



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:01 PM BST

PDB ID : 4V6Z
EMDB ID: : EMD-2472
Title : E. coli 70S-fMetVal-tRNAVal-tRNA^fMet complex in classic pre-translocation state (pre1b)
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on : 2013-10-14
Resolution : 12.00 Å(reported)
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

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

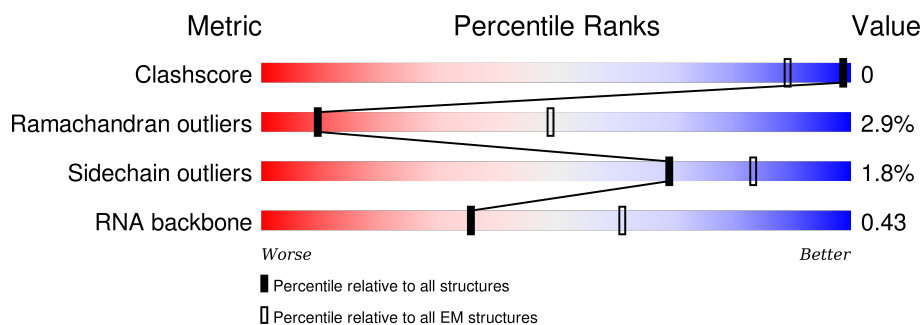
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 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.














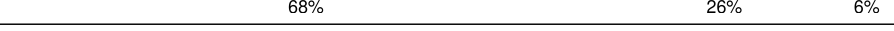

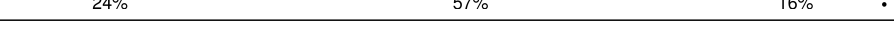

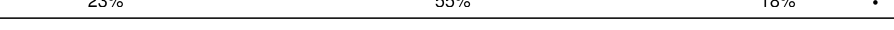



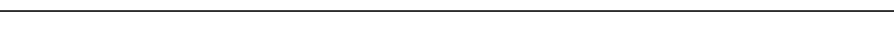

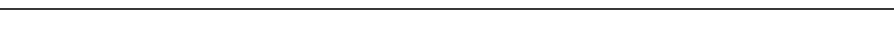
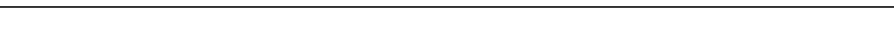


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	AB	220	94% 6%
2	AC	208	89% 10%
3	AD	206	88% 11%
4	AE	152	89% 11% .
5	AF	101	87% 12% .
6	AG	152	93% 7%
7	AH	130	92% 7% .
8	AI	128	88% 11% .











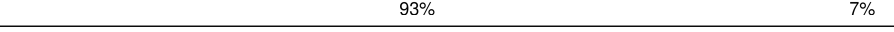
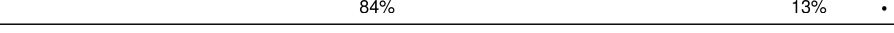
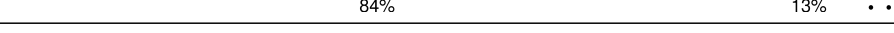
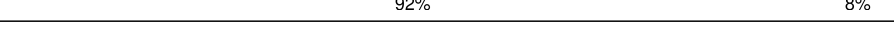

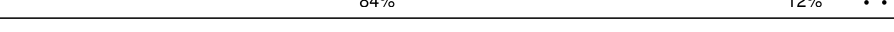



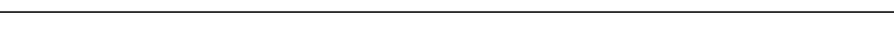


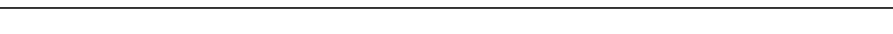
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Mol	Chain	Length	Quality of chain
9	AJ	100	 81% 16% .
10	AK	118	 90% 8% .
11	AL	124	 90% 10% .
12	AM	115	 84% 15% .
13	AN	101	 85% 14% .
14	AO	89	 87% 12% .
15	AP	81	 88% 12%
16	AQ	82	 91% 9%
17	AR	57	 88% 12%
18	AS	81	 91% 9%
19	AT	86	 86% 14%
20	AU	53	 68% 26% 6%
21	AA	1533	 13% 57% 25% 5%
22	A1	76	 24% 57% 16% .
23	A2	15	 33% 47% 20%
24	A3	77	 23% 55% 18% .
25	BC	273	 84% 14% .
26	BD	209	 88% 11% .
27	BE	201	 91% 9%
28	BF	179	 91% 8% .
29	BG	177	 89% 8% ..
30	BH	149	 94% 6%
31	BI	142	 93% 6% ..
32	BJ	142	 88% 12%
33	BK	123	 87% 11% ..

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Mol	Chain	Length	Quality of chain
34	BL	144	 81% 17% ..
35	BM	136	 89% 11%
36	BN	121	 85% 14% .
37	BO	117	 88% 11% .
38	BP	115	 84% 13% ..
39	BQ	118	 88% 10% ..
40	BR	103	 89% 11%
41	BS	110	 90% 10%
42	BT	94	 89% 11%
43	BU	104	 91% 7% ..
44	BV	94	 93% 7%
45	BW	80	 84% 13% .
46	BX	79	 84% 13% ..
47	BY	63	 92% 8%
48	BZ	59	 86% 12% .
49	B0	57	 84% 12% ..
50	B1	52	 83% 17%
51	B2	46	 74% 26%
52	B3	65	 91% 6% ..
53	B4	38	 87% 13%
54	BA	2903	 13% 57% 26% 5%
55	BB	118	 9% 57% 31% ..
56	B5	234	 90% 5% 5%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB	220	Total	C	N	O	S	0	1
			1708	1083	306	312	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	7	ACE	-	ACETYLATION	UNP P0A7V0
AB	226	NH2	-	AMIDATION	UNP P0A7V0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	207	Total	C	N	O	S	0	1
			1625	1028	306	288	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	207	NH2	-	AMIDATION	UNP P0A7V3

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	152	Total	C	N	O	S	0	1
			1109	689	212	202	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	ACETYLATION	UNP P0A7W1
AE	159	NH2	-	AMIDATION	UNP P0A7W1

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	101	Total	C	N	O	S	0	1
			818	515	149	148	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	101	NH2	-	AMIDATION	UNP P02358

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AG	152	Total	C	N	O	S	0	1
			1178	732	227	215	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	1	ACE	-	ACETYLATION	UNP P02359
AG	152	NH2	-	AMIDATION	UNP P02359

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AI	128	Total	C	N	O	S	0	0
			1025	636	206	180	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	2	ACE	-	ACETYLATION	UNP P0A7X3

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AJ	100	Total	C	N	O	S	0	1
			790	495	151	143	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	4	ACE	-	ACETYLATION	UNP P0A7R5
AJ	103	NH2	-	AMIDATION	UNP P0A7R5

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	118	Total	C	N	O	S	0	0
			880	542	174	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	11	ACE	-	ACETYLATION	UNP P0A7R9

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AM	114	Total	C	N	O	S	0	1
			877	541	178	155	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AM	114	NH2	-	AMIDATION	UNP P0A7S9

- Molecule 13 is a protein called 30S ribosomal protein S14.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	81	Total	C	N	O	S	0	1
			639	400	127	111	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	81	NH2	-	AMIDATION	UNP P0A7T3

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	82	Total	C	N	O	S	0	1
			652	413	122	114	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	2	ACE	-	ACETYLATION	UNP P0AG63
AQ	83	NH2	-	AMIDATION	UNP P0AG63

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	AR	57	Total	C	N	O	0	1
			459	290	87	82		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	18	ACE	-	ACETYLATION	UNP P0A7T7

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Chain	Residue	Modelled	Actual	Comment	Reference
AR	74	NH2	-	AMIDATION	UNP P0A7T7

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AS	81	Total	C	N	O	S	0	1
			641	410	121	108	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	ACE	-	ACETYLATION	UNP P0A7U3
AS	81	NH2	-	AMIDATION	UNP P0A7U3

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AT	86	Total	C	N	O	S	0	0
			668	413	137	115	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	1	ACE	-	ACETYLATION	UNP P0A7U7

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AU	53	Total	C	N	O	S	0	1
			429	267	87	74	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AU	2	ACE	-	ACETYLATION	UNP P68679
AU	54	NH2	-	AMIDATION	UNP P68679

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AA	1530	Total	C	N	O	P	0	0
			32828	14642	6024	10633	1529		

- Molecule 22 is a RNA chain called fMet-Val-tRNA-Val.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	A1	76	Total	C	N	O	P	S	0	0
			1627	728	292	531	75	1		

- Molecule 23 is a RNA chain called 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	15	Total	C	N	O	P	0	0
			309	140	46	109	14		

- Molecule 24 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A3	77	Total	C	N	O	P	S	0	0
			1642	734	297	534	76	1		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BC	272	Total	C	N	O	S	0	1
			2083	1288	424	364	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	272	NH2	-	AMIDATION	UNP P60422

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

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

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

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

- Molecule 31 is a protein called 50S ribosomal protein L11.

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	123	Total	C	N	O	S	0	1
			939	587	181	165	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	123	NH2	-	AMIDATION	UNP P0ADY3

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BN	121	Total	C	N	O	S	0	1
			961	593	197	166	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	121	NH2	-	AMIDATION	UNP P0AG44

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BO	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BT	94	Total	C	N	O	S	0	1
			739	466	140	131	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	94	NH2	-	AMIDATION	UNP P0ADZ0

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	BU	103	Total	C	N	O	0	1
			780	492	147	141		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	103	NH2	-	AMIDATION	UNP P60624

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BW	80	Total	C	N	O	S	0	0
			599	369	120	109	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	5	ACE	-	ACETYLATION	UNP P0A7L8

- Molecule 46 is a protein called 50S ribosomal protein L28.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BX	-1	ACE	-	ACETYLATION	UNP P0A7M2

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	B1	52	Total	C	N	O	0	1
			413	265	76	72		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	2	ACE	-	ACETYLATION	UNP P0A7N9
B1	53	NH2	-	AMIDATION	UNP P0A7N9

- Molecule 51 is a protein called 50S ribosomal protein L34.

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

- Molecule 52 is a protein called 50S ribosomal protein L35.

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

- Molecule 53 is a protein called 50S ribosomal protein L36.

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

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BA	2903	Total	C	N	O	P	0	0
			62317	27801	11467	20147	2902		

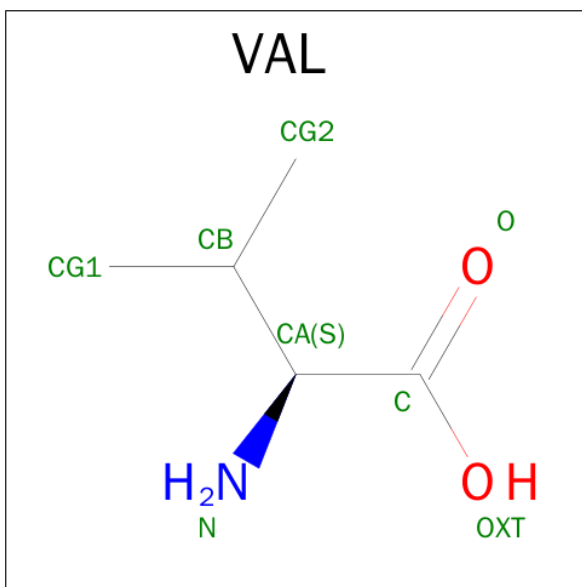
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BB	117	Total	C	N	O	P	0	0
			2504	1116	459	813	116		

- Molecule 56 is a protein called 50S ribosomal protein L1.

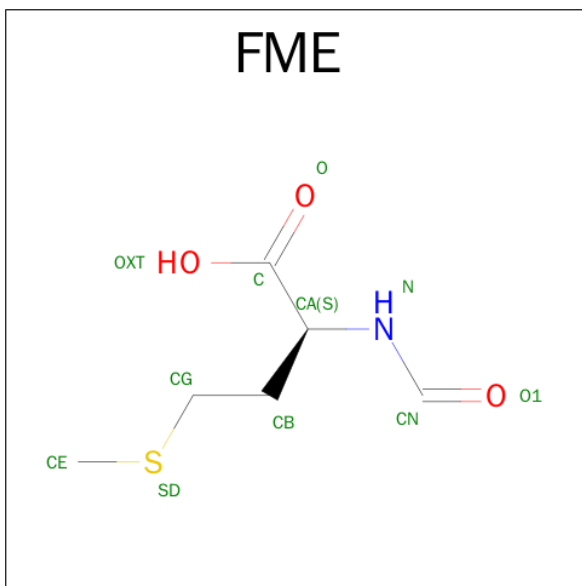
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C₅H₁₁NO₂).



Mol	Chain	Residues	Atoms				AltConf
57	A1	1	Total	C	N	O	0
			7	5	1	1	

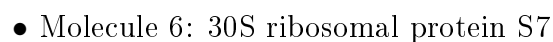
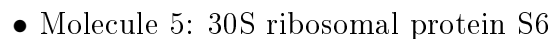
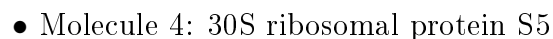
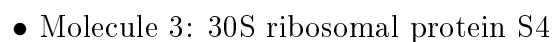
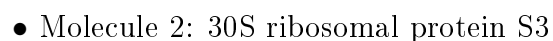
- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).

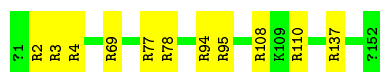


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



- Molecule 1: 30S ribosomal protein S2





- Molecule 7: 30S ribosomal protein S8

Chain AH: 92% 7%



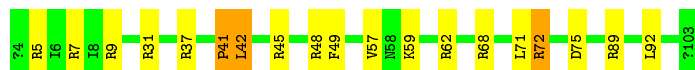
- Molecule 8: 30S ribosomal protein S9

Chain AI: 88% 11%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 81% 16%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 90% 8%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 90% 10%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 84% 15%




- Molecule 13: 30S ribosomal protein S14

Chain AN: 85% 14%



- Molecule 14: 30S ribosomal protein S15

Chain AO:  87% 12%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  88% 12%



- Molecule 16: 30S ribosomal protein S17

Chain AQ:  91% 9%



- Molecule 17: 30S ribosomal protein S18

Chain AR:  88% 12%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  91% 9%



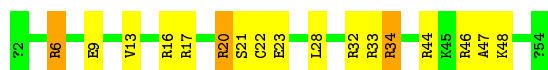
- Molecule 19: 30S ribosomal protein S20

Chain AT:  86% 14%




- Molecule 20: 30S ribosomal protein S21

Chain AU:  68% 26% 6%

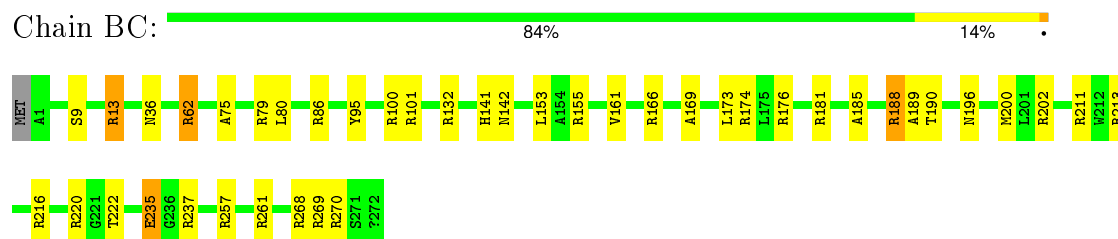


- Molecule 21: 16S ribosomal RNA

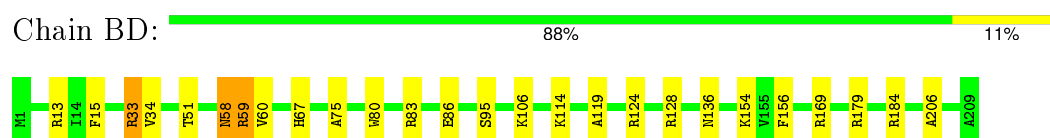
Chain AA:  13% 57% 25% 5%



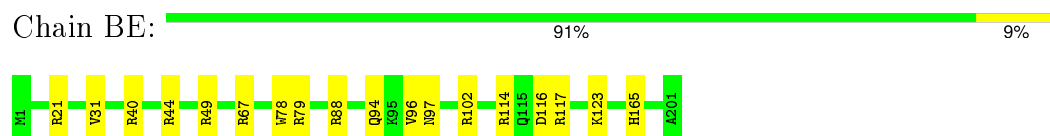

- Molecule 25: 50S ribosomal protein L2



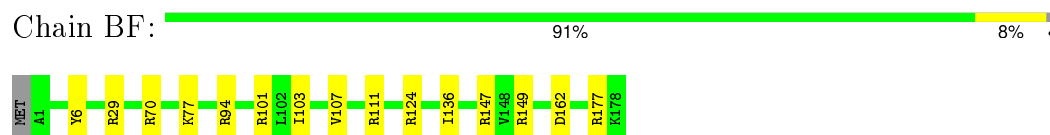
- Molecule 26: 50S ribosomal protein L3



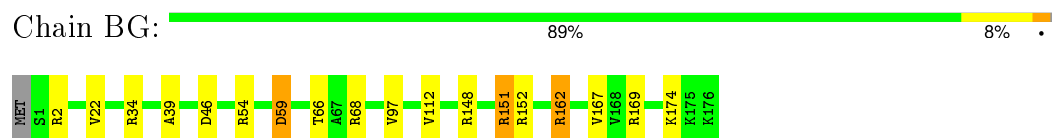
- Molecule 27: 50S ribosomal protein L4



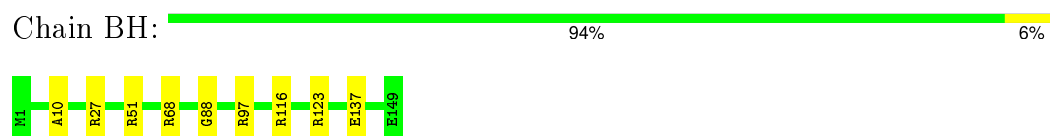
- Molecule 28: 50S ribosomal protein L5



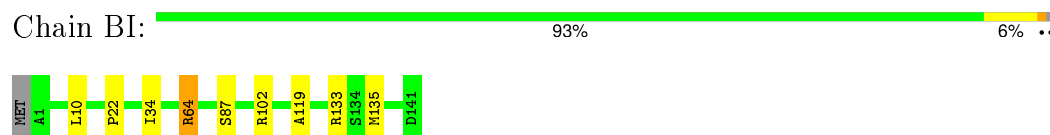
- Molecule 29: 50S ribosomal protein L6



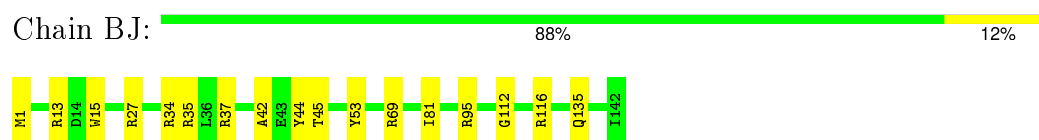
- Molecule 30: 50S ribosomal protein L9



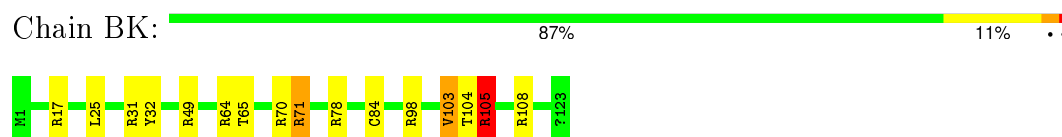
- Molecule 31: 50S ribosomal protein L11



