BE	106	LYS
35	BG	31	GLU
35	BG	47	ASN
37	BI	97	VAL
38	BJ	68	LYS
39	BK	113	MET
40	BL	66	PHE
41	BM	134	THR
42	BN	10	LEU
42	BN	32	GLU
42	BN	80	PHE
42	BN	121	LYS
43	BO	16	ARG
44	BP	35	SER
44	BP	81	ASP
45	BQ	9	ALA
46	BR	27	ILE
47	BS	31	GLN
47	BS	64	ALA
49	BU	12	VAL
49	BU	75	ALA

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Mol	Chain	Res	Type
52	BX	15	ASN
54	BZ	29	ARG
57	B2	8	SER
4	AZ	72	ASP
4	AZ	94	ILE
5	A1	157	ASP
6	AB	28	PRO
6	AB	33	ALA
7	AC	9	ILE
7	AC	47	ALA
7	AC	61	LYS
7	AC	128	MET
7	AC	218	LYS
8	AD	47	LEU
8	AD	147	LYS
9	AE	44	ARG
11	AG	2	ARG
11	AG	4	ARG
14	AJ	59	LYS
15	AK	101	ALA
17	AM	116	LYS
18	AN	28	ALA
18	AN	43	ALA
18	AN	66	THR
19	AO	73	ASP
24	AT	47	GLN
28	BA	61	ILE
28	BA	330	PHE
29	BB	65	GLY
32	BD	9	VAL
32	BD	109	VAL
33	BE	2	GLU
33	BE	83	VAL
33	BE	96	VAL
34	BF	148	VAL
35	BG	100	ASN
35	BG	136	ASP
35	BG	155	PRO
36	BH	55	GLU
36	BH	87	GLU
39	BK	92	GLU
39	BK	122	VAL

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Mol	Chain	Res	Type
41	BM	67	VAL
42	BN	72	ASP
44	BP	76	HIS
45	BQ	27	ARG
45	BQ	81	GLY
47	BS	32	ALA
47	BS	40	ASN
48	BT	10	VAL
52	BX	41	SER
56	B1	33	LEU
5	A0	47	LEU
5	A0	156	VAL
6	AB	132	GLU
7	AC	111	ASP
7	AC	205	GLU
7	AC	213	VAL
13	AI	58	GLU
13	AI	109	GLN
13	AI	110	VAL
14	AJ	48	ARG
15	AK	12	ARG
22	AR	14	ALA
28	BA	337	PHE
31	B6	59	GLN
34	BF	111	ARG
35	BG	156	TYR
36	BH	41	LYS
37	BI	30	GLN
41	BM	70	ASP
42	BN	100	CYS
48	BT	29	THR
52	BX	3	VAL
52	BX	6	VAL
55	B0	44	ALA
58	B3	53	ASP
5	A1	227	VAL
13	AI	57	VAL
18	AN	33	VAL
59	B4	16	ILE
9	AE	15	ILE
20	AP	36	VAL
39	BK	35	VAL

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Mol	Chain	Res	Type
45	BQ	33	VAL
9	AE	105	ILE
15	AK	88	PRO
21	AQ	11	VAL
28	BA	306	ILE
28	BA	403	GLY
32	BD	152	PRO
38	BJ	96	ARG
28	BA	318	VAL
51	BW	73	PRO
47	BS	45	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AZ	85/85 (100%)	72 (85%)	13 (15%)	3	22
5	A0	176/176 (100%)	174 (99%)	2 (1%)	80	91
5	A1	176/176 (100%)	173 (98%)	3 (2%)	68	87
6	AB	198/198 (100%)	194 (98%)	4 (2%)	63	85
7	AC	189/189 (100%)	183 (97%)	6 (3%)	46	76
8	AD	172/172 (100%)	166 (96%)	6 (4%)	43	74
9	AE	125/125 (100%)	122 (98%)	3 (2%)	57	82
10	AF	116/116 (100%)	111 (96%)	5 (4%)	35	70
11	AG	146/146 (100%)	146 (100%)	0	100	100
12	AH	104/104 (100%)	101 (97%)	3 (3%)	50	78
13	AI	106/106 (100%)	101 (95%)	5 (5%)	32	68
14	AJ	90/90 (100%)	88 (98%)	2 (2%)	60	83
15	AK	98/98 (100%)	95 (97%)	3 (3%)	47	77
16	AL	103/103 (100%)	102 (99%)	1 (1%)	82	92
17	AM	95/95 (100%)	92 (97%)	3 (3%)	46	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AN	83/83 (100%)	81 (98%)	2 (2%)	57	82
19	AO	76/76 (100%)	74 (97%)	2 (3%)	54	80
20	AP	65/65 (100%)	65 (100%)	0	100	100
21	AQ	77/77 (100%)	74 (96%)	3 (4%)	39	72
22	AR	64/64 (100%)	63 (98%)	1 (2%)	70	88
23	AS	78/78 (100%)	78 (100%)	0	100	100
24	AT	65/65 (100%)	65 (100%)	0	100	100
25	AU	60/60 (100%)	58 (97%)	2 (3%)	45	76
28	BA	353/353 (100%)	326 (92%)	27 (8%)	16	53
29	BB	92/92 (100%)	88 (96%)	4 (4%)	35	70
30	B5	181/181 (100%)	178 (98%)	3 (2%)	68	87
31	B6	217/217 (100%)	212 (98%)	5 (2%)	58	82
32	BD	164/164 (100%)	158 (96%)	6 (4%)	41	73
33	BE	165/165 (100%)	164 (99%)	1 (1%)	90	95
34	BF	149/149 (100%)	145 (97%)	4 (3%)	52	79
35	BG	137/137 (100%)	134 (98%)	3 (2%)	60	83
36	BH	114/114 (100%)	108 (95%)	6 (5%)	28	64
37	BI	109/109 (100%)	106 (97%)	3 (3%)	51	78
38	BJ	116/116 (100%)	113 (97%)	3 (3%)	54	80
39	BK	104/104 (100%)	99 (95%)	5 (5%)	31	67
40	BL	103/103 (100%)	102 (99%)	1 (1%)	82	92
41	BM	109/109 (100%)	109 (100%)	0	100	100
42	BN	103/103 (100%)	100 (97%)	3 (3%)	50	78
43	BO	87/87 (100%)	87 (100%)	0	100	100
44	BP	99/99 (100%)	96 (97%)	3 (3%)	48	77
45	BQ	89/89 (100%)	89 (100%)	0	100	100
46	BR	84/84 (100%)	84 (100%)	0	100	100
47	BS	93/93 (100%)	93 (100%)	0	100	100
48	BT	84/84 (100%)	79 (94%)	5 (6%)	24	60
49	BU	84/84 (100%)	82 (98%)	2 (2%)	57	82
50	BV	78/78 (100%)	77 (99%)	1 (1%)	76	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	BW	62/62 (100%)	61 (98%)	1 (2%)	70	88
52	BX	67/67 (100%)	66 (98%)	1 (2%)	72	88
53	BY	55/55 (100%)	54 (98%)	1 (2%)	66	87
54	BZ	48/48 (100%)	47 (98%)	1 (2%)	61	84
55	B0	47/47 (100%)	46 (98%)	1 (2%)	61	84
56	B1	48/48 (100%)	47 (98%)	1 (2%)	61	84
57	B2	38/38 (100%)	37 (97%)	1 (3%)	54	80
58	B3	51/51 (100%)	50 (98%)	1 (2%)	63	85
59	B4	34/34 (100%)	34 (100%)	0	100	100
All	All	5911/5911 (100%)	5749 (97%)	162 (3%)	56	79

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AZ	28	ILE
4	AZ	54	ARG
4	AZ	60	LEU
4	AZ	71	ASN
4	AZ	75	ARG
4	AZ	78	ILE
4	AZ	79	LEU
4	AZ	81	LEU
4	AZ	95	ILE
4	AZ	97	THR
4	AZ	99	ILE
4	AZ	107	ARG
4	AZ	115	HIS
5	A0	132	GLN
5	A0	133	LYS
5	A1	112	MET
5	A1	132	GLN
5	A1	237	THR
6	AB	103	TRP
6	AB	164	ASP
6	AB	169	HIS
6	AB	174	GLU
7	AC	106	ARG
7	AC	114	LEU
7	AC	131	ARG

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Mol	Chain	Res	Type
7	AC	214	GLU
7	AC	219	PRO
7	AC	225	LYS
8	AD	13	ARG
8	AD	20	LEU
8	AD	43	ARG
8	AD	110	ARG
8	AD	170	LEU
8	AD	182	LYS
9	AE	75	LEU
9	AE	89	THR
9	AE	150	GLU
10	AF	16	GLU
10	AF	44	ARG
10	AF	47	LEU
10	AF	104	LYS
10	AF	107	ASP
12	AH	2	MET
12	AH	26	MET
12	AH	123	GLU
13	AI	17	ARG
13	AI	40	ARG
13	AI	44	ARG
13	AI	58	GLU
13	AI	129	ARG
14	AJ	31	ARG
14	AJ	81	GLU
15	AK	10	ARG
15	AK	75	GLU
15	AK	79	LYS
16	AL	50	LYS
17	AM	69	ARG
17	AM	91	ARG
17	AM	113	LYS
18	AN	53	ASP
18	AN	64	ARG
19	AO	16	ARG
19	AO	87	ARG
21	AQ	5	ARG
21	AQ	17	GLU
21	AQ	26	ARG
22	AR	11	ARG

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Mol	Chain	Res	Type
25	AU	18	PHE
25	AU	69	LEU
28	BA	53	LEU
28	BA	55	GLN
28	BA	85	TYR
28	BA	130	PHE
28	BA	180	GLU
28	BA	189	ILE
28	BA	192	PHE
28	BA	195	ILE
28	BA	212	GLN
28	BA	228	PHE
28	BA	237	VAL
28	BA	252	GLN
28	BA	256	ARG
28	BA	290	ILE
28	BA	309	TYR
28	BA	317	TYR
28	BA	336	VAL
28	BA	340	ARG
28	BA	347	LYS
28	BA	352	PHE
28	BA	356	ILE
28	BA	357	ARG
28	BA	361	GLN
28	BA	372	ARG
28	BA	373	LEU
28	BA	374	THR
28	BA	441	TYR
29	BB	44	ARG
29	BB	76	ARG
29	BB	77	THR
29	BB	104	MET
30	B5	7	ARG
30	B5	9	ARG
30	B5	166	ASP
31	B6	129	LEU
31	B6	212	TRP
31	B6	227	VAL
31	B6	264	LYS
31	B6	269	ARG
32	BD	74	GLU

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Mol	Chain	Res	Type
32	BD	84	LEU
32	BD	86	GLU
32	BD	124	ARG
32	BD	128	ARG
32	BD	201	LEU
33	BE	60	TRP
34	BF	80	GLN
34	BF	119	LYS
34	BF	129	MET
34	BF	136	ILE
35	BG	34	ARG
35	BG	61	TRP
35	BG	94	ARG
36	BH	8	LYS
36	BH	21	VAL
36	BH	32	PRO
36	BH	70	GLU
36	BH	109	GLU
36	BH	144	VAL
37	BI	10	LEU
37	BI	35	MET
37	BI	95	ASP
38	BJ	23	LYS
38	BJ	35	ARG
38	BJ	129	GLU
39	BK	41	ILE
39	BK	70	ARG
39	BK	89	ASN
39	BK	114	LYS
39	BK	121	GLU
40	BL	126	ARG
42	BN	8	ARG
42	BN	49	GLU
42	BN	64	ARG
44	BP	43	GLU
44	BP	50	ARG
44	BP	87	ARG
48	BT	36	LYS
48	BT	61	LEU
48	BT	66	LYS
48	BT	69	ARG
48	BT	96	VAL