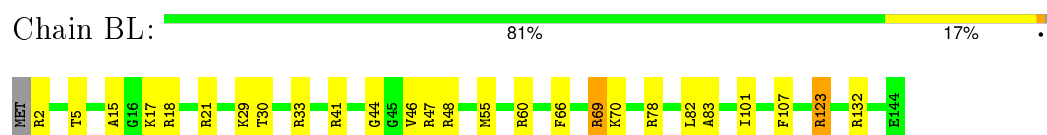
- Molecule 32: 50S ribosomal protein L13



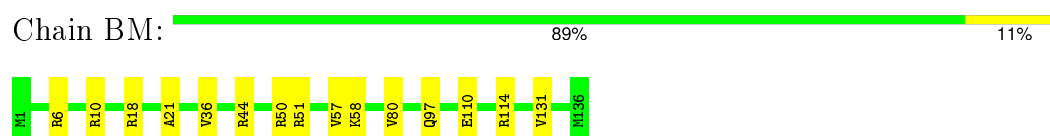
- Molecule 33: 50S ribosomal protein L14



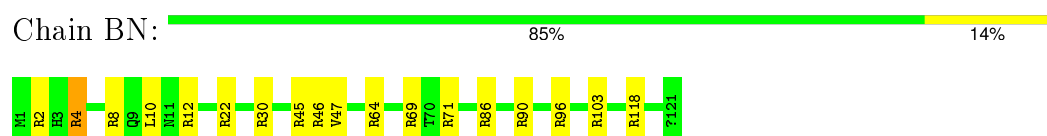
- Molecule 34: 50S ribosomal protein L15



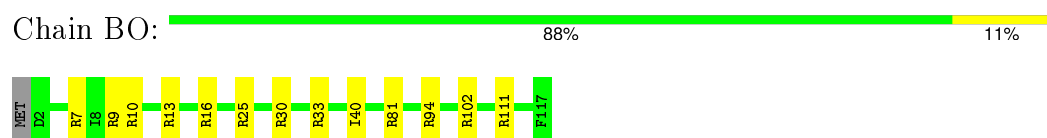
- Molecule 35: 50S ribosomal protein L16



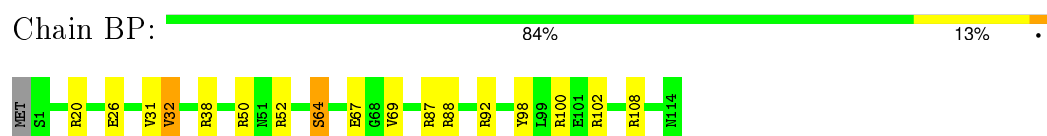
- Molecule 36: 50S ribosomal protein L17




- Molecule 37: 50S ribosomal protein L18

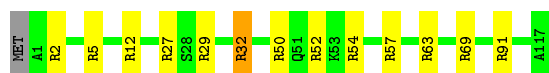


- Molecule 38: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  88% 10% ..



- Molecule 40: 50S ribosomal protein L21

Chain BR:  89% 11%



- Molecule 41: 50S ribosomal protein L22

Chain BS:  90% 10%



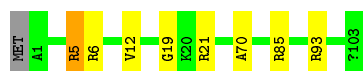
- Molecule 42: 50S ribosomal protein L23

Chain BT:  89% 11%



- Molecule 43: 50S ribosomal protein L24

Chain BU:  91% 7% ..




- Molecule 44: 50S ribosomal protein L25

Chain BV:  93% 7%




- Molecule 45: 50S ribosomal protein L27

Chain BW:  84% 13% .



- Molecule 46: 50S ribosomal protein L28

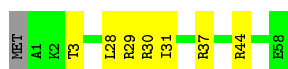
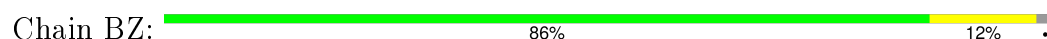
Chain BX:  84% 13% . .



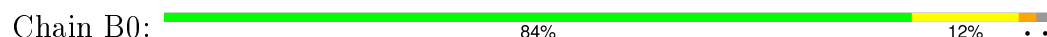
- Molecule 47: 50S ribosomal protein L29



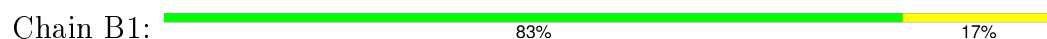
- Molecule 48: 50S ribosomal protein L30



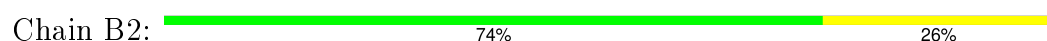
- Molecule 49: 50S ribosomal protein L32



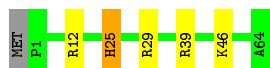
- Molecule 50: 50S ribosomal protein L33



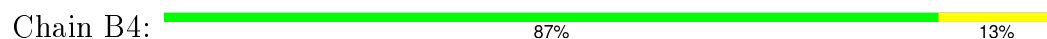
- Molecule 51: 50S ribosomal protein L34




- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36



● Molecule 54: 23S ribosomal RNA

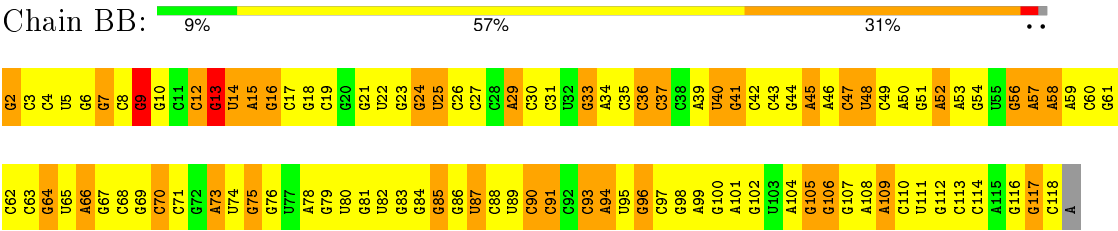
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A937	U872	G808	U747	G684	G622	U562	U499	G439	G377	G315	A251	G190	A126	G3
G938	C873	G809	G748	G685	G623	A563	G500	U440	G378	C316	G252	A191	A127	U4
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G940	A877	U811	U750	C687	G625	C565	A502	C442	G380	C318	G254	U193	C129	A6
A878		C812	A751	A688	A626	U566	A503	A443	G381	G319	A255	G194	C130	G7
G942		U813	A752	A689	A627	U568	A504	A444	G382	A320	A256	A195	A131	C8
C943	G882	C814	A753			U569	A505	A445	C383	U321	C257	A196	G132	G9
C944	G883	C815	U754	G692	A631	U569	G506	G446	A384	A322		A197	U133	A10
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		G818	G757			U572	C509	U449	G387	G325	G263	U200	G136	A13
C948	C887	A819	G758	G698	G635	U573	C510	C450	G388	G326	C264	C201	U137	A14
C949	U888	C820	G759	A699	G636	A574	U511	U451	G389	G327	A265	U202	G77	G15
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C951	C890	G822	A761	G701	G638	U576	A513	A453	A391	G329	C267	A204	C140	
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C958	C897	A829	G768	G708	C645	G583	U521	A460	C398	C336	C274	C211	C147	
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A960	A899	G831	G770	U710	C647	G585	C523	C462	G400	U339	G276	A213	A149	
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C962	C901	A833	G772	G712	G649	C587	U525	U464	A402	C341	A279	A217	U153	G30
U963			U773	G713	C650	U588	A526	C465	U403	C342	U280	A218	U154	G31
C964	G904	G836	G774	U714	G651	U589	C527	C466	A404	A343	C281	G219	A155	G32
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C968	C908	C840	U779	A718	A655	U593	C531	A470	G409	A347	U286	A223	G159	G37
G969	A909	G841	G780	C719	G656	U594	A532	A471	G410	A348	G287	U284	U160	G38
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						U596		C473	A412		U288		A161	G39
G971	A911	A844	A782	A721	G658	U596				A352		C225	A162	U00
C912	C912	U845	A783	A722	C659	G597	G536	C474	C413	C353	G291	A226	C163	A101
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G974	G914	U847	A785	U724	A661	A599	A538	C476	A415	A354	U292	A228	C164	A103
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G916		U850	A788	A727	G664	A602	C541	C479	C418	C357	G295	A231	A167	C106
A979	A918	C851	U789	G728	U665	A603	C542	C480	U419	U358	U296	G232	G168	G107
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A884	C922	G855	A793	C732	G669	G607	U546	C484	A423	A362	A300	C236	A173	G51
C985	G923	C856	A794	G733	A670	A608	U547	C485		G363	G301	C237	A111	G52
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C987	A925	U858	C796	G735	C672	C610	G549	C487	U427	U365	G303	C239	G177	G54
G988	G926	G859	G797	C736	G673	C611	C550	C488	A428	G366	U304	C240	A176	G55
G989	A927	U860	G798	C737	G674	G612	G551	C489	A429	G367	C305	A241	G180	A56
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C991	U929	G862	A739	A739	A676	A614	U554	C491	U431	U369	G307	U243	A182	G58
C992	C930	A863	G801	C740	A677	U615	G555	C492	A432	G370	G308	A244	C183	U59
G993	U931	C864	A802	U741	C678	A616	A556	C493	U428	A371	A309	G245	C184	G60
C994	C932	C865	U803	A742	G679	G617	C557	C494	U434	G372	A310	G246	G185	C61
C995	A933	A866	A804	A743	C680	G618	U558	C495	C435	U373	G247	G186	G186	A62
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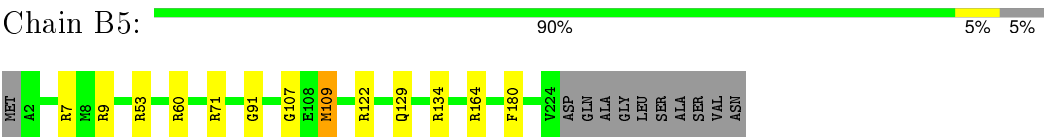
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A1928	A1866	A1802	U1742	G1681	A1618	C1558	C1498	A1437	G1317	G1256	C1196	U1132	G1071	C1006
G1929	G1867	G1803	G1743	G1682	G1619	U1559	C1499	G1438	U1318	G1257	C1197	A1133	C1072	C1007
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A1932	C1870	C1806	A1746	C1685	U1621	U1562	A1502	G1441	A1321	A1260	C1200		C1075	A1010
G1933	A1871	G1807	U1747	C1686	U1624	U1563	A1503	U1442	A1322	A1261	U1201	G1138	G1076	G1011
C1934	A1872	A1808	C1748	G1687	C1625	C1564	A1504	U1443	A1323	A1262	G1202	G1139	A1077	U1012
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A1938	A1876	G1813	C1752	C1691	U1629	U1568	A1508	C1447	A1327	G1266	C1206	A1144	U1081	A1021
U1939	A1877	G1814	G1753	U1692	A1630	G1569	A1509	G1448	A1328	U1267	G1207	A1145	U1082	G1022
U1940	G1878	A1815	A1754	U1693	G1631	U1570	G1510	G1449	U1329	A1268	C1208	C1146	U1083	U1023
C1941	C1879	C1816	A1755	C1694	A1632	A1571	G1511	G1450	U1330	A1269	U1209	C1145	A1084	G1024
C1942	U1880	G1817	G1756	G1695	G1633	A1572	C1512	G1451	G1331	G1270	G1210	A1147	A1085	G1025
U1943	C1881	U1818	A1757	G1696	A1634	G1573	U1513	G1452	G1332	G1271	G1211	U1148	A1086	G1026
C1944	U1882	A1819	U1758	G1697	A1635	C1574	G1514	A1453	G1333	A1272	G1212	G1149	G1087	A1027
G1945	U1883	U1820	A1759	U1698	U1636	C1575	G1515	G1454	G1334	U1273	A1213	C1150	A1088	A1028
U1946	G1884	C1821	C1760	G1699	A1637	U1576	G1516	C1455	C1335	A1274	A1214	A1151	A1089	A1029
C1947	A1885	G1822	C1761	U1700	C1638	C1577	G1517	G1456	U1336	A1275	G1215	C1152	A1090	C1030
G1948	U1886	G1823	A1762	A1701	C1639	U1578	C1518	U1457	G1337	A1276	G1216	C1153	G1091	G1031
G1949	A1887	G1824	G1763	G1702	A1640	A1579	G1519	U1458	C1338	G1277	U1217	G1154	C1092	A1032
G1950	C1888	U1825	C1764	G1703	A1641	A1580	U1520	G1459	G1339	C1278	G1218	A1155	G1093	U1033
U1951	G1889	G1826	U1765	G1704	G1642	U1581	G1521	U1460	U1400	U1219	G1219	A1156	U1094	G1034
A1952	A1890	U1827	G1766	A1705	G1643	C1582	U1522	C1461	G1341	G1281	G1220	G1157	A1095	U1035
A1953	G1891	G1828	C1767	C1706	C1644	U1583	U1523	G1462	A1342	U1282	C1221	C1158	A1096	G1036
G1954	C1892	A1829	C1768	G1707	G1645	U1584	G1524	C1463	G1343	G1283	U1222	U1159	U1097	G1037
U1955	C1893	C1830	U1769	C1708	C1646	C1585	A1525	G1464	U1344	A1284	G1223	G1160	A1098	G1038
U1956	C1894	U1831	G1770	U1709	U1647	A1586	C1526	U1465	C1345	A1285	U1224	C1161	G1099	A1039
C1957	G1895	G1832	C1771	G1710	U1648	G1587	G1527	U1466	G1346	A1286	G1225		C1100	A1040
G1958	G1896	C1833	A1772	A1711	G1649	U1588	A1528	U1467	A1347	A1287	A1226	C1164	G1041	G1047
G1959		U1834	A1773	U1712	A1650	U1589	G1529	U1468	C1348	G1288	G1227	A1165	G1042	G1042
A1960	A1899	G1835	C1774	A1713	G1651	A1590	C1530	G1469	U1409	C1289	G1228	G1166	A1103	C1043
A1901	A1900	C1836	U1775	U1714	A1652	A1591	G1531	A1470	C1350	G1290	C1229	C1167	C1044	G1044
G1962	C1902	G1837	G1776	G1715	G1653	C1592	A1532	G1471	C1351	G1291	A1230	G1168	U1105	G1045
U1963	G1903	C1838	U1777	U1716	A1654	A1593	C1533	C1472	U1352	G1292	U1231	A1169	G1046	A1046
G1964	C1964		U1778	U1717	A1655	U1594	U1534	G1475	A1353	C1293	G1232	C1170	G1047	G1047
G1965	G1904	C1843	U1779	G1718	C1656	C1595	A1535	A1476	A1354	U1294	C1233	G1171	A1048	A1048
A1966	C1905	U1844	A1780	G1719	U1657	A1596	C1536	U1477	U1415	C1295	U1234	C1172	C1049	C1049
G1967	G1906	G1845	U1781	U1720	C1658	A1597	G1537	A1477	G1356	G1296	G1235	U1173	A1050	A1050
G1968	G1907	U1846	U1782	G1721		U1598	G1538	G1478	C1357	G1297	G1236	U1174	G1061	G1061
A1969	C1908	G1847	A1783	A1722	U1662	U1599	U1539	G1479	G1358	C1298	A1237	A1175	C1052	C1052
A1970	C1909	A1847	G1723	G1723	G1663	C1600	G1540	A1419	A1359	G1299	G1238	U1176	C1114	C1053
U1971	U1910	A1848	G1724	A1664	A1664	G1601	U1541	U1481	G1360	G1300	G1239	G1177	A1054	A1054
G1972	G1911	C1849	U1725	A1665	U1602	U1542	G1482	G1421	A1301	A1301	U1240	C1178	G1055	G1055
G1973	C1912	G1850	G1726	G1666	G1666	A1603	G1483	G1422	C1362	A1302	A1241	G1179	G1056	G1056
C1974	A1913	U1851	C1727	G1667	A1604	A1544	G1484	G1423	C1363	G1303	U1242	U1180	C1118	A1057
G1975	C1914	U1852	C1728	A1668	C1605	A1545	U1485	G1424	G1364	A1304	C1243	U1181	U1119	U1058
U1976	A1915	A1853	U1729	A1669	C1606	A1546	U1486	G1425	A1365	C1305	A1244		G1120	G1059
A1977	A1916	C1854	U1730	C1670	C1607	G1547	U1487	G1426	A1366	C1306	G1245		C1121	U1060
A1978	U1917		G1731	G1731	A1608	A1548	C1488		A1367	A1307	A1246		G1122	U1061

G2894	G2895	G2896	G2897	G2898	G2899	G2900	G2901	G2902	G2903
G2834	A2835	A2836	A2837	G2838	G2839	G2840	G2841	G2842	G2843
G2774	G2775	G2776	G2777	A2778	A2779	G2780	A2781	G2782	G2783
G2714	G2715	G2716	G2717	G2718	G2719	G2720	A2721	G2722	G2723
C2652	G2653	G2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661
G2592	G2593	G2594	G2595	G2596	G2597	G2598	G2599	G2600	G2601
G2538	G2539	A2540	A2541	G2542	G2543	G2544	G2545	G2546	G2547
G2529	A2530	A2531	A2532	A2533	A2534	A2535	G2536	G2537	G2538
C2467	A2468	A2469	G2470	A2471	G2472	G2473	G2474	G2475	G2476
A2407	G2408	G2409	G2410	A2411	A2412	G2413	G2414	G2415	G2416
A2346	C2347	G2348	G2349	G2350	G2351	A2352	G2353	G2354	G2355
C2285	G2286	A2287	A2288	G2289	G2290	G2291	G2292	G2293	G2294
A2225	C2226	A2227	G2228	G2229	G2230	G2231	G2232	G2233	G2234
A2163	C2164	G2165	U2166	G2167	G2168	A2169	A2170	G2171	A2172
U2099	G2100	A2101	G2102	C2103	C2104		G2107	A2108	U2109
U2039	G2040	A2041	A2042	C2043	C2044	C2045	G2046	G2047	G2048
U1979	G1980	A1981	U1982	G1983	G1984	C1985	C1986	A1987	G1988

● Molecule 55: 5S ribosomal RNA



● Molecule 56: 50S ribosomal protein L1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, FME, ACE, H2U, CM0, 6MZ, NH2, 4SU, 7MG, PSU

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	AB	0.76	0/1736	1.10	10/2340 (0.4%)
10	AK	0.85	0/894	1.20	10/1207 (0.8%)
11	AL	0.85	0/969	1.25	13/1300 (1.0%)
12	AM	0.84	0/884	1.30	14/1181 (1.2%)
13	AN	0.88	1/817 (0.1%)	1.43	16/1088 (1.5%)
14	AO	0.86	0/722	1.26	12/964 (1.2%)
15	AP	0.88	0/648	1.25	6/870 (0.7%)
16	AQ	0.78	0/658	1.13	5/883 (0.6%)
17	AR	0.85	0/463	1.25	8/623 (1.3%)
18	AS	0.84	0/653	1.26	8/879 (0.9%)
19	AT	0.79	0/672	1.24	8/890 (0.9%)
2	AC	0.81	0/1651	1.19	17/2225 (0.8%)
20	AU	0.96	0/431	1.57	12/572 (2.1%)
21	AA	2.03	752/36759 (2.0%)	2.33	2571/57346 (4.5%)
22	A1	2.04	28/1668 (1.7%)	2.30	106/2595 (4.1%)
23	A2	1.81	3/343 (0.9%)	2.39	25/531 (4.7%)
24	A3	2.06	38/1722 (2.2%)	2.29	111/2685 (4.1%)
25	BC	0.85	0/2121	1.31	31/2852 (1.1%)
26	BD	0.77	0/1586	1.22	10/2134 (0.5%)
27	BE	0.75	0/1571	1.20	13/2113 (0.6%)
28	BF	0.79	0/1444	1.21	11/1937 (0.6%)
29	BG	0.76	0/1343	1.18	10/1816 (0.6%)
3	AD	0.83	0/1665	1.27	20/2227 (0.9%)
30	BH	0.72	0/1122	1.10	7/1515 (0.5%)
31	BI	0.71	0/1046	1.07	3/1410 (0.2%)
32	BJ	0.77	0/1152	1.24	12/1551 (0.8%)
33	BK	0.79	0/947	1.30	11/1268 (0.9%)
34	BL	0.82	0/1054	1.36	14/1403 (1.0%)
35	BM	0.84	0/1093	1.24	9/1460 (0.6%)
36	BN	0.89	0/973	1.43	19/1301 (1.5%)
37	BO	0.85	0/902	1.32	11/1209 (0.9%)
38	BP	0.85	0/929	1.42	13/1242 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BQ	0.86	0/960	1.33	14/1278 (1.1%)
4	AE	0.79	0/1119	1.16	9/1506 (0.6%)
40	BR	0.79	0/829	1.18	6/1107 (0.5%)
41	BS	0.76	0/864	1.20	8/1156 (0.7%)
42	BT	0.77	0/744	1.27	8/994 (0.8%)
43	BU	0.78	0/787	1.20	5/1051 (0.5%)
44	BV	0.75	0/766	1.17	6/1025 (0.6%)
45	BW	0.84	0/604	1.29	5/799 (0.6%)
46	BX	0.87	0/635	1.39	11/848 (1.3%)
47	BY	0.77	0/510	1.26	4/677 (0.6%)
48	BZ	0.84	0/453	1.29	5/605 (0.8%)
49	B0	0.85	0/450	1.33	7/599 (1.2%)
5	AF	0.79	0/835	1.15	7/1128 (0.6%)
50	B1	0.77	0/417	1.21	4/556 (0.7%)
51	B2	0.98	0/380	1.49	10/498 (2.0%)
52	B3	0.76	0/513	1.16	4/676 (0.6%)
53	B4	0.86	0/303	1.39	5/397 (1.3%)
54	BA	1.91	1309/69796 (1.9%)	2.32	5106/108888 (4.7%)
55	BB	2.03	85/2800 (3.0%)	2.33	222/4367 (5.1%)
56	B5	0.71	0/1673	1.10	10/2255 (0.4%)
6	AG	0.81	0/1188	1.19	11/1593 (0.7%)
7	AH	0.80	0/989	1.09	8/1326 (0.6%)
8	AI	0.88	0/1035	1.34	14/1377 (1.0%)
9	AJ	0.81	0/797	1.22	11/1079 (1.0%)
All	All	1.71	2216/160085 (1.4%)	2.09	8646/239402 (3.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	AK	0	1
2	AC	0	2
21	AA	0	365
22	A1	0	10
23	A2	0	1
24	A3	0	14
25	BC	0	2
33	BK	0	1
34	BL	0	1
54	BA	0	666