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Mol	Chain	Res	Type
49	BU	49	PRO
49	BU	91	LYS
50	BV	46	LYS
51	BW	23	LYS
52	BX	26	ARG
53	BY	27	ASN
54	BZ	55	LYS
55	B0	31	LYS
56	B1	27	ARG
57	B2	12	ARG
58	B3	6	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
6	AB	14	HIS
6	AB	169	HIS
6	AB	189	ASN
7	AC	175	HIS
7	AC	215	GLN
8	AD	40	HIS
8	AD	99	ASN
14	AJ	15	HIS
15	AK	108	ASN
16	AL	71	HIS
18	AN	48	GLN
20	AP	9	HIS
20	AP	18	GLN
21	AQ	50	ASN
22	AR	53	GLN
23	AS	13	HIS
24	AT	60	GLN
24	AT	67	HIS
28	BA	55	GLN
28	BA	212	GLN
31	B6	52	HIS
31	B6	57	HIS
31	B6	229	HIS
31	B6	238	ASN
33	BE	92	HIS
35	BG	100	ASN
35	BG	115	GLN

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Mol	Chain	Res	Type
36	BH	2	GLN
36	BH	20	ASN
36	BH	128	HIS
36	BH	133	GLN
38	BJ	80	HIS
38	BJ	132	HIS
39	BK	5	GLN
39	BK	89	ASN
42	BN	16	HIS
43	BO	34	HIS
45	BQ	13	HIS
46	BR	82	HIS
46	BR	87	GLN
50	BV	88	HIS
52	BX	35	HIS
55	B0	18	HIS
58	B3	42	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1541/1542 (99%)	273 (17%)	23 (1%)
2	AX	10/11 (90%)	5 (50%)	0
26	B7	119/120 (99%)	19 (15%)	2 (1%)
27	B8	2903/2904 (99%)	442 (15%)	47 (1%)
3	AV	76/77 (98%)	14 (18%)	1 (1%)
All	All	4649/4654 (99%)	753 (16%)	73 (1%)

All (753) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	5	U
1	AA	7	A
1	AA	9	G
1	AA	15	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C

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Mol	Chain	Res	Type
1	AA	51	A
1	AA	52	C
1	AA	55	A
1	AA	61	G
1	AA	66	A
1	AA	67	C
1	AA	70	U
1	AA	71	A
1	AA	75	G
1	AA	79	G
1	AA	80	A
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	91	U
1	AA	101	A
1	AA	121	U
1	AA	144	G
1	AA	149	A
1	AA	155	A
1	AA	182	A
1	AA	196	A
1	AA	197	A
1	AA	204	G
1	AA	205	A
1	AA	209	U
1	AA	210	C
1	AA	211	G
1	AA	239	U
1	AA	240	G
1	AA	243	A
1	AA	244	U
1	AA	245	U
1	AA	247	G
1	AA	252	U
1	AA	253	A
1	AA	257	G
1	AA	258	G
1	AA	266	G
1	AA	267	C

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Mol	Chain	Res	Type
1	AA	280	C
1	AA	289	G
1	AA	306	A
1	AA	308	C
1	AA	316	C
1	AA	328	C
1	AA	329	A
1	AA	332	G
1	AA	345	C
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	373	A
1	AA	374	A
1	AA	381	C
1	AA	382	A
1	AA	397	A
1	AA	398	U
1	AA	406	G
1	AA	408	A
1	AA	409	U
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	414	A
1	AA	416	G
1	AA	421	U
1	AA	424	G
1	AA	429	U
1	AA	430	A
1	AA	435	A
1	AA	451	A
1	AA	456	A
1	AA	459	A
1	AA	460	A
1	AA	461	A
1	AA	462	G
1	AA	463	U
1	AA	465	A
1	AA	466	A
1	AA	468	A
1	AA	482	A

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Mol	Chain	Res	Type
1	AA	484	G
1	AA	485	U
1	AA	486	U
1	AA	493	A
1	AA	494	G
1	AA	499	A
1	AA	508	U
1	AA	511	C
1	AA	512	U
1	AA	518	C
1	AA	524	G
1	AA	527	G
1	AA	532	A
1	AA	533	A
1	AA	535	A
1	AA	547	A
1	AA	561	U
1	AA	563	A
1	AA	564	C
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	596	A
1	AA	611	C
1	AA	633	G
1	AA	653	U
1	AA	654	G
1	AA	665	A
1	AA	666	G
1	AA	721	G
1	AA	724	G
1	AA	731	G
1	AA	747	A
1	AA	748	G
1	AA	752	G
1	AA	755	G
1	AA	781	A
1	AA	782	A
1	AA	793	U
1	AA	794	A
1	AA	812	G

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Mol	Chain	Res	Type
1	AA	815	A
1	AA	817	C
1	AA	818	G
1	AA	821	G
1	AA	828	U
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	846	G
1	AA	847	G
1	AA	849	G
1	AA	873	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	945	G
1	AA	960	U
1	AA	961	U
1	AA	966	G
1	AA	968	A
1	AA	969	A
1	AA	971	G
1	AA	974	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	981	U
1	AA	993	G
1	AA	994	A
1	AA	996	A
1	AA	1004	A
1	AA	1014	A
1	AA	1015	G
1	AA	1018	G
1	AA	1020	G
1	AA	1028	C
1	AA	1030	U
1	AA	1032	G

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Mol	Chain	Res	Type
1	AA	1034	G
1	AA	1036	A
1	AA	1043	G
1	AA	1050	G
1	AA	1053	G
1	AA	1065	U
1	AA	1066	C
1	AA	1070	U
1	AA	1085	U
1	AA	1086	U
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1112	C
1	AA	1118	U
1	AA	1119	C
1	AA	1124	G
1	AA	1125	U
1	AA	1130	A
1	AA	1133	G
1	AA	1135	U
1	AA	1136	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1143	G
1	AA	1145	A
1	AA	1146	A
1	AA	1152	A
1	AA	1154	G
1	AA	1159	U
1	AA	1160	G
1	AA	1167	A
1	AA	1181	G
1	AA	1184	G
1	AA	1191	A
1	AA	1196	A
1	AA	1197	A
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1215	G

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Mol	Chain	Res	Type
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1238	A
1	AA	1249	C
1	AA	1250	A
1	AA	1258	G
1	AA	1261	A
1	AA	1270	G
1	AA	1279	G
1	AA	1280	A
1	AA	1285	A
1	AA	1286	U
1	AA	1287	A
1	AA	1297	G
1	AA	1300	G
1	AA	1301	U
1	AA	1303	C
1	AA	1305	G
1	AA	1316	G
1	AA	1320	C
1	AA	1323	G
1	AA	1331	G
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1364	U
1	AA	1380	U
1	AA	1399	C
1	AA	1419	G
1	AA	1432	G
1	AA	1446	A
1	AA	1448	C
1	AA	1452	C
1	AA	1454	G
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A
1	AA	1506	U
1	AA	1507	A

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Mol	Chain	Res	Type
1	AA	1517	G
1	AA	1520	C
1	AA	1526	G
1	AA	1528	U
1	AA	1529	G
1	AA	1530	G
1	AA	1535	C
1	AA	1539	C
1	AA	1540	U
1	AA	1541	U
1	AA	1542	A
2	AX	13	C
2	AX	14	G
2	AX	18	C
2	AX	19	U
2	AX	22	A
3	AV	4	C
3	AV	5	A
3	AV	6	C
3	AV	8	U
3	AV	20	G
3	AV	22	A
3	AV	32	C
3	AV	44	G
3	AV	49	C
3	AV	50	G
3	AV	54	G
3	AV	68	G
3	AV	72	C
3	AV	77	A
26	B7	9	G
26	B7	13	G
26	B7	14	U
26	B7	15	A
26	B7	16	G
26	B7	26	C
26	B7	29	A
26	B7	30	C
26	B7	42	C
26	B7	45	A
26	B7	52	A
26	B7	53	A

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Mol	Chain	Res	Type
26	B7	66	A
26	B7	67	G
26	B7	90	C
26	B7	91	C
26	B7	99	A
26	B7	109	A
26	B7	120	U
27	B8	13	A
27	B8	34	U
27	B8	35	G
27	B8	46	G
27	B8	63	A
27	B8	64	A
27	B8	71	A
27	B8	74	A
27	B8	75	G
27	B8	84	A
27	B8	90	U
27	B8	91	A
27	B8	92	U
27	B8	93	G
27	B8	95	A
27	B8	100	U
27	B8	103	A
27	B8	118	A
27	B8	120	U
27	B8	136	G
27	B8	137	U
27	B8	139	U
27	B8	141	G
27	B8	143	C
27	B8	144	A
27	B8	160	A
27	B8	181	A
27	B8	196	A
27	B8	199	A
27	B8	216	A
27	B8	221	A
27	B8	222	A
27	B8	228	C
27	B8	233	A
27	B8	241	A

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Mol	Chain	Res	Type
27	B8	248	G
27	B8	252	G
27	B8	255	A
27	B8	265	A
27	B8	266	G
27	B8	268	C
27	B8	271	G
27	B8	273	G
27	B8	277	G
27	B8	278	A
27	B8	281	C
27	B8	283	G
27	B8	285	G
27	B8	286	U
27	B8	294	A
27	B8	311	A
27	B8	321	U
27	B8	329	G
27	B8	330	A
27	B8	333	G
27	B8	346	A
27	B8	352	A
27	B8	353	C
27	B8	362	A
27	B8	363	G
27	B8	364	C
27	B8	371	A
27	B8	372	G
27	B8	386	G
27	B8	387	U
27	B8	405	U
27	B8	406	G
27	B8	411	G
27	B8	412	A
27	B8	424	G
27	B8	455	C
27	B8	457	A
27	B8	479	A
27	B8	481	G
27	B8	491	G
27	B8	505	A
27	B8	508	A

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Mol	Chain	Res	Type
27	B8	509	C
27	B8	510	C
27	B8	512	G
27	B8	528	A
27	B8	531	C
27	B8	533	G
27	B8	544	C
27	B8	545	U
27	B8	546	U
27	B8	547	A
27	B8	548	G
27	B8	549	G
27	B8	555	G
27	B8	563	A
27	B8	573	U
27	B8	575	A
27	B8	586	A
27	B8	588	U
27	B8	603	A
27	B8	613	A
27	B8	637	A
27	B8	646	U
27	B8	647	G
27	B8	654	A
27	B8	655	A
27	B8	671	C
27	B8	686	U
27	B8	730	A
27	B8	747	U
27	B8	757	G
27	B8	764	A
27	B8	775	G
27	B8	776	G
27	B8	782	A
27	B8	784	G
27	B8	785	G
27	B8	788	A
27	B8	789	A
27	B8	793	A
27	B8	802	A
27	B8	805	G
27	B8	812	C