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	30
8	AI	0	1
All	All	0	1094

All (2216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1044	C	C4-N4	-7.34	1.27	1.33
54	BA	2752	C	C4-N4	-7.31	1.27	1.33
24	A3	3	C	C4-N4	-7.23	1.27	1.33
21	AA	6	G	C6-N1	-7.22	1.34	1.39
21	AA	1479	C	C4-N4	-7.20	1.27	1.33
21	AA	330	C	C4-N4	-7.18	1.27	1.33
55	BB	113	C	C4-N4	-7.17	1.27	1.33
21	AA	176	C	C4-N4	-7.17	1.27	1.33
54	BA	565	C	C4-N4	-7.17	1.27	1.33
54	BA	2723	C	C4-N4	-7.14	1.27	1.33
21	AA	1509	C	C4-N4	-7.10	1.27	1.33
21	AA	824	G	C2-N2	-7.09	1.27	1.34
54	BA	2104	C	C4-N4	-7.09	1.27	1.33
54	BA	624	C	C4-N4	-7.07	1.27	1.33
54	BA	1595	C	C4-N4	-7.05	1.27	1.33
54	BA	1558	C	C4-N4	-7.05	1.27	1.33
21	AA	341	C	C4-N4	-7.04	1.27	1.33
54	BA	1550	C	C4-N4	-7.02	1.27	1.33
54	BA	616	A	C6-N1	-7.01	1.30	1.35
54	BA	2777	G	C2-N2	-7.00	1.27	1.34
54	BA	2620	C	C4-N4	-6.99	1.27	1.33
22	A1	62	C	C4-N4	-6.98	1.27	1.33
54	BA	1793	C	C4-N4	-6.97	1.27	1.33
54	BA	527	C	C4-N4	-6.96	1.27	1.33
54	BA	1832	C	C4-N4	-6.96	1.27	1.33
21	AA	547	A	C6-N1	-6.95	1.30	1.35
54	BA	2062	A	C6-N1	-6.94	1.30	1.35
54	BA	2359	C	C4-N4	-6.92	1.27	1.33
55	BB	71	C	C4-N4	-6.88	1.27	1.33
54	BA	2045	C	C4-N4	-6.88	1.27	1.33
54	BA	2717	C	C4-N4	-6.87	1.27	1.33
54	BA	1821	A	C6-N1	-6.86	1.30	1.35
55	BB	37	C	C4-N4	-6.86	1.27	1.33
55	BB	75	G	C6-N1	-6.85	1.34	1.39
21	AA	1063	C	C4-N4	-6.84	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	675	A	C6-N1	-6.84	1.30	1.35
54	BA	433	C	C4-N4	-6.83	1.27	1.33
54	BA	1398	C	C4-N4	-6.83	1.27	1.33
22	A1	65	C	N3-C4	-6.82	1.29	1.33
21	AA	499	A	C6-N1	-6.82	1.30	1.35
54	BA	704	G	C6-N1	-6.82	1.34	1.39
54	BA	2025	C	C4-N4	-6.82	1.27	1.33
54	BA	2428	G	C6-N1	-6.81	1.34	1.39
21	AA	403	C	C4-N4	-6.80	1.27	1.33
54	BA	2863	C	C4-N4	-6.80	1.27	1.33
21	AA	58	C	C4-N4	-6.80	1.27	1.33
21	AA	1496	C	C4-N4	-6.80	1.27	1.33
54	BA	2385	C	C4-N4	-6.80	1.27	1.33
54	BA	2031	A	C6-N1	-6.80	1.30	1.35
54	BA	2795	C	C4-N4	-6.79	1.27	1.33
54	BA	2636	C	C4-N4	-6.78	1.27	1.33
21	AA	1193	G	C2-N2	-6.78	1.27	1.34
21	AA	1108	G	C2-N2	-6.77	1.27	1.34
54	BA	2452	C	C4-N4	-6.77	1.27	1.33
55	BB	19	C	C4-N4	-6.77	1.27	1.33
21	AA	392	C	C4-N4	-6.76	1.27	1.33
21	AA	277	C	C4-N4	-6.76	1.27	1.33
54	BA	2196	C	N3-C4	-6.76	1.29	1.33
21	AA	1141	C	C4-N4	-6.75	1.27	1.33
21	AA	470	C	C4-N4	-6.75	1.27	1.33
21	AA	1412	C	C4-N4	-6.75	1.27	1.33
54	BA	1704	C	C4-N4	-6.75	1.27	1.33
21	AA	188	C	C4-N4	-6.75	1.27	1.33
54	BA	2282	G	C2-N2	-6.74	1.27	1.34
21	AA	186	C	C4-N4	-6.74	1.27	1.33
54	BA	167	A	C6-N1	-6.74	1.30	1.35
55	BB	24	G	C6-N1	-6.73	1.34	1.39
24	A3	69	C	C4-N4	-6.73	1.27	1.33
54	BA	2103	C	C4-N4	-6.73	1.27	1.33
54	BA	2326	C	C4-N4	-6.73	1.27	1.33
21	AA	1094	G	C2-N2	-6.72	1.27	1.34
54	BA	645	C	C4-N4	-6.71	1.27	1.33
54	BA	2283	C	N3-C4	-6.71	1.29	1.33
54	BA	1413	A	C6-N1	-6.71	1.30	1.35
21	AA	363	A	C6-N1	-6.71	1.30	1.35
54	BA	2442	C	N3-C4	-6.70	1.29	1.33
54	BA	2901	C	C4-N4	-6.70	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	68	C	C4-N4	-6.69	1.27	1.33
54	BA	378	C	C4-N4	-6.69	1.27	1.33
54	BA	717	C	C4-N4	-6.69	1.27	1.33
54	BA	371	A	C6-N1	-6.68	1.30	1.35
55	BB	116	G	C2-N2	-6.68	1.27	1.34
54	BA	31	C	C4-N4	-6.67	1.27	1.33
54	BA	1768	C	C4-N4	-6.67	1.27	1.33
54	BA	2112	G	C2-N2	-6.67	1.27	1.34
54	BA	2175	C	C4-N4	-6.66	1.27	1.33
24	A3	62	C	C4-N4	-6.66	1.27	1.33
22	A1	1	G	C2-N2	-6.66	1.27	1.34
54	BA	781	A	C6-N1	-6.66	1.30	1.35
54	BA	2374	C	C4-N4	-6.66	1.27	1.33
54	BA	2823	A	C6-N1	-6.66	1.30	1.35
21	AA	685	G	C2-N2	-6.65	1.27	1.34
54	BA	411	G	C2-N2	-6.65	1.27	1.34
54	BA	1386	C	C4-N4	-6.64	1.27	1.33
54	BA	2428	G	C2-N2	-6.64	1.27	1.34
21	AA	1188	A	C6-N1	-6.64	1.30	1.35
54	BA	1514	G	C2-N2	-6.64	1.27	1.34
54	BA	2091	C	C4-N4	-6.64	1.27	1.33
54	BA	1556	C	C4-N4	-6.63	1.27	1.33
54	BA	2644	G	C2-N2	-6.63	1.27	1.34
21	AA	776	G	C2-N2	-6.63	1.27	1.34
54	BA	1753	G	C6-N1	-6.63	1.34	1.39
54	BA	2038	G	C6-N1	-6.63	1.34	1.39
21	AA	841	C	C4-N4	-6.62	1.27	1.33
54	BA	2623	G	C2-N2	-6.62	1.27	1.34
54	BA	1426	G	C2-N2	-6.62	1.27	1.34
54	BA	1788	C	C4-N4	-6.61	1.27	1.33
21	AA	1231	G	C2-N2	-6.61	1.27	1.34
21	AA	1482	G	C2-N2	-6.61	1.27	1.34
21	AA	292	G	C6-N1	-6.61	1.34	1.39
24	A3	73	A	C5-C4	-6.61	1.34	1.38
21	AA	359	G	C2-N2	-6.60	1.27	1.34
22	A1	72	C	C4-N4	-6.60	1.28	1.33
54	BA	2544	G	C6-N1	-6.59	1.34	1.39
54	BA	2683	C	C4-N4	-6.58	1.28	1.33
21	AA	1182	G	C2-N2	-6.58	1.27	1.34
54	BA	2043	C	N3-C4	-6.57	1.29	1.33
21	AA	930	C	N3-C4	-6.57	1.29	1.33
54	BA	54	G	C6-N1	-6.57	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	379	C	C4-N4	-6.57	1.28	1.33
21	AA	1193	G	C6-N1	-6.57	1.34	1.39
54	BA	51	G	C2-N2	-6.56	1.27	1.34
21	AA	156	C	N3-C4	-6.56	1.29	1.33
54	BA	2222	C	C4-N4	-6.56	1.28	1.33
21	AA	1066	C	C4-N4	-6.56	1.28	1.33
54	BA	2048	G	C6-N1	-6.56	1.34	1.39
54	BA	440	C	C4-N4	-6.55	1.28	1.33
21	AA	412	A	C6-N1	-6.55	1.30	1.35
24	A3	6	G	C2-N2	-6.55	1.28	1.34
54	BA	45	G	C6-N1	-6.55	1.34	1.39
54	BA	1601	G	C2-N2	-6.55	1.28	1.34
21	AA	1280	A	C6-N1	-6.54	1.30	1.35
54	BA	2638	G	C2-N2	-6.54	1.28	1.34
21	AA	926	G	C6-N1	-6.54	1.34	1.39
54	BA	623	C	C4-N4	-6.54	1.28	1.33
54	BA	1102	C	C4-N4	-6.54	1.28	1.33
54	BA	2443	C	C4-N4	-6.54	1.28	1.33
54	BA	2281	A	C6-N1	-6.53	1.30	1.35
21	AA	450	G	C6-N1	-6.53	1.34	1.39
54	BA	385	C	C4-N4	-6.53	1.28	1.33
54	BA	1614	A	C6-N1	-6.53	1.30	1.35
54	BA	2044	C	C4-N4	-6.53	1.28	1.33
54	BA	449	A	C6-N1	-6.53	1.30	1.35
54	BA	1803	A	C6-N1	-6.53	1.30	1.35
54	BA	679	C	N3-C4	-6.53	1.29	1.33
21	AA	396	C	N3-C4	-6.53	1.29	1.33
54	BA	1370	C	C4-N4	-6.51	1.28	1.33
54	BA	1759	A	C6-N1	-6.51	1.30	1.35
21	AA	1431	A	C6-N1	-6.51	1.30	1.35
55	BB	4	C	C4-N4	-6.51	1.28	1.33
21	AA	342	C	C4-N4	-6.51	1.28	1.33
21	AA	520	A	C6-N1	-6.51	1.30	1.35
54	BA	2362	C	C4-N4	-6.51	1.28	1.33
21	AA	1129	C	C4-N4	-6.50	1.28	1.33
54	BA	1414	C	N3-C4	-6.50	1.29	1.33
54	BA	32	C	C4-N4	-6.50	1.28	1.33
54	BA	275	C	C4-N4	-6.50	1.28	1.33
54	BA	1430	G	C2-N2	-6.49	1.28	1.34
21	AA	1476	A	C6-N1	-6.49	1.31	1.35
21	AA	931	C	N3-C4	-6.49	1.29	1.33
54	BA	1365	A	C6-N1	-6.49	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	207	C	N3-C4	-6.49	1.29	1.33
54	BA	456	C	C4-N4	-6.49	1.28	1.33
54	BA	1667	G	C2-N2	-6.49	1.28	1.34
54	BA	1678	A	C6-N1	-6.49	1.31	1.35
54	BA	2161	C	C4-N4	-6.49	1.28	1.33
55	BB	98	G	C2-N2	-6.48	1.28	1.34
21	AA	1084	G	C2-N2	-6.48	1.28	1.34
54	BA	2767	C	C4-N4	-6.48	1.28	1.33
21	AA	1109	C	C4-N4	-6.47	1.28	1.33
54	BA	2589	A	C6-N1	-6.47	1.31	1.35
21	AA	494	G	C2-N2	-6.47	1.28	1.34
54	BA	1395	A	C6-N1	-6.47	1.31	1.35
21	AA	347	G	C2-N2	-6.46	1.28	1.34
21	AA	113	G	C2-N2	-6.46	1.28	1.34
22	A1	1	G	C6-N1	-6.46	1.35	1.39
22	A1	52	G	C2-N2	-6.46	1.28	1.34
21	AA	778	G	C2-N2	-6.46	1.28	1.34
24	A3	73	A	C6-N6	-6.45	1.28	1.33
54	BA	295	G	C2-N2	-6.45	1.28	1.34
54	BA	704	G	C2-N2	-6.45	1.28	1.34
54	BA	2269	G	C2-N2	-6.45	1.28	1.34
54	BA	2721	A	C6-N1	-6.45	1.31	1.35
21	AA	354	G	C2-N2	-6.44	1.28	1.34
21	AA	308	C	C4-N4	-6.44	1.28	1.33
21	AA	663	A	C6-N1	-6.44	1.31	1.35
54	BA	574	A	C6-N1	-6.44	1.31	1.35
21	AA	275	G	C2-N2	-6.44	1.28	1.34
21	AA	1494	G	C2-N2	-6.44	1.28	1.34
21	AA	36	C	C4'-C3'	-6.44	1.46	1.53
22	A1	60	C	C4-N4	-6.44	1.28	1.33
54	BA	1345	C	C4-N4	-6.44	1.28	1.33
24	A3	5	G	C6-N1	-6.43	1.35	1.39
54	BA	2854	G	C2-N2	-6.43	1.28	1.34
54	BA	60	G	C6-N1	-6.43	1.35	1.39
21	AA	369	G	C2-N2	-6.43	1.28	1.34
54	BA	2201	G	C2-N2	-6.42	1.28	1.34
54	BA	1436	G	C2-N2	-6.42	1.28	1.34
54	BA	2503	A	C6-N1	-6.42	1.31	1.35
21	AA	453	G	C2-N2	-6.41	1.28	1.34
21	AA	1405	G	C2-N2	-6.41	1.28	1.34
55	BB	52	A	C6-N1	-6.41	1.31	1.35
54	BA	192	C	C4-N4	-6.41	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2595	G	C2-N2	-6.41	1.28	1.34
54	BA	1031	G	N1-C2	-6.41	1.32	1.37
21	AA	848	C	C4-N4	-6.41	1.28	1.33
21	AA	1469	C	C4-N4	-6.41	1.28	1.33
24	A3	71	G	C2-N2	-6.41	1.28	1.34
54	BA	2851	A	C5-C4	-6.41	1.34	1.38
54	BA	1950	G	C2-N2	-6.40	1.28	1.34
54	BA	37	C	C4-N4	-6.40	1.28	1.33
54	BA	1537	G	C6-N1	-6.40	1.35	1.39
54	BA	1570	A	C6-N1	-6.39	1.31	1.35
54	BA	2544	G	C2-N2	-6.39	1.28	1.34
21	AA	146	G	C2-N2	-6.39	1.28	1.34
21	AA	1281	C	N3-C4	-6.39	1.29	1.33
54	BA	422	A	C6-N1	-6.38	1.31	1.35
21	AA	1427	C	N3-C4	-6.38	1.29	1.33
21	AA	1147	C	N3-C4	-6.38	1.29	1.33
54	BA	2050	C	C4-N4	-6.38	1.28	1.33
54	BA	2083	G	C2-N2	-6.38	1.28	1.34
54	BA	2350	C	C4-N4	-6.38	1.28	1.33
21	AA	247	G	C2-N2	-6.38	1.28	1.34
55	BB	91	C	C4-N4	-6.37	1.28	1.33
21	AA	484	G	C2-N2	-6.37	1.28	1.34
21	AA	869	G	C2-N2	-6.37	1.28	1.34
54	BA	176	A	C6-N1	-6.37	1.31	1.35
54	BA	1826	G	C2-N2	-6.37	1.28	1.34
54	BA	2306	C	C4-N4	-6.37	1.28	1.33
54	BA	577	G	C6-N1	-6.37	1.35	1.39
54	BA	982	C	N3-C4	-6.36	1.29	1.33
21	AA	440	C	N3-C4	-6.36	1.29	1.33
54	BA	39	G	C2-N2	-6.36	1.28	1.34
54	BA	1349	C	C4-N4	-6.36	1.28	1.33
55	BB	34	A	C6-N1	-6.36	1.31	1.35
55	BB	61	G	N1-C2	-6.36	1.32	1.37
54	BA	2338	C	C4-N4	-6.36	1.28	1.33
54	BA	885	C	C4-N4	-6.35	1.28	1.33
21	AA	210	C	C4-N4	-6.35	1.28	1.33
21	AA	1346	A	C6-N6	-6.35	1.28	1.33
54	BA	611	C	N3-C4	-6.35	1.29	1.33
21	AA	776	G	C6-N1	-6.35	1.35	1.39
54	BA	2770	G	C2-N2	-6.35	1.28	1.34
21	AA	1531	A	C6-N1	-6.35	1.31	1.35
21	AA	941	G	C6-N1	-6.34	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2355	G	C2-N2	-6.34	1.28	1.34
24	A3	72	C	N3-C4	-6.34	1.29	1.33
54	BA	564	C	C4-N4	-6.34	1.28	1.33
54	BA	2289	G	C2-N2	-6.33	1.28	1.34
21	AA	164	G	C2-N2	-6.33	1.28	1.34
21	AA	292	G	C2-N2	-6.33	1.28	1.34
54	BA	1437	C	N3-C4	-6.33	1.29	1.33
54	BA	1965	C	C4-N4	-6.33	1.28	1.33
21	AA	779	C	N3-C4	-6.33	1.29	1.33
21	AA	1488	G	C2-N2	-6.33	1.28	1.34
54	BA	605	G	C6-N1	-6.33	1.35	1.39
54	BA	892	A	C6-N1	-6.33	1.31	1.35
21	AA	52	C	C4-N4	-6.33	1.28	1.33
21	AA	880	C	N3-C4	-6.33	1.29	1.33
54	BA	2380	C	C4-N4	-6.33	1.28	1.33
54	BA	2422	C	C4-N4	-6.32	1.28	1.33
21	AA	153	C	C4-N4	-6.32	1.28	1.33
55	BB	8	C	N3-C4	-6.32	1.29	1.33
54	BA	2759	G	C2-N2	-6.32	1.28	1.34
54	BA	2760	C	N3-C4	-6.32	1.29	1.33
21	AA	146	G	C6-N1	-6.31	1.35	1.39
54	BA	128	C	N3-C4	-6.31	1.29	1.33
54	BA	2271	G	C2-N2	-6.31	1.28	1.34
54	BA	2048	G	C2-N2	-6.31	1.28	1.34
54	BA	2224	G	C2-N2	-6.31	1.28	1.34
54	BA	291	G	C2-N2	-6.30	1.28	1.34
54	BA	2021	C	C4-N4	-6.30	1.28	1.33
54	BA	2253	G	C2-N2	-6.30	1.28	1.34
54	BA	116	C	C4-N4	-6.30	1.28	1.33
54	BA	2623	G	C6-N1	-6.30	1.35	1.39
54	BA	1470	A	C6-N1	-6.30	1.31	1.35
54	BA	2162	G	C2-N2	-6.30	1.28	1.34
54	BA	2389	G	C2-N2	-6.30	1.28	1.34
21	AA	526	C	C4-N4	-6.30	1.28	1.33
54	BA	692	C	N3-C4	-6.30	1.29	1.33
55	BB	7	G	C2-N2	-6.30	1.28	1.34
55	BB	30	C	N3-C4	-6.30	1.29	1.33
21	AA	1404	C	N3-C4	-6.29	1.29	1.33
21	AA	335	C	N3-C4	-6.29	1.29	1.33
21	AA	1320	C	C4-N4	-6.29	1.28	1.33
54	BA	1748	C	C4-N4	-6.29	1.28	1.33
54	BA	830	G	N1-C2	-6.29	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1171	A	C6-N1	-6.29	1.31	1.35
21	AA	1208	C	N3-C4	-6.29	1.29	1.33
21	AA	866	C	N3-C4	-6.29	1.29	1.33
21	AA	1501	C	N3-C4	-6.29	1.29	1.33
21	AA	449	G	C2-N2	-6.28	1.28	1.34
21	AA	443	C	N3-C4	-6.28	1.29	1.33
21	AA	865	A	C6-N1	-6.28	1.31	1.35
54	BA	2123	G	C2-N2	-6.28	1.28	1.34
21	AA	840	C	C4-N4	-6.28	1.28	1.33
21	AA	882	C	C4-N4	-6.28	1.28	1.33
21	AA	462	G	C2-N2	-6.28	1.28	1.34
21	AA	704	A	C6-N1	-6.28	1.31	1.35
54	BA	2745	C	C4-N4	-6.28	1.28	1.33
54	BA	2886	A	C6-N1	-6.28	1.31	1.35
54	BA	353	C	N3-C4	-6.27	1.29	1.33
54	BA	2800	A	C6-N1	-6.27	1.31	1.35
21	AA	778	G	C6-N1	-6.27	1.35	1.39
24	A3	63	C	C4-N4	-6.27	1.28	1.33
54	BA	2822	G	C2-N2	-6.27	1.28	1.34
54	BA	1401	G	C2-N2	-6.26	1.28	1.34
54	BA	2186	G	N1-C2	-6.26	1.32	1.37
21	AA	366	A	C6-N1	-6.26	1.31	1.35
21	AA	422	C	C4-N4	-6.26	1.28	1.33
21	AA	674	G	C2-N2	-6.26	1.28	1.34
21	AA	1366	C	N3-C4	-6.26	1.29	1.33
54	BA	2391	G	N1-C2	-6.26	1.32	1.37
54	BA	2228	G	C2-N2	-6.26	1.28	1.34
54	BA	2073	C	N3-C4	-6.26	1.29	1.33
21	AA	1421	G	C2-N2	-6.25	1.28	1.34
54	BA	1493	C	N3-C4	-6.25	1.29	1.33
21	AA	1410	A	C6-N1	-6.25	1.31	1.35
54	BA	1080	A	C6-N1	-6.25	1.31	1.35
54	BA	1695	G	C2-N2	-6.25	1.28	1.34
21	AA	314	C	C4-N4	-6.25	1.28	1.33
22	A1	61	C	C4-N4	-6.25	1.28	1.33
21	AA	1177	G	C2-N2	-6.25	1.28	1.34
54	BA	2626	C	C4-N4	-6.25	1.28	1.33
55	BB	41	G	C2-N2	-6.25	1.28	1.34
21	AA	528	C	N3-C4	-6.24	1.29	1.33
54	BA	364	C	C4-N4	-6.24	1.28	1.33
54	BA	2785	C	C4-N4	-6.24	1.28	1.33
54	BA	937	C	N3-C4	-6.24	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BB	64	G	C6-N1	-6.24	1.35	1.39
21	AA	802	A	C6-N1	-6.24	1.31	1.35
24	A3	19	G	C2-N2	-6.24	1.28	1.34
54	BA	2699	C	C4-N4	-6.24	1.28	1.33
54	BA	1537	G	C2-N2	-6.23	1.28	1.34
54	BA	1564	C	C4-N4	-6.23	1.28	1.33
21	AA	1517	G	C2-N2	-6.23	1.28	1.34
21	AA	495	A	C6-N1	-6.23	1.31	1.35
21	AA	1347	G	C2-N2	-6.23	1.28	1.34
21	AA	251	G	C2-N2	-6.23	1.28	1.34
54	BA	1446	C	N3-C4	-6.23	1.29	1.33
55	BB	31	C	C4-N4	-6.23	1.28	1.33
21	AA	1447	A	C6-N1	-6.23	1.31	1.35
54	BA	2427	C	C4-N4	-6.22	1.28	1.33
54	BA	2	G	C2-N2	-6.22	1.28	1.34
54	BA	774	G	C2-N2	-6.22	1.28	1.34
54	BA	1472	C	C4-N4	-6.22	1.28	1.33
54	BA	1990	C	N3-C4	-6.22	1.29	1.33
54	BA	343	C	C4-N4	-6.22	1.28	1.33
54	BA	1973	G	C2-N2	-6.22	1.28	1.34
55	BB	64	G	C2-N2	-6.21	1.28	1.34
21	AA	879	C	N3-C4	-6.21	1.29	1.33
21	AA	1342	C	C4-N4	-6.21	1.28	1.33
54	BA	1870	C	C4-N4	-6.21	1.28	1.33
55	BB	97	C	C4-N4	-6.21	1.28	1.33
55	BB	114	C	C4-N4	-6.20	1.28	1.33
54	BA	1609	A	C6-N1	-6.20	1.31	1.35
54	BA	2737	G	C6-N1	-6.20	1.35	1.39
54	BA	2747	G	C2-N2	-6.20	1.28	1.34
21	AA	348	G	C6-N1	-6.20	1.35	1.39
54	BA	454	A	C6-N1	-6.20	1.31	1.35
54	BA	2443	C	N3-C4	-6.20	1.29	1.33
54	BA	2885	G	C2-N2	-6.20	1.28	1.34
21	AA	637	C	N3-C4	-6.19	1.29	1.33
54	BA	2038	G	C2-N2	-6.19	1.28	1.34
55	BB	41	G	C6-N1	-6.19	1.35	1.39
21	AA	1151	A	C6-N1	-6.19	1.31	1.35
55	BB	62	C	C4-N4	-6.19	1.28	1.33
21	AA	1139	G	C2-N2	-6.19	1.28	1.34
21	AA	1484	C	C4-N4	-6.18	1.28	1.33
21	AA	494	G	C6-N1	-6.18	1.35	1.39
54	BA	412	A	C6-N1	-6.18	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	444	G	C2-N2	-6.18	1.28	1.34
54	BA	2770	G	C6-N1	-6.18	1.35	1.39
55	BB	79	G	C2-N2	-6.18	1.28	1.34
21	AA	483	C	C4-N4	-6.17	1.28	1.33
54	BA	161	A	C5-C4	-6.17	1.34	1.38
54	BA	1229	C	C4-N4	-6.17	1.28	1.33
54	BA	1774	C	C4-N4	-6.17	1.28	1.33
55	BB	29	A	C6-N1	-6.17	1.31	1.35
54	BA	2890	G	C2-N2	-6.17	1.28	1.34
54	BA	2160	C	C4-N4	-6.17	1.28	1.33
21	AA	197	A	C6-N1	-6.17	1.31	1.35
54	BA	1761	C	C4-N4	-6.17	1.28	1.33
21	AA	297	G	C2-N2	-6.17	1.28	1.34
54	BA	140	C	C4-N4	-6.16	1.28	1.33
21	AA	926	G	C2-N2	-6.16	1.28	1.34
54	BA	806	C	C4-N4	-6.16	1.28	1.33
54	BA	901	C	C4-N4	-6.16	1.28	1.33
21	AA	369	G	C6-N1	-6.16	1.35	1.39
21	AA	527	G	C6-N1	-6.16	1.35	1.39
54	BA	36	G	N1-C2	-6.16	1.32	1.37
21	AA	457	G	C2-N2	-6.16	1.28	1.34
24	A3	66	C	N3-C4	-6.16	1.29	1.33
21	AA	187	G	N1-C2	-6.15	1.32	1.37
54	BA	383	C	N3-C4	-6.15	1.29	1.33
54	BA	601	C	C4-N4	-6.15	1.28	1.33
21	AA	1534	A	C6-N1	-6.15	1.31	1.35
54	BA	1514	G	C6-N1	-6.15	1.35	1.39
54	BA	473	G	C2-N2	-6.15	1.28	1.34
21	AA	347	G	C6-N1	-6.15	1.35	1.39
21	AA	1102	A	C6-N1	-6.15	1.31	1.35
54	BA	961	C	N3-C4	-6.15	1.29	1.33
54	BA	474	G	C6-N1	-6.14	1.35	1.39
54	BA	2215	C	N3-C4	-6.14	1.29	1.33
55	BB	85	G	C2-N2	-6.14	1.28	1.34
21	AA	1526	G	C2-N2	-6.14	1.28	1.34
54	BA	1129	A	C6-N1	-6.14	1.31	1.35
54	BA	347	A	C6-N1	-6.14	1.31	1.35
54	BA	626	A	C6-N1	-6.14	1.31	1.35
54	BA	332	A	C6-N1	-6.14	1.31	1.35
54	BA	936	A	C6-N1	-6.14	1.31	1.35
54	BA	671	C	C4-N4	-6.14	1.28	1.33
54	BA	69	C	C4-N4	-6.14	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	587	C	C4-N4	-6.13	1.28	1.33
54	BA	1800	C	C4-N4	-6.13	1.28	1.33
54	BA	2628	C	C4-N4	-6.13	1.28	1.33
21	AA	481	G	C2-N2	-6.13	1.28	1.34
21	AA	1097	C	N3-C4	-6.13	1.29	1.33
21	AA	1415	G	C6-N1	-6.13	1.35	1.39
21	AA	1432	G	C2-N2	-6.13	1.28	1.34
21	AA	1521	C	N3-C4	-6.13	1.29	1.33
21	AA	376	G	C2-N2	-6.13	1.28	1.34
21	AA	1388	C	C4-N4	-6.13	1.28	1.33
55	BB	116	G	C6-N1	-6.13	1.35	1.39
21	AA	1428	A	C5-C4	-6.12	1.34	1.38
54	BA	2234	G	C2-N2	-6.12	1.28	1.34
54	BA	1036	G	C6-N1	-6.12	1.35	1.39
54	BA	2710	C	C4-N4	-6.12	1.28	1.33
54	BA	2827	C	N3-C4	-6.12	1.29	1.33
21	AA	475	C	C4-N4	-6.12	1.28	1.33
21	AA	1178	G	N1-C2	-6.12	1.32	1.37
54	BA	391	A	C6-N1	-6.12	1.31	1.35
54	BA	570	G	C2-N2	-6.12	1.28	1.34
54	BA	1077	A	C6-N1	-6.12	1.31	1.35
55	BB	23	G	C6-N1	-6.12	1.35	1.39
54	BA	2614	A	C5-C4	-6.12	1.34	1.38
54	BA	1114	C	C4-N4	-6.12	1.28	1.33
54	BA	2507	C	N3-C4	-6.12	1.29	1.33
21	AA	728	A	C5-C4	-6.12	1.34	1.38
54	BA	719	C	N3-C4	-6.12	1.29	1.33
54	BA	1075	C	C4-N4	-6.12	1.28	1.33
55	BB	102	G	N1-C2	-6.12	1.32	1.37
54	BA	223	A	C5-C4	-6.11	1.34	1.38
54	BA	423	A	C5-C4	-6.11	1.34	1.38
54	BA	1787	A	C6-N1	-6.11	1.31	1.35
54	BA	2587	A	C5-C4	-6.11	1.34	1.38
22	A1	28	C	C4-N4	-6.11	1.28	1.33
54	BA	550	C	N3-C4	-6.11	1.29	1.33
55	BB	94	A	C6-N1	-6.11	1.31	1.35
21	AA	1077	G	N1-C2	-6.11	1.32	1.37
21	AA	1344	C	C4-N4	-6.11	1.28	1.33
54	BA	226	A	C6-N1	-6.11	1.31	1.35
55	BB	7	G	C6-N1	-6.11	1.35	1.39
54	BA	585	G	C2-N2	-6.10	1.28	1.34
54	BA	1441	G	C2-N2	-6.10	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1208	C	N3-C4	-6.10	1.29	1.33
21	AA	355	C	N3-C4	-6.10	1.29	1.33
21	AA	360	G	N1-C2	-6.10	1.32	1.37
21	AA	878	A	C6-N1	-6.10	1.31	1.35
21	AA	1061	G	C6-N1	-6.10	1.35	1.39
21	AA	1369	C	C4-N4	-6.10	1.28	1.33
54	BA	2850	A	C6-N1	-6.10	1.31	1.35
21	AA	1433	A	C6-N1	-6.10	1.31	1.35
54	BA	570	G	C6-N1	-6.10	1.35	1.39
55	BB	60	C	C4-N4	-6.10	1.28	1.33
54	BA	398	C	C4-N4	-6.09	1.28	1.33
54	BA	1741	C	C4-N4	-6.09	1.28	1.33
54	BA	2870	C	C4-N4	-6.09	1.28	1.33
24	A3	6	G	C6-N1	-6.09	1.35	1.39
54	BA	121	G	C2-N2	-6.09	1.28	1.34
54	BA	1686	C	C4-N4	-6.09	1.28	1.33
54	BA	160	A	C6-N1	-6.09	1.31	1.35
54	BA	945	A	C6-N1	-6.09	1.31	1.35
54	BA	2078	C	N3-C4	-6.09	1.29	1.33
21	AA	1207	G	C2-N2	-6.08	1.28	1.34
21	AA	1038	C	C4-N4	-6.08	1.28	1.33
54	BA	54	G	C2-N2	-6.08	1.28	1.34
54	BA	393	C	C4-N4	-6.08	1.28	1.33
54	BA	2234	G	C6-N1	-6.08	1.35	1.39
21	AA	1438	G	C6-N1	-6.08	1.35	1.39
21	AA	155	A	C6-N1	-6.08	1.31	1.35
21	AA	983	A	C6-N1	-6.07	1.31	1.35
54	BA	386	G	C2-N2	-6.07	1.28	1.34
21	AA	703	G	N1-C2	-6.07	1.32	1.37
54	BA	2734	A	C6-N6	-6.07	1.29	1.33
54	BA	2828	G	N1-C2	-6.06	1.32	1.37
54	BA	1454	C	C4-N4	-6.06	1.28	1.33
21	AA	233	C	C4-N4	-6.06	1.28	1.33
21	AA	1061	G	C2-N2	-6.06	1.28	1.34
54	BA	1401	G	C6-N1	-6.06	1.35	1.39
21	AA	1407	C	C4-N4	-6.06	1.28	1.33
54	BA	1043	C	C4-N4	-6.06	1.28	1.33
55	BB	75	G	C2-N2	-6.06	1.28	1.34
21	AA	1397	C	C4-N4	-6.05	1.28	1.33
21	AA	775	G	C2-N2	-6.05	1.28	1.34
54	BA	706	A	C6-N1	-6.05	1.31	1.35
54	BA	893	C	N3-C4	-6.05	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	806	C	N3-C4	-6.05	1.29	1.33
54	BA	285	G	C2-N2	-6.05	1.28	1.34
54	BA	1646	C	C4-N4	-6.05	1.28	1.33
54	BA	2332	C	C4-N4	-6.05	1.28	1.33
21	AA	222	C	C4-N4	-6.05	1.28	1.33
54	BA	1361	G	C2-N2	-6.05	1.28	1.34
54	BA	1927	A	C6-N1	-6.05	1.31	1.35
54	BA	2618	G	C2-N2	-6.05	1.28	1.34
21	AA	489	C	N3-C4	-6.05	1.29	1.33
54	BA	738	G	C2-N2	-6.05	1.28	1.34
54	BA	1700	A	C6-N6	-6.05	1.29	1.33
21	AA	1210	C	C4-N4	-6.04	1.28	1.33
54	BA	1593	A	C6-N1	-6.04	1.31	1.35
54	BA	2367	G	C2-N2	-6.04	1.28	1.34
21	AA	32	A	C6-N1	-6.03	1.31	1.35
54	BA	1220	G	C2-N2	-6.03	1.28	1.34
21	AA	39	G	C2-N2	-6.03	1.28	1.34
54	BA	1613	G	C2-N2	-6.03	1.28	1.34
21	AA	490	C	C4-N4	-6.03	1.28	1.33
54	BA	44	A	C6-N1	-6.03	1.31	1.35
54	BA	45	G	C2-N2	-6.03	1.28	1.34
54	BA	2323	G	C2-N2	-6.03	1.28	1.34
54	BA	1046	A	C6-N1	-6.02	1.31	1.35
54	BA	33	C	C4-N4	-6.02	1.28	1.33
54	BA	443	A	C6-N1	-6.02	1.31	1.35
21	AA	1487	G	C2-N2	-6.02	1.28	1.34
54	BA	1221	C	N3-C4	-6.02	1.29	1.33
54	BA	444	C	N3-C4	-6.02	1.29	1.33
54	BA	2207	C	N3-C4	-6.02	1.29	1.33
54	BA	180	G	C2-N2	-6.02	1.28	1.34
54	BA	1121	C	C4-N4	-6.02	1.28	1.33
54	BA	1830	C	N3-C4	-6.02	1.29	1.33
54	BA	1753	G	C2-N2	-6.01	1.28	1.34
54	BA	2624	G	C6-N1	-6.01	1.35	1.39
21	AA	1507	A	C6-N1	-6.01	1.31	1.35
54	BA	60	G	C2-N2	-6.01	1.28	1.34
21	AA	370	C	N3-C4	-6.01	1.29	1.33
21	AA	519	C	C4-N4	-6.01	1.28	1.33
21	AA	1103	C	N3-C4	-6.01	1.29	1.33
54	BA	208	C	N3-C4	-6.01	1.29	1.33
54	BA	758	C	C4-N4	-6.01	1.28	1.33
54	BA	1090	A	C5-C4	-6.01	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1426	G	C6-N1	-6.01	1.35	1.39
54	BA	84	A	C6-N1	-6.00	1.31	1.35
21	AA	730	G	C2-N2	-6.00	1.28	1.34
54	BA	1512	C	C4-N4	-6.00	1.28	1.33
54	BA	2	G	C6-N1	-6.00	1.35	1.39
21	AA	1169	A	C5-C4	-6.00	1.34	1.38
54	BA	2821	A	C6-N1	-6.00	1.31	1.35
21	AA	453	G	C6-N1	-6.00	1.35	1.39
54	BA	382	A	C6-N1	-6.00	1.31	1.35
54	BA	2801	G	C2-N2	-6.00	1.28	1.34
21	AA	192	A	C5-C4	-6.00	1.34	1.38
54	BA	2342	C	N3-C4	-5.99	1.29	1.33
21	AA	614	C	C4-N4	-5.99	1.28	1.33
54	BA	729	G	C2-N2	-5.99	1.28	1.34
54	BA	1561	C	N3-C4	-5.99	1.29	1.33
54	BA	2704	C	N3-C4	-5.99	1.29	1.33
54	BA	2712	C	C4-N4	-5.99	1.28	1.33
54	BA	2323	G	C6-N1	-5.99	1.35	1.39
54	BA	2692	G	C6-N1	-5.99	1.35	1.39
55	BB	117	G	C2-N2	-5.99	1.28	1.34