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Mol	Chain	Res	Type
27	B8	819	A
27	B8	827	U
27	B8	828	U
27	B8	830	G
27	B8	846	U
27	B8	847	U
27	B8	859	G
27	B8	869	G
27	B8	871	U
27	B8	875	G
27	B8	876	C
27	B8	881	G
27	B8	887	U
27	B8	891	G
27	B8	896	A
27	B8	897	C
27	B8	900	A
27	B8	901	C
27	B8	910	A
27	B8	912	C
27	B8	919	U
27	B8	931	U
27	B8	932	U
27	B8	941	A
27	B8	945	A
27	B8	946	C
27	B8	961	C
27	B8	973	A
27	B8	974	G
27	B8	980	A
27	B8	982	C
27	B8	983	A
27	B8	985	C
27	B8	991	C
27	B8	995	C
27	B8	996	A
27	B8	1005	C
27	B8	1012	U
27	B8	1013	C
27	B8	1022	G
27	B8	1025	G
27	B8	1033	U

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Mol	Chain	Res	Type
27	B8	1054	A
27	B8	1056	G
27	B8	1061	U
27	B8	1062	G
27	B8	1070	A
27	B8	1071	G
27	B8	1078	U
27	B8	1088	A
27	B8	1090	A
27	B8	1095	A
27	B8	1096	A
27	B8	1104	C
27	B8	1112	G
27	B8	1116	G
27	B8	1130	U
27	B8	1132	U
27	B8	1133	A
27	B8	1134	A
27	B8	1135	C
27	B8	1136	G
27	B8	1139	G
27	B8	1142	A
27	B8	1176	U
27	B8	1206	G
27	B8	1237	A
27	B8	1238	G
27	B8	1241	A
27	B8	1242	U
27	B8	1248	G
27	B8	1250	G
27	B8	1253	A
27	B8	1256	G
27	B8	1266	G
27	B8	1271	G
27	B8	1272	A
27	B8	1273	U
27	B8	1275	A
27	B8	1276	A
27	B8	1300	G
27	B8	1301	A
27	B8	1312	U
27	B8	1313	U

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Mol	Chain	Res	Type
27	B8	1316	U
27	B8	1325	U
27	B8	1326	U
27	B8	1334	G
27	B8	1336	A
27	B8	1337	G
27	B8	1352	U
27	B8	1365	A
27	B8	1374	G
27	B8	1379	U
27	B8	1386	C
27	B8	1394	U
27	B8	1396	U
27	B8	1416	G
27	B8	1419	A
27	B8	1420	A
27	B8	1421	G
27	B8	1427	A
27	B8	1428	C
27	B8	1451	C
27	B8	1454	C
27	B8	1459	G
27	B8	1460	U
27	B8	1461	C
27	B8	1469	A
27	B8	1476	U
27	B8	1477	A
27	B8	1478	G
27	B8	1482	G
27	B8	1490	A
27	B8	1497	U
27	B8	1504	A
27	B8	1505	A
27	B8	1507	C
27	B8	1508	A
27	B8	1509	A
27	B8	1523	U
27	B8	1524	G
27	B8	1532	A
27	B8	1535	A
27	B8	1538	G
27	B8	1552	A

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Mol	Chain	Res	Type
27	B8	1560	G
27	B8	1569	A
27	B8	1578	U
27	B8	1583	A
27	B8	1585	C
27	B8	1608	A
27	B8	1609	A
27	B8	1610	A
27	B8	1618	A
27	B8	1634	A
27	B8	1635	A
27	B8	1640	A
27	B8	1647	U
27	B8	1648	U
27	B8	1654	A
27	B8	1674	G
27	B8	1677	A
27	B8	1700	A
27	B8	1714	U
27	B8	1715	G
27	B8	1729	U
27	B8	1730	C
27	B8	1731	G
27	B8	1733	G
27	B8	1738	G
27	B8	1756	G
27	B8	1758	U
27	B8	1761	C
27	B8	1764	C
27	B8	1773	A
27	B8	1776	G
27	B8	1781	U
27	B8	1782	U
27	B8	1784	A
27	B8	1800	C
27	B8	1801	A
27	B8	1808	A
27	B8	1809	A
27	B8	1816	C
27	B8	1819	A
27	B8	1829	A
27	B8	1870	C

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Mol	Chain	Res	Type
27	B8	1896	G
27	B8	1906	G
27	B8	1913	A
27	B8	1914	C
27	B8	1929	G
27	B8	1930	G
27	B8	1940	U
27	B8	1955	U
27	B8	1965	C
27	B8	1966	A
27	B8	1967	C
27	B8	1970	A
27	B8	1971	U
27	B8	1972	G
27	B8	1991	U
27	B8	1993	U
27	B8	1997	C
27	B8	2020	A
27	B8	2022	U
27	B8	2023	C
27	B8	2031	A
27	B8	2033	A
27	B8	2043	C
27	B8	2055	C
27	B8	2056	G
27	B8	2059	A
27	B8	2061	G
27	B8	2062	A
27	B8	2065	C
27	B8	2069	G
27	B8	2077	A
27	B8	2102	G
27	B8	2104	C
27	B8	2111	U
27	B8	2116	G
27	B8	2117	A
27	B8	2118	U
27	B8	2119	A
27	B8	2120	G
27	B8	2128	G
27	B8	2133	G
27	B8	2135	A

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Mol	Chain	Res	Type
27	B8	2136	G
27	B8	2137	U
27	B8	2138	G
27	B8	2145	C
27	B8	2146	C
27	B8	2147	A
27	B8	2148	G
27	B8	2149	U
27	B8	2153	C
27	B8	2155	U
27	B8	2158	A
27	B8	2164	C
27	B8	2165	C
27	B8	2166	U
27	B8	2167	U
27	B8	2176	A
27	B8	2179	C
27	B8	2181	U
27	B8	2192	U
27	B8	2198	A
27	B8	2199	A
27	B8	2204	G
27	B8	2212	A
27	B8	2213	U
27	B8	2214	C
27	B8	2225	A
27	B8	2238	G
27	B8	2239	G
27	B8	2250	G
27	B8	2251	G
27	B8	2266	A
27	B8	2271	G
27	B8	2278	A
27	B8	2279	G
27	B8	2283	C
27	B8	2286	G
27	B8	2287	A
27	B8	2297	A
27	B8	2305	U
27	B8	2307	G
27	B8	2308	G
27	B8	2311	A

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Mol	Chain	Res	Type
27	B8	2322	A
27	B8	2324	U
27	B8	2325	G
27	B8	2333	A
27	B8	2335	A
27	B8	2336	A
27	B8	2337	G
27	B8	2347	C
27	B8	2357	G
27	B8	2383	G
27	B8	2385	C
27	B8	2396	G
27	B8	2407	A
27	B8	2426	A
27	B8	2429	G
27	B8	2430	A
27	B8	2434	A
27	B8	2441	U
27	B8	2448	A
27	B8	2458	G
27	B8	2472	G
27	B8	2473	U
27	B8	2476	A
27	B8	2478	A
27	B8	2491	U
27	B8	2498	C
27	B8	2505	G
27	B8	2506	U
27	B8	2518	A
27	B8	2529	G
27	B8	2530	A
27	B8	2534	A
27	B8	2535	G
27	B8	2554	U
27	B8	2566	A
27	B8	2567	G
27	B8	2573	C
27	B8	2585	U
27	B8	2586	U
27	B8	2602	A
27	B8	2609	U
27	B8	2613	U

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Mol	Chain	Res	Type
27	B8	2629	U
27	B8	2630	G
27	B8	2689	U
27	B8	2690	U
27	B8	2714	G
27	B8	2726	A
27	B8	2729	G
27	B8	2744	G
27	B8	2748	A
27	B8	2757	A
27	B8	2765	A
27	B8	2778	A
27	B8	2791	G
27	B8	2793	C
27	B8	2799	A
27	B8	2800	A
27	B8	2808	G
27	B8	2809	A
27	B8	2820	A
27	B8	2821	A
27	B8	2832	U
27	B8	2836	U
27	B8	2849	U
27	B8	2850	A
27	B8	2867	G
27	B8	2872	A
27	B8	2873	A
27	B8	2883	A
27	B8	2904	U

All (73) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	51	A
1	AA	60	A
1	AA	85	U
1	AA	243	A
1	AA	279	A
1	AA	328	C
1	AA	366	A
1	AA	372	C
1	AA	428	G

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Mol	Chain	Res	Type
1	AA	429	U
1	AA	484	G
1	AA	653	U
1	AA	700	G
1	AA	960	U
1	AA	1049	U
1	AA	1065	U
1	AA	1159	U
1	AA	1201	A
1	AA	1226	C
1	AA	1300	G
1	AA	1301	U
1	AA	1319	A
1	AA	1541	U
3	AV	16	C
26	B7	14	U
26	B7	66	A
27	B8	91	A
27	B8	241	A
27	B8	320	A
27	B8	329	G
27	B8	507	A
27	B8	670	A
27	B8	792	A
27	B8	827	U
27	B8	858	G
27	B8	876	C
27	B8	880	G
27	B8	890	C
27	B8	891	G
27	B8	973	A
27	B8	984	A
27	B8	1061	U
27	B8	1133	A
27	B8	1205	A
27	B8	1272	A
27	B8	1312	U
27	B8	1608	A
27	B8	1699	G
27	B8	1730	C
27	B8	1786	A
27	B8	1808	A

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Mol	Chain	Res	Type
27	B8	2076	U
27	B8	2116	G
27	B8	2118	U
27	B8	2144	G
27	B8	2145	C
27	B8	2152	G
27	B8	2159	G
27	B8	2164	C
27	B8	2172	U
27	B8	2282	G
27	B8	2286	G
27	B8	2324	U
27	B8	2336	A
27	B8	2402	U
27	B8	2425	A
27	B8	2430	A
27	B8	2491	U
27	B8	2601	C
27	B8	2713	U
27	B8	2756	U
27	B8	2797	U
27	B8	2903	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