54	BA	2369	A	C6-N6	-5.99	1.29	1.33
54	BA	2597	G	C2-N2	-5.99	1.28	1.34
55	BB	105	G	C6-N1	-5.99	1.35	1.39
21	AA	451	A	C6-N1	-5.98	1.31	1.35
21	AA	747	A	C6-N1	-5.98	1.31	1.35
54	BA	1987	A	C6-N6	-5.98	1.29	1.33
22	A1	52	G	C6-N1	-5.98	1.35	1.39
21	AA	348	G	C2-N2	-5.98	1.28	1.34
21	AA	825	A	C6-N1	-5.98	1.31	1.35
21	AA	1409	C	N3-C4	-5.98	1.29	1.33
22	A1	41	A	C6-N1	-5.98	1.31	1.35
55	BB	105	G	C2-N2	-5.98	1.28	1.34
21	AA	1226	C	C4-N4	-5.97	1.28	1.33
54	BA	1037	G	N1-C2	-5.97	1.32	1.37
21	AA	1416	G	C2-N2	-5.97	1.28	1.34
21	AA	940	C	N3-C4	-5.97	1.29	1.33
54	BA	2090	A	C5-C4	-5.97	1.34	1.38
54	BA	2855	C	N3-C4	-5.97	1.29	1.33
54	BA	145	C	C4-N4	-5.96	1.28	1.33
54	BA	620	G	C2-N2	-5.96	1.28	1.34
54	BA	2285	C	C4-N4	-5.96	1.28	1.33
54	BA	2301	C	C4-N4	-5.96	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2379	G	C2-N2	-5.96	1.28	1.34
21	AA	868	C	C4-N4	-5.96	1.28	1.33
54	BA	845	A	C6-N1	-5.96	1.31	1.35
54	BA	58	G	C2-N2	-5.96	1.28	1.34
54	BA	1703	G	N1-C2	-5.96	1.32	1.37
21	AA	1113	C	C4-N4	-5.96	1.28	1.33
21	AA	1133	G	C6-N1	-5.96	1.35	1.39
54	BA	730	A	C6-N1	-5.96	1.31	1.35
54	BA	1347	A	C6-N1	-5.96	1.31	1.35
54	BA	1452	G	C2-N2	-5.96	1.28	1.34
21	AA	712	A	C4'-C3'	-5.95	1.46	1.52
54	BA	1740	G	C6-N1	-5.95	1.35	1.39
54	BA	2737	G	C2-N2	-5.95	1.28	1.34
54	BA	2824	C	N3-C4	-5.95	1.29	1.33
21	AA	1133	G	C2-N2	-5.95	1.28	1.34
21	AA	783	C	N3-C4	-5.95	1.29	1.33
54	BA	1592	C	N3-C4	-5.95	1.29	1.33
54	BA	2023	C	N3-C4	-5.95	1.29	1.33
54	BA	2136	G	C2-N2	-5.95	1.28	1.34
54	BA	2358	A	C6-N6	-5.95	1.29	1.33
21	AA	1084	G	C6-N1	-5.95	1.35	1.39
54	BA	2330	G	C6-N1	-5.95	1.35	1.39
21	AA	319	G	N1-C2	-5.95	1.32	1.37
54	BA	341	C	C4-N4	-5.95	1.28	1.33
54	BA	2341	G	C2-N2	-5.94	1.28	1.34
54	BA	1276	A	C6-N1	-5.94	1.31	1.35
54	BA	1362	C	N3-C4	-5.94	1.29	1.33
21	AA	838	G	C2-N2	-5.94	1.28	1.34
54	BA	647	G	C2-N2	-5.94	1.28	1.34
54	BA	217	A	C6-N1	-5.93	1.31	1.35
54	BA	1674	G	N1-C2	-5.93	1.33	1.37
21	AA	509	A	C5-C4	-5.93	1.34	1.38
54	BA	2896	C	C4-N4	-5.93	1.28	1.33
21	AA	394	G	C2-N2	-5.93	1.28	1.34
21	AA	1041	G	C2-N2	-5.93	1.28	1.34
54	BA	1822	C	C4-N4	-5.93	1.28	1.33
54	BA	2208	C	N3-C4	-5.93	1.29	1.33
54	BA	2339	C	C4-N4	-5.93	1.28	1.33
21	AA	999	C	C4-N4	-5.92	1.28	1.33
54	BA	1833	C	C4-N4	-5.92	1.28	1.33
54	BA	516	C	C4-N4	-5.92	1.28	1.33
54	BA	557	C	C4-N4	-5.92	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1773	A	C6-N1	-5.92	1.31	1.35
21	AA	1150	A	C6-N1	-5.92	1.31	1.35
21	AA	1422	G	C2-N2	-5.92	1.28	1.34
21	AA	449	G	C6-N1	-5.92	1.35	1.39
54	BA	316	C	C4-N4	-5.92	1.28	1.33
54	BA	1408	G	C2-N2	-5.92	1.28	1.34
54	BA	2597	G	C6-N1	-5.92	1.35	1.39
21	AA	372	C	C4-N4	-5.91	1.28	1.33
21	AA	469	C	N3-C4	-5.91	1.29	1.33
54	BA	1134	A	C6-N1	-5.91	1.31	1.35
54	BA	1587	G	C2-N2	-5.91	1.28	1.34
55	BB	118	C	C4-N4	-5.91	1.28	1.33
21	AA	929	G	C2-N2	-5.91	1.28	1.34
21	AA	939	G	C2-N2	-5.91	1.28	1.34
54	BA	882	G	C2-N2	-5.91	1.28	1.34
21	AA	63	C	C4-N4	-5.91	1.28	1.33
24	A3	53	G	C2-N2	-5.91	1.28	1.34
54	BA	757	G	N1-C2	-5.91	1.33	1.37
21	AA	1228	C	C4-N4	-5.91	1.28	1.33
21	AA	528	C	C4-N4	-5.91	1.28	1.33
21	AA	1164	G	N1-C2	-5.91	1.33	1.37
54	BA	1980	G	N1-C2	-5.91	1.33	1.37
54	BA	2736	A	C6-N1	-5.90	1.31	1.35
54	BA	2851	A	C6-N6	-5.90	1.29	1.33
55	BB	86	G	C2-N2	-5.90	1.28	1.34
21	AA	349	A	C5-C4	-5.90	1.34	1.38
54	BA	1036	G	C2-N2	-5.90	1.28	1.34
21	AA	145	G	C2-N2	-5.90	1.28	1.34
54	BA	1679	A	C5-C4	-5.90	1.34	1.38
21	AA	179	A	C6-N1	-5.90	1.31	1.35
54	BA	2890	G	C6-N1	-5.89	1.35	1.39
21	AA	40	C	C4-N4	-5.89	1.28	1.33
21	AA	1524	C	C4-N4	-5.89	1.28	1.33
54	BA	1373	A	C6-N1	-5.89	1.31	1.35
54	BA	2201	G	C6-N1	-5.89	1.35	1.39
21	AA	1375	A	C5-C4	-5.89	1.34	1.38
21	AA	1132	C	N3-C4	-5.89	1.29	1.33
22	A1	42	G	C6-N1	-5.89	1.35	1.39
21	AA	1411	C	N3-C4	-5.89	1.29	1.33
54	BA	585	G	C6-N1	-5.89	1.35	1.39
54	BA	2762	C	N3-C4	-5.89	1.29	1.33
55	BB	53	A	C6-N1	-5.89	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1482	G	C6-N1	-5.88	1.35	1.39
54	BA	536	G	C2-N2	-5.88	1.28	1.34
54	BA	1799	G	N1-C2	-5.88	1.33	1.37
54	BA	2638	G	C6-N1	-5.88	1.35	1.39
54	BA	2854	G	C6-N1	-5.88	1.35	1.39
21	AA	1473	G	N1-C2	-5.88	1.33	1.37
54	BA	474	G	C2-N2	-5.88	1.28	1.34
54	BA	891	G	C2-N2	-5.88	1.28	1.34
54	BA	1874	C	C4-N4	-5.88	1.28	1.33
54	BA	2633	G	C2-N2	-5.88	1.28	1.34
21	AA	1156	G	C6-N1	-5.88	1.35	1.39
54	BA	1954	G	C6-N1	-5.88	1.35	1.39
21	AA	1031	C	N3-C4	-5.88	1.29	1.33
21	AA	478	A	C6-N1	-5.87	1.31	1.35
54	BA	450	G	N1-C2	-5.87	1.33	1.37
54	BA	2358	A	C5-C4	-5.87	1.34	1.38
54	BA	2794	C	C4-N4	-5.87	1.28	1.33
21	AA	1340	A	C6-N1	-5.87	1.31	1.35
21	AA	1367	C	C4-N4	-5.87	1.28	1.33
54	BA	1519	G	C2-N2	-5.87	1.28	1.34
54	BA	1527	G	C6-N1	-5.87	1.35	1.39
54	BA	2174	C	C4-N4	-5.87	1.28	1.33
54	BA	2676	C	C4-N4	-5.87	1.28	1.33
54	BA	2813	A	C6-N1	-5.87	1.31	1.35
55	BB	16	G	C2-N2	-5.87	1.28	1.34
21	AA	658	C	C4-N4	-5.87	1.28	1.33
54	BA	1156	A	C6-N1	-5.87	1.31	1.35
54	BA	1361	G	C6-N1	-5.87	1.35	1.39
54	BA	1587	G	C6-N1	-5.87	1.35	1.39
21	AA	127	G	C2-N2	-5.86	1.28	1.34
54	BA	1084	A	C5-C4	-5.86	1.34	1.38
21	AA	498	A	C5-C4	-5.86	1.34	1.38
21	AA	1177	G	C6-N1	-5.86	1.35	1.39
54	BA	2602	A	C5-C4	-5.86	1.34	1.38
55	BB	70	C	C4-N4	-5.86	1.28	1.33
54	BA	2140	G	C2-N2	-5.86	1.28	1.34
54	BA	2619	C	C4-N4	-5.86	1.28	1.33
55	BB	27	C	C4-N4	-5.86	1.28	1.33
21	AA	1418	A	C5-C4	-5.86	1.34	1.38
54	BA	1548	A	C6-N1	-5.86	1.31	1.35
54	BA	2708	G	C2-N2	-5.86	1.28	1.34
54	BA	2618	G	C6-N1	-5.86	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2667	C	C4-N4	-5.86	1.28	1.33
54	BA	2887	A	C6-N6	-5.86	1.29	1.33
21	AA	506	G	C2-N2	-5.85	1.28	1.34
55	BB	49	C	C4-N4	-5.85	1.28	1.33
21	AA	664	G	C2-N2	-5.85	1.28	1.34
24	A3	17	C	C4-N4	-5.85	1.28	1.33
54	BA	651	G	C2-N2	-5.85	1.28	1.34
54	BA	420	C	N3-C4	-5.85	1.29	1.33
54	BA	1434	A	C6-N6	-5.85	1.29	1.33
21	AA	1192	C	C4-N4	-5.85	1.28	1.33
54	BA	1389	G	C2-N2	-5.85	1.28	1.34
54	BA	1545	A	C5-C4	-5.85	1.34	1.38
21	AA	527	G	C2-N2	-5.84	1.28	1.34
21	AA	623	C	C4-N4	-5.84	1.28	1.33
21	AA	419	C	C4-N4	-5.84	1.28	1.33
21	AA	846	G	C2-N2	-5.84	1.28	1.34
21	AA	1152	A	C5-C4	-5.84	1.34	1.38
21	AA	708	C	N3-C4	-5.84	1.29	1.33
54	BA	1677	A	C6-N1	-5.84	1.31	1.35
21	AA	290	C	C4-N4	-5.84	1.28	1.33
54	BA	1407	G	C2-N2	-5.84	1.28	1.34
54	BA	1947	C	C4-N4	-5.84	1.28	1.33
54	BA	2330	G	C2-N2	-5.84	1.28	1.34
54	BA	1090	A	C6-N6	-5.83	1.29	1.33
54	BA	1691	C	N3-C4	-5.83	1.29	1.33
21	AA	1483	A	C6-N1	-5.83	1.31	1.35
54	BA	439	A	C5-C4	-5.83	1.34	1.38
54	BA	544	C	C4-N4	-5.83	1.28	1.33
54	BA	1374	G	N1-C2	-5.83	1.33	1.37
54	BA	1339	G	C2-N2	-5.83	1.28	1.34
54	BA	1382	G	C2-N2	-5.83	1.28	1.34
54	BA	2405	G	C2-N2	-5.83	1.28	1.34
54	BA	1569	A	C6-N1	-5.83	1.31	1.35
54	BA	1598	A	C5-C4	-5.83	1.34	1.38
21	AA	175	C	C4-N4	-5.83	1.28	1.33
54	BA	1738	G	C2-N2	-5.83	1.28	1.34
54	BA	2254	C	N3-C4	-5.83	1.29	1.33
54	BA	2815	C	C4-N4	-5.83	1.28	1.33
21	AA	359	G	C6-N1	-5.82	1.35	1.39
54	BA	2655	G	C2-N2	-5.82	1.28	1.34
21	AA	6	G	C2-N2	-5.82	1.28	1.34
21	AA	124	C	C4-N4	-5.82	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	363	G	N1-C2	-5.82	1.33	1.37
54	BA	2040	G	N1-C2	-5.82	1.33	1.37
54	BA	2063	C	N3-C4	-5.82	1.29	1.33
55	BB	3	C	C4-N4	-5.82	1.28	1.33
55	BB	24	G	C2-N2	-5.82	1.28	1.34
21	AA	1349	A	C6-N1	-5.82	1.31	1.35
54	BA	1901	A	C6-N1	-5.82	1.31	1.35
54	BA	2097	A	C6-N1	-5.82	1.31	1.35
54	BA	42	A	C6-N6	-5.82	1.29	1.33
21	AA	356	A	C5-C4	-5.81	1.34	1.38
54	BA	2682	A	C6-N1	-5.81	1.31	1.35
54	BA	2872	A	C6-N6	-5.81	1.29	1.33
21	AA	1510	C	C4-N4	-5.81	1.28	1.33
21	AA	1184	G	N1-C2	-5.81	1.33	1.37
54	BA	187	G	C2-N2	-5.81	1.28	1.34
54	BA	445	C	C4-N4	-5.81	1.28	1.33
54	BA	651	G	C6-N1	-5.81	1.35	1.39
54	BA	2239	G	C2-N2	-5.81	1.28	1.34
21	AA	1438	G	C2-N2	-5.81	1.28	1.34
54	BA	1120	G	N1-C2	-5.81	1.33	1.37
54	BA	2032	G	C2-N2	-5.81	1.28	1.34
21	AA	385	C	N3-C4	-5.81	1.29	1.33
21	AA	395	C	N3-C4	-5.80	1.29	1.33
54	BA	7	G	C2-N2	-5.80	1.28	1.34
54	BA	2270	A	C6-N1	-5.80	1.31	1.35
54	BA	439	A	C6-N6	-5.80	1.29	1.33
21	AA	484	G	C6-N1	-5.80	1.35	1.39
21	AA	1181	G	C2-N2	-5.80	1.28	1.34
21	AA	1331	G	C2-N2	-5.80	1.28	1.34
54	BA	209	C	C4-N4	-5.80	1.28	1.33
55	BB	33	G	C2-N2	-5.80	1.28	1.34
21	AA	305	G	C2-N2	-5.80	1.28	1.34
54	BA	2499	C	C4-N4	-5.80	1.28	1.33
21	AA	215	C	N3-C4	-5.79	1.29	1.33
24	A3	67	C	C4-N4	-5.79	1.28	1.33
54	BA	1317	G	C2-N2	-5.79	1.28	1.34
54	BA	2282	G	C6-N1	-5.79	1.35	1.39
54	BA	2900	A	C5-C4	-5.79	1.34	1.38
54	BA	2364	C	C4-N4	-5.79	1.28	1.33
21	AA	1365	G	C2-N2	-5.79	1.28	1.34
54	BA	1447	C	N3-C4	-5.79	1.29	1.33
21	AA	141	G	C2-N2	-5.79	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1182	G	C6-N1	-5.79	1.35	1.39
54	BA	2738	A	C5-C4	-5.79	1.34	1.38
54	BA	1348	C	N3-C4	-5.78	1.29	1.33
54	BA	2080	A	C5-C4	-5.78	1.34	1.38
54	BA	1069	A	C6-N1	-5.78	1.31	1.35
54	BA	1339	G	C6-N1	-5.78	1.35	1.39
54	BA	1684	G	C2-N2	-5.78	1.28	1.34
21	AA	852	G	C2-N2	-5.78	1.28	1.34
21	AA	1051	C	C4-N4	-5.78	1.28	1.33
24	A3	5	G	C2-N2	-5.78	1.28	1.34
54	BA	2208	C	C4-N4	-5.78	1.28	1.33
54	BA	2263	C	N3-C4	-5.78	1.29	1.33
54	BA	122	G	C2-N2	-5.78	1.28	1.34
54	BA	2899	A	C6-N1	-5.78	1.31	1.35
21	AA	522	C	C4-N4	-5.78	1.28	1.33
54	BA	1770	G	C2-N2	-5.78	1.28	1.34
54	BA	1961	C	C4-N4	-5.78	1.28	1.33
54	BA	2226	C	C4-N4	-5.78	1.28	1.33
54	BA	2591	C	C4-N4	-5.78	1.28	1.33
55	BB	6	G	C2-N2	-5.78	1.28	1.34
54	BA	605	G	C2-N2	-5.77	1.28	1.34
54	BA	1073	A	C5-C4	-5.77	1.34	1.38
54	BA	2856	A	C5-C4	-5.77	1.34	1.38
21	AA	1517	G	C6-N1	-5.77	1.35	1.39
54	BA	2369	A	C5-C4	-5.77	1.34	1.38
54	BA	417	C	C4-N4	-5.77	1.28	1.33
54	BA	2846	G	C2-N2	-5.77	1.28	1.34
54	BA	1441	G	C6-N1	-5.77	1.35	1.39
54	BA	1975	G	N1-C2	-5.76	1.33	1.37
54	BA	837	C	N3-C4	-5.76	1.29	1.33
55	BB	101	A	C6-N1	-5.76	1.31	1.35
21	AA	34	C	C4-N4	-5.76	1.28	1.33
21	AA	1437	A	C6-N1	-5.76	1.31	1.35
54	BA	410	G	C2-N2	-5.76	1.28	1.34
54	BA	1334	G	C2-N2	-5.76	1.28	1.34
21	AA	376	G	C6-N1	-5.76	1.35	1.39
21	AA	703	G	C2-N2	-5.76	1.28	1.34
21	AA	1415	G	C2-N2	-5.76	1.28	1.34
54	BA	2357	G	N1-C2	-5.76	1.33	1.37
54	BA	1760	C	N3-C4	-5.76	1.29	1.33
21	AA	976	G	C2-N2	-5.76	1.28	1.34
21	AA	1467	C	C4-N4	-5.76	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1427	A	C5-C4	-5.76	1.34	1.38
54	BA	2607	G	C2-N2	-5.75	1.28	1.34
21	AA	839	C	C4-N4	-5.75	1.28	1.33
21	AA	1117	A	C5-C4	-5.75	1.34	1.38
21	AA	1128	C	C4-N4	-5.75	1.28	1.33
54	BA	129	C	C4-N4	-5.75	1.28	1.33
54	BA	1123	C	N3-C4	-5.75	1.29	1.33
54	BA	2077	A	C6-N1	-5.75	1.31	1.35
21	AA	1502	A	C6-N1	-5.75	1.31	1.35
21	AA	1504	G	N1-C2	-5.75	1.33	1.37
54	BA	1243	C	N3-C4	-5.75	1.29	1.33
54	BA	1359	A	C5-C4	-5.75	1.34	1.38
54	BA	1771	C	N3-C4	-5.75	1.29	1.33
21	AA	313	A	C6-N6	-5.75	1.29	1.33
21	AA	383	A	C5-C4	-5.75	1.34	1.38
54	BA	2590	A	C6-N1	-5.75	1.31	1.35
21	AA	1174	G	N1-C2	-5.75	1.33	1.37
54	BA	2241	A	C5-C4	-5.75	1.34	1.38
54	BA	2349	G	N1-C2	-5.75	1.33	1.37
21	AA	826	C	N3-C4	-5.74	1.29	1.33
54	BA	104	A	C6-N6	-5.74	1.29	1.33
21	AA	1047	G	C2-N2	-5.74	1.28	1.34
54	BA	2297	A	C6-N1	-5.74	1.31	1.35
54	BA	612	G	N1-C2	-5.74	1.33	1.37
54	BA	1985	C	N3-C4	-5.74	1.29	1.33
21	AA	1209	C	C4-N4	-5.74	1.28	1.33
54	BA	57	C	C4-N4	-5.74	1.28	1.33
54	BA	1989	G	C2-N2	-5.74	1.28	1.34
54	BA	2521	C	C4-N4	-5.74	1.28	1.33
21	AA	1449	C	N3-C4	-5.73	1.29	1.33
54	BA	2030	A	C5-C4	-5.73	1.34	1.38
21	AA	354	G	C6-N1	-5.73	1.35	1.39
21	AA	496	A	C6-N1	-5.73	1.31	1.35
21	AA	447	G	C2-N2	-5.73	1.28	1.34
55	BB	79	G	C6-N1	-5.73	1.35	1.39
54	BA	1968	G	C2-N2	-5.73	1.28	1.34
21	AA	521	G	C2-N2	-5.73	1.28	1.34
22	A1	66	A	C5-C4	-5.73	1.34	1.38
54	BA	64	A	C6-N6	-5.73	1.29	1.33
54	BA	2088	A	C6-N1	-5.73	1.31	1.35
54	BA	2217	G	N1-C2	-5.73	1.33	1.37
54	BA	2602	A	C6-N6	-5.73	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1094	G	C6-N1	-5.73	1.35	1.39
24	A3	77	A	C6-N1	-5.73	1.31	1.35
55	BB	96	G	N1-C2	-5.72	1.33	1.37
21	AA	1093	A	C6-N1	-5.72	1.31	1.35
21	AA	1421	G	C6-N1	-5.72	1.35	1.39
54	BA	1630	A	C5-C4	-5.72	1.34	1.38
21	AA	468	A	C6-N6	-5.72	1.29	1.33
54	BA	352	A	C6-N1	-5.72	1.31	1.35
21	AA	450	G	C2-N2	-5.72	1.28	1.34
21	AA	799	G	N1-C2	-5.72	1.33	1.37
21	AA	803	G	N1-C2	-5.72	1.33	1.37
54	BA	14	A	C6-N1	-5.72	1.31	1.35
54	BA	1477	A	C5-C4	-5.72	1.34	1.38
54	BA	2361	G	C2-N2	-5.72	1.28	1.34
54	BA	2425	A	C6-N1	-5.72	1.31	1.35
21	AA	371	A	C6-N6	-5.71	1.29	1.33
24	A3	54	G	C6-N1	-5.71	1.35	1.39
54	BA	55	G	N1-C2	-5.71	1.33	1.37
54	BA	1112	G	C2-N2	-5.71	1.28	1.34
54	BA	2368	C	C4-N4	-5.71	1.28	1.33
54	BA	2862	G	N1-C2	-5.71	1.33	1.37
55	BB	2	G	C2-N2	-5.71	1.28	1.34
54	BA	2354	C	N3-C4	-5.71	1.29	1.33
21	AA	313	A	C5-C4	-5.71	1.34	1.38
21	AA	328	C	C4-N4	-5.71	1.28	1.33
21	AA	784	A	C6-N1	-5.71	1.31	1.35
24	A3	50	G	N1-C2	-5.71	1.33	1.37
54	BA	2072	C	N3-C4	-5.71	1.29	1.33
54	BA	2304	G	C2-N2	-5.71	1.28	1.34
54	BA	1996	C	N3-C4	-5.71	1.29	1.33
54	BA	2260	C	C4-N4	-5.71	1.28	1.33
54	BA	668	A	C6-N1	-5.71	1.31	1.35
54	BA	1645	G	C2-N2	-5.71	1.28	1.34
54	BA	173	A	C5-C4	-5.71	1.34	1.38
21	AA	445	G	N1-C2	-5.71	1.33	1.37
21	AA	568	G	C2-N2	-5.71	1.28	1.34
54	BA	63	A	C5-C4	-5.71	1.34	1.38
21	AA	237	G	C2-N2	-5.70	1.28	1.34
21	AA	353	A	C6-N6	-5.70	1.29	1.33
55	BB	117	G	C6-N1	-5.70	1.35	1.39
54	BA	2697	G	C2-N2	-5.70	1.28	1.34
54	BA	164	C	C4-N4	-5.70	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	959	A	C5-C4	-5.70	1.34	1.38
21	AA	1466	C	N3-C4	-5.70	1.29	1.33
21	AA	1519	A	C5-C4	-5.70	1.34	1.38
54	BA	1987	A	C5-C4	-5.70	1.34	1.38
21	AA	521	G	N1-C2	-5.69	1.33	1.37
54	BA	789	A	C6-N1	-5.69	1.31	1.35
21	AA	498	A	C6-N6	-5.69	1.29	1.33
54	BA	529	A	C5-C4	-5.69	1.34	1.38
54	BA	1087	G	C2-N2	-5.69	1.28	1.34
21	AA	553	A	C6-N6	-5.69	1.29	1.33
21	AA	1111	A	C6-N1	-5.69	1.31	1.35
54	BA	1549	A	C5-C4	-5.69	1.34	1.38
54	BA	2190	G	C2-N2	-5.69	1.28	1.34
21	AA	226	G	C2-N2	-5.69	1.28	1.34
54	BA	377	G	C2-N2	-5.69	1.28	1.34
54	BA	1819	A	C5-C4	-5.69	1.34	1.38
54	BA	1404	C	N3-C4	-5.69	1.29	1.33
54	BA	2639	A	C6-N1	-5.69	1.31	1.35
54	BA	2706	A	C6-N1	-5.69	1.31	1.35
21	AA	941	G	C2-N2	-5.68	1.28	1.34
54	BA	161	A	C6-N6	-5.68	1.29	1.33
54	BA	1204	A	C6-N6	-5.68	1.29	1.33
21	AA	364	A	C5-C4	-5.68	1.34	1.38
54	BA	228	C	N3-C4	-5.68	1.29	1.33
54	BA	2498	C	C4-N4	-5.68	1.28	1.33
21	AA	844	G	C2-N2	-5.68	1.28	1.34
54	BA	1124	G	N1-C2	-5.68	1.33	1.37
21	AA	33	A	C5-C4	-5.68	1.34	1.38
54	BA	1822	C	N3-C4	-5.68	1.29	1.33
54	BA	2090	A	C6-N6	-5.68	1.29	1.33
54	BA	2315	G	C2-N2	-5.68	1.28	1.34
54	BA	2888	C	C4-N4	-5.68	1.28	1.33
54	BA	134	G	C2-N2	-5.67	1.28	1.34
54	BA	2748	A	C6-N1	-5.67	1.31	1.35
21	AA	1516	G	C2-N2	-5.67	1.28	1.34
54	BA	9	G	N1-C2	-5.67	1.33	1.37
54	BA	2083	G	C6-N1	-5.67	1.35	1.39
21	AA	248	C	N3-C4	-5.67	1.29	1.33
24	A3	54	G	C2-N2	-5.67	1.28	1.34
54	BA	1210	G	C2-N2	-5.67	1.28	1.34
21	AA	111	G	N1-C2	-5.67	1.33	1.37
21	AA	569	C	N3-C4	-5.67	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1371	G	C2-N2	-5.67	1.28	1.34
54	BA	48	G	C6-N1	-5.67	1.35	1.39
54	BA	291	G	C6-N1	-5.67	1.35	1.39
54	BA	617	G	N1-C2	-5.67	1.33	1.37
54	BA	1382	G	C6-N1	-5.67	1.35	1.39
54	BA	1959	G	C2-N2	-5.67	1.28	1.34
54	BA	2608	G	C2-N2	-5.67	1.28	1.34
21	AA	1169	A	C6-N6	-5.67	1.29	1.33
54	BA	1355	G	C2-N2	-5.67	1.28	1.34
54	BA	1404	C	C4-N4	-5.67	1.28	1.33
54	BA	2726	A	C6-N1	-5.67	1.31	1.35
21	AA	554	A	N9-C4	-5.67	1.34	1.37
54	BA	42	A	C5-C4	-5.67	1.34	1.38
21	AA	68	G	C2-N2	-5.66	1.28	1.34
54	BA	1389	G	C6-N1	-5.66	1.35	1.39
21	AA	748	G	C2-N2	-5.66	1.28	1.34
54	BA	198	C	C4-N4	-5.66	1.28	1.33
54	BA	1630	A	C6-N6	-5.66	1.29	1.33
54	BA	2371	G	C2-N2	-5.66	1.28	1.34
22	A1	2	G	C6-N1	-5.66	1.35	1.39
21	AA	77	A	C6-N1	-5.66	1.31	1.35
21	AA	442	G	C2-N2	-5.66	1.28	1.34
22	A1	66	A	C6-N6	-5.66	1.29	1.33
54	BA	362	A	C6-N1	-5.66	1.31	1.35
54	BA	1335	C	C4-N4	-5.66	1.28	1.33
54	BA	1538	G	N1-C2	-5.66	1.33	1.37
54	BA	2228	G	C6-N1	-5.66	1.35	1.39
54	BA	2426	A	C6-N1	-5.66	1.31	1.35
54	BA	2872	A	C5-C4	-5.66	1.34	1.38
21	AA	191	G	C6-N1	-5.65	1.35	1.39
54	BA	1314	C	C4-N4	-5.65	1.28	1.33
54	BA	1428	C	C4-N4	-5.65	1.28	1.33
54	BA	2855	C	C4-N4	-5.65	1.28	1.33
21	AA	621	A	C6-N1	-5.65	1.31	1.35
21	AA	1500	A	C6-N1	-5.65	1.31	1.35
54	BA	2293	G	C2-N2	-5.65	1.28	1.34
54	BA	2614	A	C6-N6	-5.65	1.29	1.33
54	BA	1295	C	C4-N4	-5.65	1.28	1.33
54	BA	2315	G	C6-N1	-5.65	1.35	1.39
54	BA	2643	G	C2-N2	-5.65	1.28	1.34
54	BA	729	G	C6-N1	-5.65	1.35	1.39
54	BA	2651	C	C4-N4	-5.65	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2708	G	C6-N1	-5.65	1.35	1.39
24	A3	19	G	C6-N1	-5.65	1.35	1.39
54	BA	1204	A	C5-C4	-5.65	1.34	1.38
21	AA	481	G	C6-N1	-5.65	1.35	1.39
21	AA	1140	C	C4-N4	-5.64	1.28	1.33
54	BA	1252	G	C2-N2	-5.64	1.28	1.34
54	BA	2127	G	C2-N2	-5.64	1.28	1.34
55	BB	39	A	C6-N1	-5.64	1.31	1.35
21	AA	1037	C	C4-N4	-5.64	1.28	1.33
54	BA	432	A	C5-C4	-5.64	1.34	1.38
54	BA	674	G	C2-N2	-5.64	1.28	1.34
54	BA	1471	G	N1-C2	-5.64	1.33	1.37
21	AA	1338	G	N1-C2	-5.64	1.33	1.37
54	BA	809	G	C2-N2	-5.64	1.28	1.34
54	BA	1376	C	C4-N4	-5.64	1.28	1.33
21	AA	518	C	N3-C4	-5.64	1.30	1.33
21	AA	893	C	N3-C4	-5.64	1.30	1.33
21	AA	1375	A	C6-N6	-5.64	1.29	1.33
54	BA	1351	C	N3-C4	-5.64	1.30	1.33
54	BA	1436	G	C6-N1	-5.64	1.35	1.39
54	BA	1669	A	C6-N1	-5.64	1.31	1.35
54	BA	1681	G	C2-N2	-5.64	1.28	1.34
54	BA	2084	C	C4-N4	-5.64	1.28	1.33
54	BA	731	C	C4-N4	-5.64	1.28	1.33
54	BA	927	A	C6-N1	-5.64	1.31	1.35
54	BA	2757	A	C5-C4	-5.64	1.34	1.38
21	AA	136	C	C4-N4	-5.64	1.28	1.33
21	AA	560	A	C5-C4	-5.64	1.34	1.38
54	BA	2693	G	N1-C2	-5.64	1.33	1.37
54	BA	1122	G	C2-N2	-5.63	1.28	1.34
21	AA	192	A	C6-N6	-5.63	1.29	1.33
21	AA	563	A	C6-N1	-5.63	1.31	1.35
54	BA	2061	G	C2-N2	-5.63	1.28	1.34
21	AA	1042	A	C6-N1	-5.63	1.31	1.35
54	BA	104	A	C5-C4	-5.63	1.34	1.38
54	BA	109	C	C4-N4	-5.63	1.28	1.33
54	BA	281	C	N3-C4	-5.63	1.30	1.33
54	BA	1772	A	C5-C4	-5.63	1.34	1.38
54	BA	2237	G	C2-N2	-5.63	1.28	1.34
54	BA	2824	C	C4-N4	-5.63	1.28	1.33
24	A3	65	G	C2-N2	-5.62	1.28	1.34
54	BA	1448	G	N1-C2	-5.62	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	53	G	C6-N1	-5.62	1.35	1.39
21	AA	168	G	C2-N2	-5.62	1.28	1.34
54	BA	1802	A	C6-N1	-5.62	1.31	1.35
55	BB	26	C	C4-N4	-5.62	1.28	1.33
21	AA	984	C	N3-C4	-5.62	1.30	1.33
21	AA	371	A	C5-C4	-5.62	1.34	1.38
21	AA	1402	C	C4-N4	-5.62	1.28	1.33
22	A1	2	G	N1-C2	-5.62	1.33	1.37
54	BA	2224	G	C6-N1	-5.62	1.35	1.39
54	BA	105	C	C4-N4	-5.62	1.28	1.33
54	BA	338	G	N1-C2	-5.62	1.33	1.37
54	BA	604	G	C2-N2	-5.62	1.28	1.34
54	BA	2084	C	N3-C4	-5.62	1.30	1.33
54	BA	1582	C	C4-N4	-5.61	1.28	1.33
54	BA	1675	C	N3-C4	-5.61	1.30	1.33
54	BA	1008	A	C6-N1	-5.61	1.31	1.35
21	AA	915	A	C6-N6	-5.61	1.29	1.33
54	BA	144	A	C6-N1	-5.61	1.31	1.35
54	BA	282	A	C6-N6	-5.61	1.29	1.33
54	BA	1089	A	C5-C4	-5.61	1.34	1.38
54	BA	1723	G	C2-N2	-5.61	1.28	1.34
54	BA	2789	C	N3-C4	-5.61	1.30	1.33
54	BA	172	A	C6-N1	-5.61	1.31	1.35
54	BA	285	G	C6-N1	-5.61	1.35	1.39
54	BA	2730	C	N3-C4	-5.61	1.30	1.33
55	BB	90	C	C4-N4	-5.61	1.28	1.33
21	AA	106	C	N3-C4	-5.61	1.30	1.33
21	AA	110	C	N3-C4	-5.61	1.30	1.33
21	AA	874	G	C2-N2	-5.61	1.28	1.34
21	AA	962	C	N3-C4	-5.61	1.30	1.33
21	AA	248	C	C4-N4	-5.60	1.28	1.33
21	AA	553	A	C5-C4	-5.60	1.34	1.38
21	AA	281	G	C2-N2	-5.60	1.28	1.34
54	BA	155	A	C5-C4	-5.60	1.34	1.38
54	BA	619	G	C2-N2	-5.60	1.28	1.34
21	AA	346	G	N1-C2	-5.60	1.33	1.37
54	BA	1371	G	C2-N2	-5.60	1.28	1.34
54	BA	203	A	C6-N1	-5.60	1.31	1.35
54	BA	1084	A	C6-N6	-5.60	1.29	1.33
54	BA	1475	G	N1-C2	-5.60	1.33	1.37
54	BA	2128	G	C6-N1	-5.60	1.35	1.39
54	BA	2761	A	C6-N1	-5.60	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	728	A	C6-N6	-5.60	1.29	1.33
21	AA	1350	A	C5-C4	-5.60	1.34	1.38
54	BA	1601	G	C6-N1	-5.60	1.35	1.39
54	BA	2355	G	C6-N1	-5.60	1.35	1.39
54	BA	2640	G	N1-C2	-5.60	1.33	1.37
22	A1	71	C	C4-N4	-5.59	1.28	1.33
54	BA	2365	G	C2-N2	-5.59	1.28	1.34
54	BA	2808	G	N1-C2	-5.59	1.33	1.37
54	BA	563	A	C6-N1	-5.59	1.31	1.35
54	BA	2209	G	N1-C2	-5.59	1.33	1.37
54	BA	216	A	C6-N1	-5.59	1.31	1.35
54	BA	784	G	C2-N2	-5.59	1.28	1.34
54	BA	1878	G	C6-N1	-5.59	1.35	1.39
54	BA	2668	G	C2-N2	-5.59	1.28	1.34
21	AA	339	C	N3-C4	-5.59	1.30	1.33
21	AA	1108	G	C6-N1	-5.59	1.35	1.39
54	BA	173	A	C6-N6	-5.59	1.29	1.33
54	BA	2232	C	C4-N4	-5.59	1.28	1.33
54	BA	2069	G	N1-C2	-5.58	1.33	1.37
21	AA	744	C	C4-N4	-5.58	1.28	1.33
54	BA	107	G	C2-N2	-5.58	1.28	1.34
21	AA	39	G	C6-N1	-5.58	1.35	1.39
55	BB	100	G	C2-N2	-5.58	1.28	1.34
21	AA	441	A	C5-C4	-5.58	1.34	1.38
54	BA	97	C	O3'-P	-5.58	1.54	1.61
21	AA	954	G	C2-N2	-5.58	1.28	1.34
54	BA	281	C	C4-N4	-5.57	1.28	1.33
54	BA	1710	G	C6-N1	-5.57	1.35	1.39
55	BB	51	G	C2-N2	-5.57	1.28	1.34
54	BA	207	A	C6-N1	-5.57	1.31	1.35
54	BA	2140	G	C6-N1	-5.57	1.35	1.39
21	AA	1446	A	C6-N1	-5.57	1.31	1.35
54	BA	410	G	C6-N1	-5.57	1.35	1.39
54	BA	2289	G	C6-N1	-5.57	1.35	1.39
21	AA	601	G	C4'-O4'	-5.57	1.38	1.45
21	AA	1346	A	C5-C4	-5.57	1.34	1.38