133 ligands 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	$\# Z > 2$
60	PEV	A0	301	-	47,48,48	0.78	1 (2%)	48,53,53	0.67	2 (4%)
60	PEV	A0	302	-	47,48,48	0.78	1 (2%)	48,53,53	0.70	2 (4%)
60	PEV	A0	303	-	47,48,48	0.80	2 (4%)	48,53,53	0.69	2 (4%)
61	PGV	A0	304	-	50,50,50	1.08	2 (4%)	51,56,56	0.83	2 (3%)
61	PGV	A0	305	-	50,50,50	1.07	2 (4%)	51,56,56	0.75	2 (3%)
61	PGV	A0	306	-	50,50,50	1.07	2 (4%)	51,56,56	0.77	2 (3%)
60	PEV	A0	307	-	47,48,48	0.78	1 (2%)	48,53,53	0.65	2 (4%)
60	PEV	A0	308	-	47,48,48	0.79	2 (4%)	48,53,53	0.74	2 (4%)
60	PEV	A0	309	-	47,48,48	0.80	2 (4%)	48,53,53	0.69	2 (4%)
60	PEV	A0	310	-	47,48,48	0.79	2 (4%)	48,53,53	0.83	2 (4%)
60	PEV	A0	311	-	47,48,48	0.78	1 (2%)	48,53,53	0.66	2 (4%)
60	PEV	A0	312	-	47,48,48	0.79	1 (2%)	48,53,53	0.60	2 (4%)
60	PEV	A0	313	-	47,48,48	0.81	2 (4%)	48,53,53	0.73	2 (4%)
60	PEV	A0	314	-	47,48,48	0.80	2 (4%)	48,53,53	0.69	2 (4%)
60	PEV	A0	315	-	47,48,48	0.76	1 (2%)	48,53,53	0.63	2 (4%)
60	PEV	A0	316	-	47,48,48	0.80	1 (2%)	48,53,53	0.84	2 (4%)
61	PGV	A0	317	-	50,50,50	1.07	2 (4%)	51,56,56	0.85	2 (3%)
61	PGV	A0	318	-	50,50,50	1.08	2 (4%)	51,56,56	0.76	2 (3%)
60	PEV	A0	319	-	47,48,48	0.79	1 (2%)	48,53,53	0.74	2 (4%)
60	PEV	A0	320	-	47,48,48	0.80	1 (2%)	48,53,53	0.64	2 (4%)
60	PEV	A0	321	-	47,48,48	0.79	1 (2%)	48,53,53	0.80	4 (8%)
60	PEV	A0	322	-	47,48,48	0.79	1 (2%)	48,53,53	0.74	2 (4%)
60	PEV	A0	323	-	47,48,48	0.77	1 (2%)	48,53,53	0.70	2 (4%)
60	PEV	A0	324	-	47,48,48	0.79	1 (2%)	48,53,53	0.71	2 (4%)
61	PGV	A0	325	-	50,50,50	1.08	2 (4%)	51,56,56	0.88	2 (3%)
60	PEV	A0	326	-	47,48,48	0.75	1 (2%)	48,53,53	0.68	2 (4%)
61	PGV	A0	327	-	50,50,50	1.09	2 (4%)	51,56,56	0.73	2 (3%)
61	PGV	A0	328	-	50,50,50	1.07	2 (4%)	51,56,56	0.78	2 (3%)
60	PEV	A0	329	-	47,48,48	0.78	1 (2%)	48,53,53	0.71	2 (4%)
60	PEV	A0	330	-	47,48,48	0.78	1 (2%)	48,53,53	0.64	2 (4%)
61	PGV	A0	331	-	50,50,50	1.07	2 (4%)	51,56,56	0.78	2 (3%)
61	PGV	A0	332	-	50,50,50	1.08	2 (4%)	51,56,56	0.78	2 (3%)
60	PEV	A1	301	-	47,48,48	0.78	2 (4%)	48,53,53	0.71	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	A1	302	-	47,48,48	0.79	2 (4%)	48,53,53	0.70	2 (4%)
61	PGV	A1	303	-	50,50,50	1.07	2 (4%)	51,56,56	0.77	2 (3%)
60	PEV	A1	304	-	47,48,48	0.77	1 (2%)	48,53,53	0.62	2 (4%)
60	PEV	A1	305	-	47,48,48	0.78	1 (2%)	48,53,53	0.68	2 (4%)
60	PEV	A1	306	-	47,48,48	0.79	1 (2%)	48,53,53	0.62	2 (4%)
60	PEV	A1	307	-	47,48,48	0.78	1 (2%)	48,53,53	0.69	2 (4%)
60	PEV	A1	308	-	47,48,48	0.79	2 (4%)	48,53,53	0.64	2 (4%)
60	PEV	A1	309	-	47,48,48	0.79	1 (2%)	48,53,53	0.73	2 (4%)
60	PEV	A1	310	-	47,48,48	0.77	1 (2%)	48,53,53	0.72	2 (4%)
61	PGV	A1	311	-	50,50,50	1.08	2 (4%)	51,56,56	0.82	2 (3%)
60	PEV	A1	312	-	47,48,48	0.79	2 (4%)	48,53,53	0.68	2 (4%)
60	PEV	A1	313	-	47,48,48	0.77	1 (2%)	48,53,53	0.72	2 (4%)
60	PEV	A1	314	-	47,48,48	0.78	1 (2%)	48,53,53	0.69	2 (4%)
61	PGV	A1	315	-	50,50,50	1.09	2 (4%)	51,56,56	0.81	2 (3%)
60	PEV	A1	316	-	47,48,48	0.79	2 (4%)	48,53,53	0.74	2 (4%)
60	PEV	A1	317	-	47,48,48	0.79	2 (4%)	48,53,53	0.69	2 (4%)
61	PGV	A1	318	-	50,50,50	1.08	2 (4%)	51,56,56	0.81	2 (3%)
60	PEV	A1	319	-	47,48,48	0.77	1 (2%)	48,53,53	0.64	1 (2%)
60	PEV	A1	320	-	47,48,48	0.79	2 (4%)	48,53,53	0.71	2 (4%)
60	PEV	A1	321	-	47,48,48	0.79	1 (2%)	48,53,53	0.67	2 (4%)
60	PEV	A1	322	-	47,48,48	0.76	1 (2%)	48,53,53	0.69	2 (4%)
60	PEV	A1	323	-	47,48,48	0.76	1 (2%)	48,53,53	0.66	2 (4%)
60	PEV	A1	324	-	47,48,48	0.79	1 (2%)	48,53,53	0.64	2 (4%)
60	PEV	A1	325	-	47,48,48	0.78	1 (2%)	48,53,53	0.66	2 (4%)
60	PEV	A1	326	-	47,48,48	0.77	1 (2%)	48,53,53	0.68	2 (4%)
60	PEV	A1	327	-	47,48,48	0.77	1 (2%)	48,53,53	0.68	2 (4%)
60	PEV	A1	328	-	47,48,48	0.76	1 (2%)	48,53,53	0.67	2 (4%)
60	PEV	A1	329	-	47,48,48	0.79	1 (2%)	48,53,53	0.71	2 (4%)
60	PEV	AZ	201	-	47,48,48	0.76	1 (2%)	48,53,53	0.70	2 (4%)
60	PEV	AZ	202	-	47,48,48	0.78	1 (2%)	48,53,53	0.71	2 (4%)
60	PEV	AZ	203	-	47,48,48	0.78	1 (2%)	48,53,53	0.61	2 (4%)
60	PEV	AZ	204	-	47,48,48	0.78	1 (2%)	48,53,53	0.68	2 (4%)
61	PGV	AZ	205	-	50,50,50	1.08	2 (4%)	51,56,56	0.78	2 (3%)
60	PEV	AZ	206	-	47,48,48	0.78	1 (2%)	48,53,53	0.61	2 (4%)
61	PGV	AZ	207	-	50,50,50	1.07	2 (4%)	51,56,56	0.77	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	B8	3001	-	47,48,48	0.79	1 (2%)	48,53,53	0.71	2 (4%)
60	PEV	B8	3002	-	47,48,48	0.77	1 (2%)	48,53,53	0.65	2 (4%)
60	PEV	B8	3003	-	47,48,48	0.79	1 (2%)	48,53,53	0.71	2 (4%)
60	PEV	B8	3004	-	47,48,48	0.78	1 (2%)	48,53,53	0.67	2 (4%)
61	PGV	B8	3005	-	50,50,50	1.07	2 (4%)	51,56,56	0.74	2 (3%)
60	PEV	B8	3006	-	47,48,48	0.79	1 (2%)	48,53,53	0.64	2 (4%)
60	PEV	B8	3007	-	47,48,48	0.77	1 (2%)	48,53,53	0.63	2 (4%)
61	PGV	BA	501	-	50,50,50	1.07	2 (4%)	51,56,56	0.82	2 (3%)
60	PEV	BA	502	-	47,48,48	0.78	1 (2%)	48,53,53	0.70	2 (4%)
60	PEV	BA	503	-	47,48,48	0.80	3 (6%)	48,53,53	0.73	2 (4%)
60	PEV	BA	504	-	47,48,48	0.80	2 (4%)	48,53,53	0.79	2 (4%)
61	PGV	BA	505	-	50,50,50	1.07	2 (4%)	51,56,56	0.78	2 (3%)
60	PEV	BA	506	-	47,48,48	0.75	1 (2%)	48,53,53	0.69	2 (4%)
60	PEV	BA	507	-	47,48,48	0.78	1 (2%)	48,53,53	0.68	2 (4%)
60	PEV	BA	508	-	47,48,48	0.78	1 (2%)	48,53,53	0.67	2 (4%)
60	PEV	BA	509	-	47,48,48	0.79	2 (4%)	48,53,53	0.73	2 (4%)
60	PEV	BA	510	-	47,48,48	0.77	1 (2%)	48,53,53	0.68	2 (4%)
60	PEV	BA	511	-	47,48,48	0.74	1 (2%)	48,53,53	0.67	2 (4%)
61	PGV	BA	512	-	50,50,50	1.06	2 (4%)	51,56,56	0.77	2 (3%)
60	PEV	BA	513	-	47,48,48	0.78	1 (2%)	48,53,53	0.68	2 (4%)
60	PEV	BA	514	-	47,48,48	0.80	2 (4%)	48,53,53	0.73	2 (4%)
61	PGV	BA	515	-	50,50,50	1.07	2 (4%)	51,56,56	0.75	2 (3%)
61	PGV	BA	516	-	50,50,50	1.08	2 (4%)	51,56,56	0.71	2 (3%)
60	PEV	BA	517	-	47,48,48	0.78	1 (2%)	48,53,53	0.68	2 (4%)
60	PEV	BA	518	-	47,48,48	0.77	1 (2%)	48,53,53	0.66	2 (4%)
60	PEV	BA	519	-	47,48,48	0.78	2 (4%)	48,53,53	0.72	2 (4%)
60	PEV	BA	520	-	47,48,48	0.78	1 (2%)	48,53,53	0.64	2 (4%)
60	PEV	BA	521	-	47,48,48	0.78	1 (2%)	48,53,53	0.66	2 (4%)
61	PGV	BA	522	-	50,50,50	1.08	2 (4%)	51,56,56	0.72	2 (3%)
60	PEV	BA	523	-	47,48,48	0.78	1 (2%)	48,53,53	0.74	2 (4%)
60	PEV	BA	524	-	47,48,48	0.80	2 (4%)	48,53,53	0.69	2 (4%)
60	PEV	BA	525	-	47,48,48	0.79	1 (2%)	48,53,53	0.73	2 (4%)
60	PEV	BA	526	-	47,48,48	0.77	1 (2%)	48,53,53	0.68	2 (4%)
60	PEV	BA	527	-	47,48,48	0.79	1 (2%)	48,53,53	0.76	2 (4%)
60	PEV	BA	528	-	47,48,48	0.78	1 (2%)	48,53,53	0.70	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	BA	529	-	47,48,48	0.80	2 (4%)	48,53,53	0.70	2 (4%)
60	PEV	BA	530	-	47,48,48	0.77	1 (2%)	48,53,53	0.65	2 (4%)
60	PEV	BA	531	-	47,48,48	0.77	1 (2%)	48,53,53	0.65	2 (4%)
60	PEV	BA	532	-	47,48,48	0.76	1 (2%)	48,53,53	0.74	2 (4%)
60	PEV	BA	533	-	47,48,48	2.68	1 (2%)	48,53,53	1.32	2 (4%)
60	PEV	BA	534	-	47,48,48	0.81	3 (6%)	48,53,53	0.76	3 (6%)
60	PEV	BA	535	-	47,48,48	0.79	1 (2%)	48,53,53	0.67	2 (4%)
61	PGV	BA	536	-	50,50,50	1.07	2 (4%)	51,56,56	0.74	2 (3%)
60	PEV	BA	537	-	47,48,48	0.81	2 (4%)	48,53,53	0.73	2 (4%)
60	PEV	BA	538	-	47,48,48	0.75	1 (2%)	48,53,53	0.65	2 (4%)
60	PEV	BA	539	-	47,48,48	0.78	2 (4%)	48,53,53	0.79	2 (4%)
61	PGV	BA	540	-	50,50,50	1.06	2 (4%)	51,56,56	0.79	2 (3%)
60	PEV	BB	201	-	47,48,48	0.79	1 (2%)	48,53,53	0.69	2 (4%)
60	PEV	BB	202	-	47,48,48	0.79	2 (4%)	48,53,53	0.70	2 (4%)
61	PGV	BB	203	-	50,50,50	1.08	2 (4%)	51,56,56	0.79	2 (3%)
61	PGV	BB	204	-	50,50,50	1.09	3 (6%)	51,56,56	0.83	3 (5%)
61	PGV	BB	205	-	50,50,50	1.07	2 (4%)	51,56,56	0.82	2 (3%)
60	PEV	BB	206	-	47,48,48	0.77	1 (2%)	48,53,53	0.67	2 (4%)
61	PGV	BB	207	-	50,50,50	1.08	2 (4%)	51,56,56	0.78	2 (3%)
61	PGV	BB	208	-	50,50,50	1.08	2 (4%)	51,56,56	0.75	2 (3%)
60	PEV	BB	209	-	47,48,48	0.76	1 (2%)	48,53,53	0.68	2 (4%)
60	PEV	BB	210	-	47,48,48	0.77	1 (2%)	48,53,53	0.72	2 (4%)
60	PEV	BB	211	-	47,48,48	0.77	1 (2%)	48,53,53	0.72	2 (4%)
60	PEV	BB	212	-	47,48,48	0.78	1 (2%)	48,53,53	0.65	2 (4%)
61	PGV	BB	213	-	50,50,50	1.08	2 (4%)	51,56,56	0.81	2 (3%)
60	PEV	BB	214	-	47,48,48	0.78	1 (2%)	48,53,53	0.70	2 (4%)
60	PEV	BB	215	-	47,48,48	0.77	1 (2%)	48,53,53	0.69	2 (4%)
60	PEV	BB	216	-	47,48,48	0.78	2 (4%)	48,53,53	0.76	2 (4%)
61	PGV	BB	217	-	50,50,50	1.07	2 (4%)	51,56,56	0.77	2 (3%)
60	PEV	BB	218	-	47,48,48	0.78	1 (2%)	48,53,53	0.69	2 (4%)

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
60	PEV	A0	301	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	302	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	303	-	-	0/52/52/52	0/0/0/0
61	PGV	A0	304	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	A0	305	-	1/1/5/7	0/55/55/55	0/0/0/0
61	PGV	A0	306	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A0	307	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	308	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	A0	309	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	310	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	311	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	312	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	313	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	314	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	A0	315	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	316	-	-	0/52/52/52	0/0/0/0
61	PGV	A0	317	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	A0	318	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A0	319	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	320	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	321	-	-	2/52/52/52	0/0/0/0
60	PEV	A0	322	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	323	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	A0	324	-	-	0/52/52/52	0/0/0/0
61	PGV	A0	325	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A0	326	-	-	0/52/52/52	0/0/0/0
61	PGV	A0	327	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	A0	328	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A0	329	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	330	-	-	0/52/52/52	0/0/0/0
61	PGV	A0	331	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	A0	332	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A1	301	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	A1	302	-	-	0/52/52/52	0/0/0/0
61	PGV	A1	303	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A1	304	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	305	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	A1	306	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	307	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	308	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	309	-	-	0/52/52/52	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	A1	310	-	-	0/52/52/52	0/0/0/0
61	PGV	A1	311	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A1	312	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	313	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	A1	314	-	-	0/52/52/52	0/0/0/0
61	PGV	A1	315	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A1	316	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	317	-	1/1/4/4	0/52/52/52	0/0/0/0
61	PGV	A1	318	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A1	319	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	320	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	321	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	322	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	323	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	324	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	325	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	326	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	327	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	328	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	329	-	-	0/52/52/52	0/0/0/0
60	PEV	AZ	201	-	-	0/52/52/52	0/0/0/0
60	PEV	AZ	202	-	-	0/52/52/52	0/0/0/0
60	PEV	AZ	203	-	-	0/52/52/52	0/0/0/0
60	PEV	AZ	204	-	1/1/4/4	0/52/52/52	0/0/0/0
61	PGV	AZ	205	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	AZ	206	-	-	0/52/52/52	0/0/0/0
61	PGV	AZ	207	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	B8	3001	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	B8	3002	-	-	0/52/52/52	0/0/0/0
60	PEV	B8	3003	-	-	0/52/52/52	0/0/0/0
60	PEV	B8	3004	-	-	0/52/52/52	0/0/0/0
61	PGV	B8	3005	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	B8	3006	-	-	0/52/52/52	0/0/0/0
60	PEV	B8	3007	-	-	0/52/52/52	0/0/0/0
61	PGV	BA	501	-	1/1/5/7	0/55/55/55	0/0/0/0
60	PEV	BA	502	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	BA	503	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	504	-	-	0/52/52/52	0/0/0/0
61	PGV	BA	505	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BA	506	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	507	-	-	0/52/52/52	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	BA	508	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	BA	509	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	510	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	511	-	-	0/52/52/52	0/0/0/0
61	PGV	BA	512	-	1/1/5/7	0/55/55/55	0/0/0/0
60	PEV	BA	513	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	514	-	-	0/52/52/52	0/0/0/0
61	PGV	BA	515	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	BA	516	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BA	517	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	518	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	519	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	520	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	521	-	-	0/52/52/52	0/0/0/0
61	PGV	BA	522	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BA	523	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	524	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	525	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	526	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	BA	527	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	528	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	529	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	530	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	BA	531	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	532	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	533	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	534	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	535	-	1/1/4/4	0/52/52/52	0/0/0/0
61	PGV	BA	536	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BA	537	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	BA	538	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	BA	539	-	-	0/52/52/52	0/0/0/0
61	PGV	BA	540	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BB	201	-	-	0/52/52/52	0/0/0/0
60	PEV	BB	202	-	1/1/4/4	0/52/52/52	0/0/0/0
61	PGV	BB	203	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	BB	204	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	BB	205	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BB	206	-	1/1/4/4	0/52/52/52	0/0/0/0
61	PGV	BB	207	-	2/2/5/7	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PGV	BB	208	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BB	209	-	-	0/52/52/52	0/0/0/0
60	PEV	BB	210	-	-	0/52/52/52	0/0/0/0
60	PEV	BB	211	-	-	0/52/52/52	0/0/0/0
60	PEV	BB	212	-	-	0/52/52/52	0/0/0/0
61	PGV	BB	213	-	1/1/5/7	0/55/55/55	0/0/0/0
60	PEV	BB	214	-	-	0/52/52/52	0/0/0/0
60	PEV	BB	215	-	-	0/52/52/52	0/0/0/0
60	PEV	BB	216	-	-	0/52/52/52	0/0/0/0
61	PGV	BB	217	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BB	218	-	-	0/52/52/52	0/0/0/0

All (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BA	516	PGV	C9-C10	-4.72	1.34	1.52
61	BB	213	PGV	C9-C10	-4.70	1.34	1.52
61	BA	522	PGV	C9-C10	-4.66	1.34	1.52
61	A1	315	PGV	C9-C10	-4.65	1.34	1.52
61	BB	204	PGV	C9-C10	-4.65	1.34	1.52
61	BA	501	PGV	C9-C10	-4.65	1.34	1.52
61	BB	205	PGV	C9-C10	-4.64	1.34	1.52
61	AZ	207	PGV	C9-C10	-4.63	1.34	1.52
61	BA	515	PGV	C9-C10	-4.63	1.34	1.52
61	A0	327	PGV	C9-C10	-4.62	1.34	1.52
61	A0	331	PGV	C9-C10	-4.62	1.35	1.52
61	A0	318	PGV	C9-C10	-4.62	1.35	1.52
61	BB	208	PGV	C9-C10	-4.61	1.35	1.52
61	BA	540	PGV	C9-C10	-4.61	1.35	1.52
61	A0	305	PGV	C9-C10	-4.61	1.35	1.52
61	AZ	205	PGV	C9-C10	-4.60	1.35	1.52
61	BB	207	PGV	C9-C10	-4.60	1.35	1.52
61	A1	303	PGV	C9-C10	-4.59	1.35	1.52
61	A1	311	PGV	C9-C10	-4.59	1.35	1.52
61	A0	317	PGV	C9-C10	-4.59	1.35	1.52
61	BB	217	PGV	C9-C10	-4.57	1.35	1.52
61	BA	512	PGV	C9-C10	-4.57	1.35	1.52
61	A0	328	PGV	C9-C10	-4.57	1.35	1.52
61	BA	536	PGV	C9-C10	-4.57	1.35	1.52
61	A0	306	PGV	C9-C10	-4.56	1.35	1.52
61	A0	304	PGV	C9-C10	-4.56	1.35	1.52
61	B8	3005	PGV	C9-C10	-4.56	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	A1	318	PGV	C9-C10	-4.56	1.35	1.52
61	BA	505	PGV	C9-C10	-4.55	1.35	1.52
61	BB	203	PGV	C9-C10	-4.55	1.35	1.52
61	A0	332	PGV	C9-C10	-4.54	1.35	1.52
61	A0	325	PGV	C9-C10	-4.53	1.35	1.52
60	A1	319	PEV	C39-C40	-2.94	1.34	1.51
60	B8	3004	PEV	C39-C40	-2.94	1.34	1.51
60	A0	309	PEV	C39-C40	-2.93	1.34	1.51
60	B8	3002	PEV	C39-C40	-2.92	1.34	1.51
60	BA	519	PEV	C39-C40	-2.92	1.34	1.51
60	BA	531	PEV	C39-C40	-2.92	1.34	1.51
60	A1	308	PEV	C39-C40	-2.92	1.34	1.51
60	A1	326	PEV	C39-C40	-2.92	1.34	1.51
60	AZ	204	PEV	C39-C40	-2.91	1.34	1.51
60	A0	314	PEV	C39-C40	-2.91	1.34	1.51
60	A1	301	PEV	C39-C40	-2.91	1.34	1.51
60	A0	308	PEV	C39-C40	-2.91	1.34	1.51
60	B8	3007	PEV	C39-C40	-2.91	1.34	1.51
60	BA	518	PEV	C39-C40	-2.91	1.34	1.51
60	BA	528	PEV	C39-C40	-2.91	1.34	1.51
60	BA	532	PEV	C39-C40	-2.91	1.34	1.51
60	BA	514	PEV	C39-C40	-2.91	1.34	1.51
60	BA	507	PEV	C39-C40	-2.91	1.34	1.51
60	A0	330	PEV	C39-C40	-2.90	1.34	1.51
60	AZ	206	PEV	C39-C40	-2.90	1.35	1.51
60	BA	530	PEV	C39-C40	-2.90	1.35	1.51
60	AZ	202	PEV	C39-C40	-2.90	1.35	1.51
60	A1	323	PEV	C39-C40	-2.90	1.35	1.51
60	BA	534	PEV	C39-C40	-2.90	1.35	1.51
60	A1	310	PEV	C39-C40	-2.90	1.35	1.51
60	A1	305	PEV	C39-C40	-2.90	1.35	1.51
60	A1	322	PEV	C39-C40	-2.90	1.35	1.51
60	BA	521	PEV	C39-C40	-2.90	1.35	1.51
60	A0	310	PEV	C39-C40	-2.90	1.35	1.51
60	BA	539	PEV	C39-C40	-2.90	1.35	1.51
60	BB	211	PEV	C39-C40	-2.90	1.35	1.51
60	A0	322	PEV	C39-C40	-2.90	1.35	1.51
60	A1	324	PEV	C39-C40	-2.89	1.35	1.51
60	A1	304	PEV	C39-C40	-2.89	1.35	1.51
60	A0	315	PEV	C39-C40	-2.89	1.35	1.51
60	A1	306	PEV	C39-C40	-2.89	1.35	1.51
60	A1	329	PEV	C39-C40	-2.89	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BB	201	PEV	C39-C40	-2.89	1.35	1.51
60	A0	319	PEV	C39-C40	-2.89	1.35	1.51
60	B8	3006	PEV	C39-C40	-2.89	1.35	1.51
60	A0	326	PEV	C39-C40	-2.89	1.35	1.51
60	A1	328	PEV	C39-C40	-2.89	1.35	1.51
60	BA	517	PEV	C39-C40	-2.89	1.35	1.51
60	BA	535	PEV	C39-C40	-2.89	1.35	1.51
60	BA	504	PEV	C39-C40	-2.89	1.35	1.51
60	A0	313	PEV	C39-C40	-2.89	1.35	1.51
60	A0	329	PEV	C39-C40	-2.89	1.35	1.51
60	AZ	201	PEV	C39-C40	-2.89	1.35	1.51
60	A1	327	PEV	C39-C40	-2.89	1.35	1.51
60	BB	212	PEV	C39-C40	-2.89	1.35	1.51
60	BB	218	PEV	C39-C40	-2.88	1.35	1.51
60	A0	302	PEV	C39-C40	-2.88	1.35	1.51
60	BB	216	PEV	C39-C40	-2.88	1.35	1.51
60	A0	324	PEV	C39-C40	-2.88	1.35	1.51
60	BA	538	PEV	C39-C40	-2.88	1.35	1.51
60	AZ	203	PEV	C39-C40	-2.88	1.35	1.51
60	A0	312	PEV	C39-C40	-2.88	1.35	1.51
60	BA	527	PEV	C39-C40	-2.88	1.35	1.51
60	BB	202	PEV	C39-C40	-2.88	1.35	1.51
60	BA	508	PEV	C39-C40	-2.88	1.35	1.51
60	BB	210	PEV	C39-C40	-2.88	1.35	1.51
60	A1	302	PEV	C39-C40	-2.88	1.35	1.51
60	A1	314	PEV	C39-C40	-2.88	1.35	1.51
60	BA	537	PEV	C39-C40	-2.88	1.35	1.51
60	A0	303	PEV	C39-C40	-2.88	1.35	1.51
60	BA	509	PEV	C39-C40	-2.88	1.35	1.51
60	BB	214	PEV	C39-C40	-2.88	1.35	1.51
60	BA	526	PEV	C39-C40	-2.88	1.35	1.51
60	BA	520	PEV	C39-C40	-2.88	1.35	1.51
60	BA	506	PEV	C39-C40	-2.88	1.35	1.51
60	B8	3003	PEV	C39-C40	-2.87	1.35	1.51
60	BA	513	PEV	C39-C40	-2.87	1.35	1.51
60	A0	301	PEV	C39-C40	-2.87	1.35	1.51
60	A1	321	PEV	C39-C40	-2.87	1.35	1.51
60	BA	503	PEV	C39-C40	-2.87	1.35	1.51
60	BA	529	PEV	C39-C40	-2.87	1.35	1.51
60	BA	502	PEV	C39-C40	-2.87	1.35	1.51
60	A0	311	PEV	C39-C40	-2.87	1.35	1.51
60	A0	320	PEV	C39-C40	-2.87	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	510	PEV	C39-C40	-2.87	1.35	1.51
60	BA	523	PEV	C39-C40	-2.86	1.35	1.51
60	A1	317	PEV	C39-C40	-2.86	1.35	1.51
60	A1	309	PEV	C39-C40	-2.86	1.35	1.51
60	A1	316	PEV	C39-C40	-2.86	1.35	1.51
60	B8	3001	PEV	C39-C40	-2.86	1.35	1.51
60	A0	321	PEV	C39-C40	-2.86	1.35	1.51
60	A1	320	PEV	C39-C40	-2.86	1.35	1.51
60	A1	307	PEV	C39-C40	-2.86	1.35	1.51
60	BB	209	PEV	C39-C40	-2.86	1.35	1.51
60	A1	312	PEV	C39-C40	-2.86	1.35	1.51
60	BA	525	PEV	C39-C40	-2.85	1.35	1.51
60	A0	307	PEV	C39-C40	-2.85	1.35	1.51
60	A0	323	PEV	C39-C40	-2.85	1.35	1.51
60	A1	313	PEV	C39-C40	-2.85	1.35	1.51
60	BA	524	PEV	C39-C40	-2.85	1.35	1.51
60	BB	206	PEV	C39-C40	-2.85	1.35	1.51
60	BB	215	PEV	C39-C40	-2.84	1.35	1.51
60	A1	325	PEV	C39-C40	-2.84	1.35	1.51
60	BA	511	PEV	C39-C40	-2.82	1.35	1.51
60	A0	316	PEV	C39-C40	-2.81	1.35	1.51
60	BA	524	PEV	C3-C2	2.00	1.56	1.50
60	BA	539	PEV	C3-C2	2.01	1.56	1.50
60	A0	314	PEV	C3-C2	2.01	1.56	1.50
60	A1	320	PEV	C3-C2	2.01	1.56	1.50
60	A0	313	PEV	C3-C2	2.01	1.56	1.50
60	A1	312	PEV	C3-C2	2.01	1.56	1.50
60	BA	534	PEV	C1-C2	2.02	1.56	1.50
60	A0	310	PEV	C3-C2	2.02	1.56	1.50
60	A1	308	PEV	C3-C2	2.02	1.56	1.50
60	BA	519	PEV	C3-C2	2.02	1.56	1.50
60	BB	216	PEV	C3-C2	2.02	1.56	1.50
60	A1	302	PEV	C3-C2	2.03	1.56	1.50
60	A1	316	PEV	C1-C2	2.03	1.56	1.50
60	BA	503	PEV	C1-C2	2.03	1.56	1.50
60	BA	503	PEV	C3-C2	2.03	1.56	1.50
60	A0	309	PEV	C3-C2	2.03	1.56	1.50
60	BA	529	PEV	C3-C2	2.04	1.56	1.50
60	BA	514	PEV	C1-C2	2.05	1.56	1.50
60	BB	202	PEV	C3-C2	2.06	1.56	1.50
60	BA	509	PEV	C1-C2	2.07	1.56	1.50
60	BA	534	PEV	C3-C2	2.07	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	A0	303	PEV	C3-C2	2.09	1.56	1.50
60	BA	504	PEV	C3-C2	2.10	1.56	1.50
61	BB	204	PGV	C01-C02	2.12	1.56	1.50
60	A0	308	PEV	C3-C2	2.13	1.56	1.50
60	A1	301	PEV	C3-C2	2.17	1.57	1.50
60	BA	537	PEV	C3-C2	2.19	1.57	1.50
60	A1	317	PEV	C3-C2	2.20	1.57	1.50
61	BB	205	PGV	C12-C11	3.80	1.54	1.31
61	BA	515	PGV	C12-C11	3.81	1.54	1.31
61	B8	3005	PGV	C12-C11	3.82	1.54	1.31
61	BA	512	PGV	C12-C11	3.82	1.54	1.31
61	A0	305	PGV	C12-C11	3.83	1.54	1.31
61	BA	501	PGV	C12-C11	3.83	1.54	1.31
61	BB	207	PGV	C12-C11	3.84	1.54	1.31
61	A0	331	PGV	C12-C11	3.84	1.54	1.31
61	AZ	207	PGV	C12-C11	3.85	1.54	1.31
61	AZ	205	PGV	C12-C11	3.85	1.54	1.31
61	A0	317	PGV	C12-C11	3.85	1.54	1.31
61	BB	208	PGV	C12-C11	3.85	1.54	1.31
61	A0	328	PGV	C12-C11	3.86	1.54	1.31
61	A1	318	PGV	C12-C11	3.86	1.54	1.31
61	BA	540	PGV	C12-C11	3.86	1.54	1.31
61	BB	217	PGV	C12-C11	3.86	1.54	1.31
61	BA	536	PGV	C12-C11	3.87	1.54	1.31
61	A0	318	PGV	C12-C11	3.87	1.54	1.31
61	A0	304	PGV	C12-C11	3.88	1.54	1.31
61	A0	332	PGV	C12-C11	3.88	1.54	1.31
61	A1	311	PGV	C12-C11	3.88	1.54	1.31
61	BB	204	PGV	C12-C11	3.88	1.54	1.31
61	A0	306	PGV	C12-C11	3.88	1.54	1.31
61	A0	327	PGV	C12-C11	3.89	1.54	1.31
61	A1	315	PGV	C12-C11	3.90	1.54	1.31
61	A1	303	PGV	C12-C11	3.90	1.54	1.31
61	BB	213	PGV	C12-C11	3.91	1.54	1.31
61	BA	516	PGV	C12-C11	3.91	1.54	1.31
61	BA	505	PGV	C12-C11	3.91	1.54	1.31
61	BB	203	PGV	C12-C11	3.92	1.54	1.31
61	BA	522	PGV	C12-C11	3.92	1.54	1.31
61	A0	325	PGV	C12-C11	3.93	1.55	1.31
60	BA	533	PEV	C39-C40	17.65	2.52	1.51

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	BB	204	PGV	O01-C1-C2	-2.01	107.28	111.53
60	A0	321	PEV	O2-C31-C32	2.00	115.75	111.53
60	BA	534	PEV	O3-C3-C2	2.04	114.21	108.70
60	A1	304	PEV	C39-C40-C41	2.06	125.24	114.54
60	AZ	203	PEV	C38-C39-C40	2.06	125.25	114.54
60	A0	330	PEV	C38-C39-C40	2.08	125.34	114.54
60	A0	312	PEV	C39-C40-C41	2.09	125.38	114.54
60	AZ	203	PEV	C39-C40-C41	2.12	125.55	114.54
60	AZ	206	PEV	C38-C39-C40	2.12	125.57	114.54
60	A0	330	PEV	C39-C40-C41	2.18	125.88	114.54
60	A1	304	PEV	C38-C39-C40	2.20	125.99	114.54
60	BA	529	PEV	C38-C39-C40	2.21	126.02	114.54
60	BA	518	PEV	C39-C40-C41	2.22	126.08	114.54
60	BA	537	PEV	C39-C40-C41	2.23	126.11	114.54
60	A0	310	PEV	C39-C40-C41	2.25	126.21	114.54
60	A0	302	PEV	C38-C39-C40	2.25	126.22	114.54
60	A0	312	PEV	C38-C39-C40	2.25	126.24	114.54
60	AZ	204	PEV	C38-C39-C40	2.25	126.24	114.54
61	BA	516	PGV	C9-C10-C11	2.25	125.61	112.08
60	AZ	206	PEV	C39-C40-C41	2.26	126.27	114.54
60	BA	513	PEV	C38-C39-C40	2.27	126.32	114.54
60	A0	302	PEV	C39-C40-C41	2.27	126.35	114.54
60	B8	3007	PEV	C38-C39-C40	2.27	126.35	114.54
60	BB	218	PEV	C39-C40-C41	2.27	126.35	114.54
60	A1	312	PEV	C38-C39-C40	2.28	126.37	114.54
60	BA	519	PEV	C38-C39-C40	2.28	126.38	114.54
60	BA	518	PEV	C38-C39-C40	2.28	126.38	114.54
60	A1	308	PEV	C39-C40-C41	2.28	126.38	114.54
60	BA	529	PEV	C39-C40-C41	2.28	126.40	114.54
60	A0	314	PEV	C39-C40-C41	2.28	126.41	114.54
60	A1	319	PEV	C38-C39-C40	2.29	126.44	114.54
61	B8	3005	PGV	C9-C10-C11	2.30	125.86	112.08
60	BA	537	PEV	C38-C39-C40	2.30	126.47	114.54
60	BB	201	PEV	C38-C39-C40	2.30	126.47	114.54
60	BB	215	PEV	C38-C39-C40	2.30	126.48	114.54
60	A0	303	PEV	C39-C40-C41	2.30	126.49	114.54
61	A0	305	PGV	C9-C10-C11	2.30	125.90	112.08
60	A1	308	PEV	C38-C39-C40	2.31	126.53	114.54
60	A1	312	PEV	C39-C40-C41	2.32	126.61	114.54
60	A0	315	PEV	C38-C39-C40	2.32	126.61	114.54
60	A0	314	PEV	C38-C39-C40	2.33	126.63	114.54
60	B8	3007	PEV	C39-C40-C41	2.33	126.63	114.54
60	A1	302	PEV	C38-C39-C40	2.33	126.65	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	531	PEV	C38-C39-C40	2.34	126.67	114.54
60	A1	310	PEV	C39-C40-C41	2.34	126.69	114.54
60	A1	320	PEV	C39-C40-C41	2.34	126.69	114.54
60	A1	320	PEV	C38-C39-C40	2.34	126.71	114.54
60	A1	305	PEV	C39-C40-C41	2.35	126.75	114.54
60	BA	520	PEV	C39-C40-C41	2.35	126.75	114.54
60	A1	326	PEV	C38-C39-C40	2.35	126.75	114.54
61	BA	515	PGV	C9-C10-C11	2.35	126.20	112.08
60	BB	215	PEV	C39-C40-C41	2.35	126.77	114.54
60	A1	306	PEV	C39-C40-C41	2.36	126.79	114.54
60	A1	327	PEV	C38-C39-C40	2.36	126.80	114.54
60	A1	324	PEV	C39-C40-C41	2.36	126.81	114.54
61	A0	318	PGV	C9-C10-C11	2.36	126.26	112.08
60	AZ	204	PEV	C39-C40-C41	2.36	126.82	114.54
60	BA	531	PEV	C39-C40-C41	2.37	126.84	114.54
60	BB	209	PEV	C38-C39-C40	2.37	126.85	114.54
60	B8	3002	PEV	C38-C39-C40	2.37	126.85	114.54
60	A0	324	PEV	C38-C39-C40	2.37	126.87	114.54
60	A0	303	PEV	C38-C39-C40	2.38	126.88	114.54
60	A1	306	PEV	C38-C39-C40	2.38	126.88	114.54
60	A1	326	PEV	C39-C40-C41	2.38	126.88	114.54
60	A0	309	PEV	C38-C39-C40	2.38	126.89	114.54
60	BA	530	PEV	C39-C40-C41	2.38	126.90	114.54
60	A0	321	PEV	C38-C39-C40	2.38	126.92	114.54
60	A1	317	PEV	C38-C39-C40	2.38	126.92	114.54
60	BB	201	PEV	C39-C40-C41	2.39	126.95	114.54
60	BB	209	PEV	C39-C40-C41	2.39	126.95	114.54
60	A0	315	PEV	C39-C40-C41	2.39	126.96	114.54
60	BA	538	PEV	C38-C39-C40	2.39	126.97	114.54
61	AZ	205	PGV	C9-C10-C11	2.39	126.44	112.08
60	A1	317	PEV	C39-C40-C41	2.39	126.97	114.54
60	BA	513	PEV	C39-C40-C41	2.40	126.99	114.54
60	A1	302	PEV	C39-C40-C41	2.40	127.00	114.54
61	BB	217	PGV	C9-C10-C11	2.40	126.48	112.08
60	A0	313	PEV	C39-C40-C41	2.40	127.00	114.54
60	BA	523	PEV	C38-C39-C40	2.40	127.01	114.54
60	A1	316	PEV	C38-C39-C40	2.40	127.03	114.54
60	A0	321	PEV	C39-C40-C41	2.40	127.03	114.54
61	BB	204	PGV	C9-C10-C11	2.41	126.52	112.08
60	A0	313	PEV	C38-C39-C40	2.41	127.04	114.54
60	A1	323	PEV	C39-C40-C41	2.41	127.04	114.54
60	A1	310	PEV	C38-C39-C40	2.41	127.04	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	511	PEV	C38-C39-C40	2.41	127.05	114.54
60	A0	309	PEV	C39-C40-C41	2.41	127.05	114.54
61	A0	327	PGV	C9-C10-C11	2.41	126.54	112.08
60	BA	519	PEV	C39-C40-C41	2.41	127.06	114.54
60	A0	322	PEV	C38-C39-C40	2.41	127.07	114.54
60	A0	324	PEV	C39-C40-C41	2.41	127.08	114.54
60	B8	3001	PEV	C38-C39-C40	2.42	127.09	114.54
60	A1	316	PEV	C39-C40-C41	2.42	127.12	114.54
60	BA	520	PEV	C38-C39-C40	2.42	127.13	114.54
60	A1	321	PEV	C38-C39-C40	2.43	127.14	114.54
60	B8	3003	PEV	C38-C39-C40	2.43	127.14	114.54
60	BA	514	PEV	C39-C40-C41	2.43	127.17	114.54
60	BA	521	PEV	C39-C40-C41	2.43	127.18	114.54
60	BA	504	PEV	C38-C39-C40	2.43	127.19	114.54
60	B8	3006	PEV	C38-C39-C40	2.44	127.19	114.54
61	A0	306	PGV	C9-C10-C11	2.44	126.70	112.08
60	BB	202	PEV	C38-C39-C40	2.44	127.20	114.54
60	A0	307	PEV	C38-C39-C40	2.44	127.23	114.54
60	A1	301	PEV	C39-C40-C41	2.44	127.24	114.54
61	A1	318	PGV	C9-C10-C11	2.45	126.76	112.08
60	A1	321	PEV	C39-C40-C41	2.45	127.24	114.54
60	BA	538	PEV	C39-C40-C41	2.45	127.25	114.54
60	BB	202	PEV	C39-C40-C41	2.45	127.25	114.54
60	BB	212	PEV	C39-C40-C41	2.45	127.27	114.54
61	A0	304	PGV	C9-C10-C11	2.45	126.80	112.08
60	A1	325	PEV	C38-C39-C40	2.45	127.29	114.54
60	BB	216	PEV	C39-C40-C41	2.46	127.29	114.54
60	A0	310	PEV	C38-C39-C40	2.46	127.31	114.54
61	A1	315	PGV	C9-C10-C11	2.46	126.83	112.08
61	BA	536	PGV	C9-C10-C11	2.46	126.84	112.08
60	A1	329	PEV	C39-C40-C41	2.46	127.33	114.54
60	BA	524	PEV	C38-C39-C40	2.47	127.35	114.54
60	BA	530	PEV	C38-C39-C40	2.47	127.35	114.54
60	A1	327	PEV	C39-C40-C41	2.47	127.35	114.54
60	A1	324	PEV	C38-C39-C40	2.47	127.35	114.54
60	A1	313	PEV	C38-C39-C40	2.47	127.35	114.54
60	B8	3006	PEV	C39-C40-C41	2.47	127.35	114.54
60	A0	322	PEV	C39-C40-C41	2.47	127.37	114.54
60	BA	502	PEV	C38-C39-C40	2.47	127.38	114.54
60	BA	521	PEV	C38-C39-C40	2.47	127.38	114.54
60	A1	328	PEV	C38-C39-C40	2.47	127.39	114.54
60	A0	307	PEV	C39-C40-C41	2.47	127.39	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	A0	311	PEV	C38-C39-C40	2.47	127.39	114.54
60	BA	539	PEV	C39-C40-C41	2.48	127.40	114.54
60	B8	3002	PEV	C39-C40-C41	2.48	127.42	114.54
60	BA	508	PEV	C39-C40-C41	2.48	127.43	114.54
60	A1	328	PEV	C39-C40-C41	2.48	127.43	114.54
60	A1	322	PEV	C38-C39-C40	2.48	127.44	114.54
61	A1	303	PGV	C9-C10-C11	2.48	126.99	112.08
60	BA	509	PEV	C39-C40-C41	2.48	127.45	114.54
61	A0	317	PGV	C9-C10-C11	2.49	127.00	112.08
61	AZ	207	PGV	C9-C10-C11	2.49	127.02	112.08
60	A0	320	PEV	C38-C39-C40	2.49	127.47	114.54
60	A0	301	PEV	C38-C39-C40	2.49	127.47	114.54
60	A1	301	PEV	C38-C39-C40	2.49	127.47	114.54
60	A1	325	PEV	C39-C40-C41	2.49	127.49	114.54
60	BA	509	PEV	C38-C39-C40	2.49	127.49	114.54
60	A1	313	PEV	C39-C40-C41	2.49	127.50	114.54
60	BA	502	PEV	C39-C40-C41	2.50	127.52	114.54
61	BA	501	PGV	C9-C10-C11	2.50	127.09	112.08
61	BA	540	PGV	C9-C10-C11	2.50	127.09	112.08
60	BB	212	PEV	C38-C39-C40	2.50	127.55	114.54
60	BA	507	PEV	C38-C39-C40	2.51	127.55	114.54
60	BA	508	PEV	C38-C39-C40	2.51	127.55	114.54
60	A1	309	PEV	C38-C39-C40	2.51	127.56	114.54
60	BA	523	PEV	C39-C40-C41	2.51	127.57	114.54
60	A1	314	PEV	C38-C39-C40	2.51	127.58	114.54
60	B8	3003	PEV	C39-C40-C41	2.51	127.58	114.54
60	A0	320	PEV	C39-C40-C41	2.51	127.60	114.54
60	BA	510	PEV	C38-C39-C40	2.51	127.60	114.54
60	BB	214	PEV	C38-C39-C40	2.52	127.61	114.54
60	A0	326	PEV	C38-C39-C40	2.52	127.62	114.54
60	BB	206	PEV	C39-C40-C41	2.52	127.62	114.54
60	B8	3001	PEV	C39-C40-C41	2.52	127.62	114.54
61	A0	328	PGV	C9-C10-C11	2.52	127.19	112.08
60	BA	510	PEV	C39-C40-C41	2.52	127.63	114.54
60	A1	309	PEV	C39-C40-C41	2.52	127.63	114.54
60	BA	526	PEV	C38-C39-C40	2.52	127.64	114.54
61	BA	512	PGV	C9-C10-C11	2.52	127.22	112.08
61	BA	505	PGV	C9-C10-C11	2.53	127.24	112.08
61	BA	522	PGV	C9-C10-C11	2.53	127.24	112.08
60	BB	216	PEV	C38-C39-C40	2.53	127.67	114.54
60	BA	535	PEV	C38-C39-C40	2.53	127.68	114.54
60	BA	514	PEV	C38-C39-C40	2.53	127.68	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	504	PEV	C39-C40-C41	2.53	127.69	114.54
60	BA	524	PEV	C39-C40-C41	2.53	127.69	114.54
60	A0	326	PEV	C39-C40-C41	2.53	127.69	114.54
60	BA	511	PEV	C39-C40-C41	2.53	127.69	114.54
60	BA	539	PEV	C38-C39-C40	2.53	127.69	114.54
60	BA	527	PEV	C39-C40-C41	2.54	127.72	114.54
60	A0	311	PEV	C39-C40-C41	2.54	127.72	114.54
60	A1	305	PEV	C38-C39-C40	2.54	127.73	114.54
60	BA	507	PEV	C39-C40-C41	2.54	127.73	114.54
60	A1	322	PEV	C39-C40-C41	2.54	127.73	114.54
60	BA	517	PEV	C39-C40-C41	2.54	127.73	114.54
61	BB	208	PGV	C9-C10-C11	2.54	127.34	112.08
60	BB	214	PEV	C39-C40-C41	2.54	127.75	114.54
60	AZ	201	PEV	C39-C40-C41	2.55	127.79	114.54
60	BA	528	PEV	C38-C39-C40	2.55	127.81	114.54
60	A0	308	PEV	C39-C40-C41	2.56	127.81	114.54
60	A1	314	PEV	C39-C40-C41	2.56	127.82	114.54
61	BA	522	PGV	C8-C9-C10	2.56	124.19	113.79
60	BA	525	PEV	C39-C40-C41	2.56	127.83	114.54
60	BA	535	PEV	C39-C40-C41	2.56	127.84	114.54
60	BA	525	PEV	C38-C39-C40	2.56	127.85	114.54
60	A0	319	PEV	C39-C40-C41	2.56	127.85	114.54
61	A0	331	PGV	C9-C10-C11	2.56	127.46	112.08
60	AZ	201	PEV	C38-C39-C40	2.57	127.87	114.54
60	A1	323	PEV	C38-C39-C40	2.57	127.87	114.54
61	BB	203	PGV	C9-C10-C11	2.57	127.49	112.08
60	BA	506	PEV	C38-C39-C40	2.58	127.95	114.54
60	A0	329	PEV	C38-C39-C40	2.59	127.98	114.54
60	BA	526	PEV	C39-C40-C41	2.59	127.98	114.54
60	B8	3004	PEV	C38-C39-C40	2.59	127.99	114.54
61	BB	213	PGV	C9-C10-C11	2.59	127.62	112.08
60	BB	218	PEV	C38-C39-C40	2.59	128.00	114.54
60	A0	301	PEV	C39-C40-C41	2.59	128.00	114.54
60	A0	329	PEV	C39-C40-C41	2.59	128.00	114.54
61	A1	311	PGV	C9-C10-C11	2.59	127.65	112.08
60	AZ	202	PEV	C38-C39-C40	2.60	128.05	114.54
60	BA	528	PEV	C39-C40-C41	2.60	128.05	114.54
60	BB	206	PEV	C38-C39-C40	2.60	128.06	114.54
60	BA	534	PEV	C38-C39-C40	2.60	128.06	114.54
60	AZ	202	PEV	C39-C40-C41	2.60	128.07	114.54
60	BA	506	PEV	C39-C40-C41	2.61	128.08	114.54
60	BA	532	PEV	C39-C40-C41	2.61	128.10	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	B8	3004	PEV	C39-C40-C41	2.61	128.11	114.54
60	BB	210	PEV	C38-C39-C40	2.62	128.16	114.54
60	A0	319	PEV	C38-C39-C40	2.62	128.16	114.54
60	A1	307	PEV	C39-C40-C41	2.63	128.19	114.54
60	BA	527	PEV	C38-C39-C40	2.63	128.23	114.54
60	BA	503	PEV	C39-C40-C41	2.64	128.25	114.54
60	A0	323	PEV	C39-C40-C41	2.64	128.28	114.54
60	BB	211	PEV	C39-C40-C41	2.65	128.28	114.54
61	A0	332	PGV	C9-C10-C11	2.65	127.98	112.08
60	BB	210	PEV	C39-C40-C41	2.66	128.37	114.54
60	A0	323	PEV	C38-C39-C40	2.66	128.37	114.54
60	BA	517	PEV	C38-C39-C40	2.67	128.40	114.54
60	BA	534	PEV	C39-C40-C41	2.67	128.41	114.54
60	A1	307	PEV	C38-C39-C40	2.68	128.44	114.54
61	A0	325	PGV	C9-C10-C11	2.68	128.18	112.08
60	A1	329	PEV	C38-C39-C40	2.68	128.47	114.54
60	BA	503	PEV	C38-C39-C40	2.69	128.49	114.54
61	BB	207	PGV	C9-C10-C11	2.69	128.21	112.08
60	BA	532	PEV	C38-C39-C40	2.71	128.64	114.54
60	BB	211	PEV	C38-C39-C40	2.72	128.67	114.54
60	A0	308	PEV	C38-C39-C40	2.72	128.67	114.54
61	BB	205	PGV	C9-C10-C11	2.73	128.44	112.08
61	BA	516	PGV	C8-C9-C10	2.82	125.25	113.79
61	A0	305	PGV	C8-C9-C10	2.85	125.37	113.79
61	A0	327	PGV	C8-C9-C10	2.96	125.81	113.79
60	A0	321	PEV	C2-O2-C31	2.98	125.27	117.91
61	BA	515	PGV	C8-C9-C10	3.07	126.25	113.79
61	B8	3005	PGV	C8-C9-C10	3.08	126.31	113.79
61	BB	204	PGV	C8-C9-C10	3.08	126.31	113.79
61	BA	536	PGV	C8-C9-C10	3.09	126.34	113.79
60	A0	316	PEV	C39-C40-C41	3.10	130.63	114.54
61	A1	303	PGV	C8-C9-C10	3.14	126.54	113.79
61	AZ	207	PGV	C8-C9-C10	3.14	126.57	113.79
61	A0	331	PGV	C8-C9-C10	3.16	126.63	113.79
61	BB	207	PGV	C8-C9-C10	3.16	126.65	113.79
61	BB	217	PGV	C8-C9-C10	3.18	126.69	113.79
61	BA	540	PGV	C8-C9-C10	3.18	126.73	113.79
61	AZ	205	PGV	C8-C9-C10	3.19	126.77	113.79
61	A1	318	PGV	C8-C9-C10	3.22	126.88	113.79
61	A0	306	PGV	C8-C9-C10	3.23	126.90	113.79
61	A0	317	PGV	C8-C9-C10	3.24	126.94	113.79
61	A0	318	PGV	C8-C9-C10	3.26	127.03	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	A1	315	PGV	C8-C9-C10	3.27	127.08	113.79
61	BB	208	PGV	C8-C9-C10	3.28	127.10	113.79
61	BA	501	PGV	C8-C9-C10	3.29	127.16	113.79
61	A0	304	PGV	C8-C9-C10	3.30	127.21	113.79
61	BB	203	PGV	C8-C9-C10	3.31	127.24	113.79
61	BA	512	PGV	C8-C9-C10	3.32	127.27	113.79
61	BA	505	PGV	C8-C9-C10	3.38	127.53	113.79
61	BB	213	PGV	C8-C9-C10	3.43	127.73	113.79
61	A0	328	PGV	C8-C9-C10	3.44	127.78	113.79
61	A1	311	PGV	C8-C9-C10	3.45	127.80	113.79
61	A0	332	PGV	C8-C9-C10	3.46	127.84	113.79
60	A0	316	PEV	C38-C39-C40	3.47	132.56	114.54
61	BB	205	PGV	C8-C9-C10	3.49	127.98	113.79
61	A0	325	PGV	C8-C9-C10	3.58	128.33	113.79
60	BA	533	PEV	C38-C39-C40	5.39	142.55	114.54
60	BA	533	PEV	C39-C40-C41	5.90	145.17	114.54

All (78) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
60	A1	301	PEV	C2
61	BA	540	PGV	C05
61	BA	540	PGV	C02
61	A1	318	PGV	C05
61	A1	318	PGV	C02
61	A0	327	PGV	C05
61	A0	327	PGV	C02
61	BB	208	PGV	C05
61	BB	208	PGV	C02
61	A1	303	PGV	C05
61	A1	303	PGV	C02
60	A0	323	PEV	C2
61	BA	512	PGV	C05
60	A1	313	PEV	C2
61	A1	311	PGV	C05
61	A1	311	PGV	C02
60	BA	538	PEV	C2
61	BA	515	PGV	C05
61	BA	515	PGV	C02
61	BB	207	PGV	C05
61	BB	207	PGV	C02
61	BA	505	PGV	C05

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Mol	Chain	Res	Type	Atom
61	BA	505	PGV	C02
61	A0	304	PGV	C05
61	A0	304	PGV	C02
61	A0	325	PGV	C05
61	A0	325	PGV	C02
61	A0	305	PGV	C05
61	BA	501	PGV	C05
61	A0	317	PGV	C05
61	A0	317	PGV	C02
61	A0	318	PGV	C05
61	A0	318	PGV	C02
61	A0	332	PGV	C05
61	A0	332	PGV	C02
60	BA	502	PEV	C2
61	BB	204	PGV	C05
61	BB	204	PGV	C02
61	AZ	207	PGV	C05
61	AZ	207	PGV	C02
60	BB	202	PEV	C2
60	A0	314	PEV	C2
60	A0	308	PEV	C2
61	B8	3005	PGV	C05
61	B8	3005	PGV	C02
60	A1	305	PEV	C2
61	BA	536	PGV	C05
61	BA	536	PGV	C02
60	BA	535	PEV	C2
61	BA	522	PGV	C05
61	BA	522	PGV	C02
61	A1	315	PGV	C05
61	A1	315	PGV	C02
60	BB	206	PEV	C2
60	BA	537	PEV	C2
61	A0	331	PGV	C05
61	A0	331	PGV	C02
60	AZ	204	PEV	C2
60	BA	526	PEV	C2
61	BB	203	PGV	C05
61	BB	203	PGV	C02
60	A1	317	PEV	C2
60	B8	3001	PEV	C2
61	BB	217	PGV	C05

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Mol	Chain	Res	Type	Atom
61	BB	217	PGV	C02
61	A0	328	PGV	C05
61	A0	328	PGV	C02
60	BA	508	PEV	C2
61	BB	205	PGV	C05
61	BB	205	PGV	C02
61	BA	516	PGV	C05
61	BA	516	PGV	C02
61	A0	306	PGV	C05
61	A0	306	PGV	C02
60	BA	530	PEV	C2
61	AZ	205	PGV	C05
61	AZ	205	PGV	C02
61	BB	213	PGV	C05

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	A0	321	PEV	C2-O2-C31-O31
60	A0	321	PEV	C2-O2-C31-C32

There are no ring outliers.

17 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	A0	315	PEV	1	0
60	A1	301	PEV	1	0
60	A1	302	PEV	1	0
61	A1	303	PGV	1	0
61	A1	315	PGV	1	0
60	A1	319	PEV	1	0
60	A1	323	PEV	1	0
60	B8	3001	PEV	1	0
60	B8	3002	PEV	2	0
60	BA	503	PEV	1	0
61	BA	512	PGV	1	0
60	BA	513	PEV	1	0
60	BA	514	PEV	1	0
60	BA	520	PEV	1	0
60	BA	526	PEV	1	0
60	BA	531	PEV	1	0
60	BA	533	PEV	29	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.