21	AA	1355	G	C2-N2	-5.57	1.28	1.34
54	BA	1718	G	C2-N2	-5.57	1.28	1.34
54	BA	299	A	C5-C4	-5.57	1.34	1.38
21	AA	1071	C	N3-C4	-5.56	1.30	1.33
21	AA	1429	A	C5-C4	-5.56	1.34	1.38
22	A1	53	G	C2-N2	-5.56	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2108	A	C6-N1	-5.56	1.31	1.35
21	AA	833	G	N1-C2	-5.56	1.33	1.37
21	AA	1336	C	C4-N4	-5.56	1.28	1.33
54	BA	517	C	C4-N4	-5.56	1.28	1.33
54	BA	1378	A	C6-N1	-5.56	1.31	1.35
54	BA	1756	G	N1-C2	-5.56	1.33	1.37
21	AA	1462	C	C4-N4	-5.56	1.28	1.33
54	BA	2227	A	C6-N6	-5.56	1.29	1.33
54	BA	2368	C	N3-C4	-5.56	1.30	1.33
54	BA	2565	A	C6-N1	-5.56	1.31	1.35
54	BA	2782	G	C2-N2	-5.56	1.28	1.34
54	BA	210	C	C4-N4	-5.55	1.28	1.33
54	BA	883	G	N1-C2	-5.55	1.33	1.37
54	BA	1800	C	N3-C4	-5.55	1.30	1.33
54	BA	1973	G	C6-N1	-5.55	1.35	1.39
21	AA	329	A	C6-N1	-5.55	1.31	1.35
54	BA	184	C	C4-N4	-5.55	1.28	1.33
54	BA	680	C	N3-C4	-5.55	1.30	1.33
21	AA	165	G	N1-C2	-5.55	1.33	1.37
54	BA	1986	C	C4-N4	-5.55	1.28	1.33
54	BA	2089	C	N3-C4	-5.55	1.30	1.33
54	BA	2112	G	C6-N1	-5.55	1.35	1.39
54	BA	2616	C	C4-N4	-5.55	1.28	1.33
21	AA	105	G	C2-N2	-5.55	1.29	1.34
21	AA	1489	G	N1-C2	-5.55	1.33	1.37
22	A1	42	G	C2-N2	-5.55	1.29	1.34
54	BA	1056	G	C2-N2	-5.55	1.29	1.34
54	BA	1752	C	N3-C4	-5.55	1.30	1.33
54	BA	1950	G	C6-N1	-5.55	1.35	1.39
54	BA	2692	G	C2-N2	-5.55	1.29	1.34
21	AA	174	A	C6-N1	-5.54	1.31	1.35
54	BA	282	A	C5-C4	-5.54	1.34	1.38
54	BA	732	C	C4-N4	-5.54	1.28	1.33
54	BA	2660	A	C6-N1	-5.54	1.31	1.35
55	BB	23	G	C2-N2	-5.54	1.29	1.34
54	BA	1071	G	C2-N2	-5.54	1.29	1.34
54	BA	1700	A	C5-C4	-5.54	1.34	1.38
54	BA	2606	C	C4-N4	-5.54	1.28	1.33
54	BA	2731	G	C2-N2	-5.54	1.29	1.34
55	BB	30	C	C4-N4	-5.54	1.28	1.33
21	AA	386	C	N3-C4	-5.54	1.30	1.33
22	A1	30	C	C4-N4	-5.54	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	228	C	C4-N4	-5.54	1.28	1.33
54	BA	473	G	C6-N1	-5.54	1.35	1.39
54	BA	532	A	C5-C4	-5.54	1.34	1.38
54	BA	1958	C	N3-C4	-5.54	1.30	1.33
54	BA	2814	A	C5-C4	-5.54	1.34	1.38
21	AA	193	C	C4-N4	-5.54	1.28	1.33
54	BA	2080	A	C6-N6	-5.54	1.29	1.33
54	BA	1986	C	N3-C4	-5.54	1.30	1.33
21	AA	732	C	C4-N4	-5.53	1.28	1.33
21	AA	1374	A	C6-N1	-5.53	1.31	1.35
21	AA	1399	C	N3-C4	-5.53	1.30	1.33
54	BA	145	C	N3-C4	-5.53	1.30	1.33
54	BA	201	C	C4-N4	-5.53	1.28	1.33
54	BA	1431	A	C6-N1	-5.53	1.31	1.35
54	BA	1732	C	C4-N4	-5.53	1.28	1.33
54	BA	2454	G	C2-N2	-5.53	1.29	1.34
21	AA	713	G	C4'-C3'	-5.53	1.47	1.52
54	BA	1465	G	N1-C2	-5.53	1.33	1.37
54	BA	1996	C	C4-N4	-5.53	1.28	1.33
54	BA	2624	G	C2-N2	-5.53	1.29	1.34
54	BA	1878	G	C2-N2	-5.53	1.29	1.34
21	AA	41	G	N1-C2	-5.53	1.33	1.37
21	AA	234	C	C4-N4	-5.53	1.28	1.33
54	BA	71	A	C6-N6	-5.53	1.29	1.33
54	BA	1098	A	C5-C4	-5.53	1.34	1.38
21	AA	1170	A	C6-N6	-5.53	1.29	1.33
54	BA	295	G	C6-N1	-5.53	1.35	1.39
54	BA	467	G	C2-N2	-5.53	1.29	1.34
54	BA	728	G	C2-N2	-5.53	1.29	1.34
21	AA	1104	G	C2-N2	-5.52	1.29	1.34
21	AA	382	A	C5-C4	-5.52	1.34	1.38
54	BA	149	A	C5-C4	-5.52	1.34	1.38
54	BA	608	A	C5-C4	-5.52	1.34	1.38
54	BA	1797	G	C2-N2	-5.52	1.29	1.34
54	BA	2777	G	C6-N1	-5.52	1.35	1.39
54	BA	63	A	C6-N6	-5.52	1.29	1.33
54	BA	386	G	C6-N1	-5.52	1.35	1.39
54	BA	445	C	N3-C4	-5.52	1.30	1.33
54	BA	684	G	C2-N2	-5.52	1.29	1.34
54	BA	1925	C	C4-N4	-5.52	1.28	1.33
54	BA	2110	G	N1-C2	-5.52	1.33	1.37
21	AA	336	A	C5-C4	-5.52	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	49	A	C5-C4	-5.52	1.34	1.38
54	BA	1447	C	C4-N4	-5.52	1.28	1.33
54	BA	1527	G	C2-N2	-5.52	1.29	1.34
21	AA	1081	A	C5-C4	-5.52	1.34	1.38
54	BA	447	A	C5-C4	-5.52	1.34	1.38
21	AA	44	A	C6-N1	-5.51	1.31	1.35
21	AA	312	C	C4-N4	-5.51	1.28	1.33
21	AA	1343	G	N1-C2	-5.51	1.33	1.37
54	BA	1359	A	C6-N1	-5.51	1.31	1.35
54	BA	2543	G	C2-N2	-5.51	1.29	1.34
21	AA	1057	G	N1-C2	-5.51	1.33	1.37
24	A3	57	C	N3-C4	-5.51	1.30	1.33
54	BA	1071	G	C6-N1	-5.51	1.35	1.39
21	AA	242	G	C2-N2	-5.51	1.29	1.34
54	BA	68	G	N1-C2	-5.51	1.33	1.37
21	AA	1147	C	C4-N4	-5.51	1.28	1.33
24	A3	2	G	N1-C2	-5.51	1.33	1.37
54	BA	426	C	N3-C4	-5.51	1.30	1.33
54	BA	1269	A	C6-N1	-5.51	1.31	1.35
54	BA	1560	G	C2-N2	-5.51	1.29	1.34
54	BA	2379	G	C6-N1	-5.51	1.35	1.39
54	BA	2657	A	C6-N1	-5.51	1.31	1.35
54	BA	1817	G	C2-N2	-5.50	1.29	1.34
21	AA	1343	G	C4'-O4'	-5.50	1.38	1.45
54	BA	41	C	N3-C4	-5.50	1.30	1.33
54	BA	377	G	C6-N1	-5.50	1.35	1.39
54	BA	1432	G	N1-C2	-5.50	1.33	1.37
54	BA	2221	G	C2-N2	-5.50	1.29	1.34
54	BA	2733	A	C6-N1	-5.50	1.31	1.35
54	BA	2771	C	C4-N4	-5.50	1.28	1.33
54	BA	2822	G	C6-N1	-5.50	1.35	1.39
21	AA	164	G	C6-N1	-5.50	1.35	1.39
21	AA	1418	A	C6-N6	-5.50	1.29	1.33
54	BA	41	C	C4-N4	-5.50	1.29	1.33
24	A3	53	G	C6-N1	-5.50	1.35	1.39
54	BA	938	G	N1-C2	-5.50	1.33	1.37
54	BA	1767	G	N1-C2	-5.50	1.33	1.37
21	AA	468	A	C5-C4	-5.49	1.34	1.38
54	BA	1710	G	C2-N2	-5.49	1.29	1.34
54	BA	2856	A	C6-N6	-5.49	1.29	1.33
21	AA	377	G	N1-C2	-5.49	1.33	1.37
54	BA	2154	A	C6-N1	-5.49	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	322	A	C5-C4	-5.49	1.34	1.38
54	BA	647	G	C6-N1	-5.49	1.35	1.39
54	BA	1740	G	C2-N2	-5.49	1.29	1.34
54	BA	2591	C	N3-C4	-5.49	1.30	1.33
21	AA	335	C	C4-N4	-5.49	1.29	1.33
21	AA	546	A	C4'-C3'	-5.49	1.47	1.52
21	AA	998	C	C4-N4	-5.49	1.29	1.33
21	AA	1191	A	C6-N6	-5.49	1.29	1.33
54	BA	79	C	C4-N4	-5.49	1.29	1.33
54	BA	801	G	N1-C2	-5.49	1.33	1.37
54	BA	1836	C	C4-N4	-5.49	1.29	1.33
54	BA	2179	C	N3-C4	-5.49	1.30	1.33
21	AA	873	A	C5-C4	-5.49	1.34	1.38
54	BA	1451	C	N3-C4	-5.49	1.30	1.33
54	BA	1552	A	C6-N1	-5.49	1.31	1.35
54	BA	1696	G	N1-C2	-5.49	1.33	1.37
54	BA	115	C	N3-C4	-5.48	1.30	1.33
54	BA	2264	C	N3-C4	-5.48	1.30	1.33
54	BA	301	G	C2-N2	-5.48	1.29	1.34
54	BA	1954	G	C2-N2	-5.48	1.29	1.34
54	BA	2060	A	C5-C4	-5.48	1.34	1.38
54	BA	71	A	C5-C4	-5.48	1.34	1.38
21	AA	1163	A	C6-N1	-5.48	1.31	1.35
21	AA	1428	A	C6-N6	-5.48	1.29	1.33
21	AA	800	G	C2-N2	-5.48	1.29	1.34
54	BA	1867	G	C2-N2	-5.48	1.29	1.34
54	BA	2349	G	C2-N2	-5.48	1.29	1.34
54	BA	2633	G	C6-N1	-5.48	1.35	1.39
54	BA	1665	A	C6-N6	-5.48	1.29	1.33
54	BA	2176	A	C6-N6	-5.48	1.29	1.33
54	BA	2496	C	C4-N4	-5.47	1.29	1.33
54	BA	2755	C	N3-C4	-5.47	1.30	1.33
21	AA	418	C	C4-N4	-5.47	1.29	1.33
21	AA	474	G	N1-C2	-5.47	1.33	1.37
21	AA	1071	C	C4-N4	-5.47	1.29	1.33
54	BA	2012	G	C2-N2	-5.47	1.29	1.34
21	AA	970	C	C4-N4	-5.47	1.29	1.33
54	BA	2608	G	C6-N1	-5.47	1.35	1.39
21	AA	386	C	C4-N4	-5.47	1.29	1.33
21	AA	1426	G	C2-N2	-5.47	1.29	1.34
54	BA	2691	C	N3-C4	-5.47	1.30	1.33
55	BB	24	G	N1-C2	-5.47	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1155	A	C6-N1	-5.46	1.31	1.35
54	BA	2258	C	N3-C4	-5.46	1.30	1.33
54	BA	2688	G	N1-C2	-5.46	1.33	1.37
54	BA	442	G	C2-N2	-5.46	1.29	1.34
21	AA	1072	G	N1-C2	-5.46	1.33	1.37
54	BA	2373	G	C2-N2	-5.46	1.29	1.34
54	BA	2719	G	C2-N2	-5.46	1.29	1.34
54	BA	2353	G	C2-N2	-5.46	1.29	1.34
21	AA	336	A	C6-N6	-5.46	1.29	1.33
21	AA	604	G	C2-N2	-5.46	1.29	1.34
54	BA	1555	G	N1-C2	-5.46	1.33	1.37
54	BA	625	G	C2-N2	-5.46	1.29	1.34
54	BA	2136	G	C6-N1	-5.46	1.35	1.39
54	BA	1788	C	N3-C4	-5.46	1.30	1.33
21	AA	914	A	C6-N1	-5.45	1.31	1.35
21	AA	735	C	N3-C4	-5.45	1.30	1.33
54	BA	299	A	C6-N6	-5.45	1.29	1.33
54	BA	5	A	C6-N6	-5.45	1.29	1.33
54	BA	1857	G	C2-N2	-5.45	1.29	1.34
54	BA	2123	G	C6-N1	-5.45	1.35	1.39
21	AA	1322	C	C4-N4	-5.45	1.29	1.33
54	BA	1407	G	C6-N1	-5.45	1.35	1.39
54	BA	2253	G	C6-N1	-5.45	1.35	1.39
54	BA	208	C	C4-N4	-5.45	1.29	1.33
54	BA	1320	C	C4-N4	-5.45	1.29	1.33
21	AA	311	C	N3-C4	-5.44	1.30	1.33
54	BA	1238	G	N1-C2	-5.44	1.33	1.37
54	BA	2226	C	N3-C4	-5.44	1.30	1.33
21	AA	620	C	C4-N4	-5.44	1.29	1.33
21	AA	1190	G	C2-N2	-5.44	1.29	1.34
54	BA	531	C	N3-C4	-5.44	1.30	1.33
54	BA	2587	A	C6-N6	-5.44	1.29	1.33
54	BA	2782	G	C6-N1	-5.44	1.35	1.39
54	BA	2808	G	C2-N2	-5.44	1.29	1.34
54	BA	2902	C	C4-N4	-5.44	1.29	1.33
55	BB	106	G	N1-C2	-5.44	1.33	1.37
54	BA	608	A	C6-N6	-5.44	1.29	1.33
54	BA	1063	G	C2-N2	-5.44	1.29	1.34
21	AA	212	G	N1-C2	-5.44	1.33	1.37
54	BA	48	G	C2-N2	-5.44	1.29	1.34
54	BA	2663	G	C2-N2	-5.44	1.29	1.34
54	BA	2762	C	C4-N4	-5.44	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	56	A	C6-N6	-5.44	1.29	1.33
54	BA	1632	A	C6-N1	-5.44	1.31	1.35
54	BA	1902	C	N3-C4	-5.43	1.30	1.33
21	AA	353	A	C5-C4	-5.43	1.34	1.38
21	AA	383	A	C6-N6	-5.43	1.29	1.33
21	AA	1112	C	N3-C4	-5.43	1.30	1.33
22	A1	68	C	C4-N4	-5.43	1.29	1.33
54	BA	804	A	C6-N1	-5.43	1.31	1.35
21	AA	92	U	C4'-O4'	-5.43	1.38	1.45
21	AA	839	C	N3-C4	-5.43	1.30	1.33
54	BA	1357	C	C4-N4	-5.43	1.29	1.33
54	BA	2053	G	C2-N2	-5.43	1.29	1.34
21	AA	664	G	N1-C2	-5.43	1.33	1.37
54	BA	301	G	C6-N1	-5.43	1.35	1.39
54	BA	372	G	C2-N2	-5.43	1.29	1.34
21	AA	1143	G	C2-N2	-5.43	1.29	1.34
54	BA	147	C	C4-N4	-5.43	1.29	1.33
54	BA	164	C	N3-C4	-5.43	1.30	1.33
54	BA	2102	G	C2-N2	-5.43	1.29	1.34
54	BA	2444	G	N1-C2	-5.43	1.33	1.37
54	BA	2894	G	N1-C2	-5.43	1.33	1.37
54	BA	1929	G	C2-N2	-5.42	1.29	1.34
21	AA	441	A	C6-N6	-5.42	1.29	1.33
54	BA	2014	A	C6-N1	-5.42	1.31	1.35
21	AA	566	G	C2-N2	-5.42	1.29	1.34
21	AA	1082	A	C6-N6	-5.42	1.29	1.33
54	BA	1654	A	C6-N6	-5.42	1.29	1.33
21	AA	355	C	C4-N4	-5.42	1.29	1.33
21	AA	674	G	C6-N1	-5.42	1.35	1.39
21	AA	784	A	C5-C4	-5.42	1.34	1.38
54	BA	396	G	C2-N2	-5.42	1.29	1.34
21	AA	171	A	C5-C4	-5.42	1.34	1.38
21	AA	980	C	C4-N4	-5.42	1.29	1.33
21	AA	1365	G	C6-N1	-5.42	1.35	1.39
54	BA	277	G	N1-C2	-5.42	1.33	1.37
54	BA	1319	C	C4-N4	-5.42	1.29	1.33
54	BA	1356	G	C2-N2	-5.42	1.29	1.34
55	BB	8	C	C4-N4	-5.42	1.29	1.33
21	AA	275	G	C6-N1	-5.42	1.35	1.39
21	AA	152	A	C6-N1	-5.41	1.31	1.35
21	AA	821	G	N1-C2	-5.41	1.33	1.37
21	AA	127	G	C6-N1	-5.41	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	155	A	C6-N6	-5.41	1.29	1.33
54	BA	637	A	C6-N1	-5.41	1.31	1.35
21	AA	1156	G	C2-N2	-5.41	1.29	1.34
24	A3	20	G	N1-C2	-5.41	1.33	1.37
54	BA	2625	G	N1-C2	-5.41	1.33	1.37
21	AA	57	G	C2-N2	-5.41	1.29	1.34
21	AA	550	G	C2-N2	-5.41	1.29	1.34
21	AA	838	G	C6-N1	-5.41	1.35	1.39
21	AA	1136	C	C4-N4	-5.41	1.29	1.33
21	AA	1187	G	C2-N2	-5.41	1.29	1.34
21	AA	1511	G	C2-N2	-5.41	1.29	1.34
54	BA	334	C	N3-C4	-5.41	1.30	1.33
54	BA	614	A	C6-N1	-5.41	1.31	1.35
54	BA	716	A	C5-C4	-5.41	1.34	1.38
54	BA	2191	A	C6-N1	-5.41	1.31	1.35
54	BA	2435	A	C6-N1	-5.41	1.31	1.35
54	BA	2644	G	C6-N1	-5.41	1.35	1.39
54	BA	2705	A	C6-N6	-5.41	1.29	1.33
21	AA	145	G	C6-N1	-5.41	1.35	1.39
21	AA	570	G	N1-C2	-5.41	1.33	1.37
22	A1	32	C	N3-C4	-5.41	1.30	1.33
54	BA	396	G	C6-N1	-5.41	1.35	1.39
54	BA	103	A	C6-N1	-5.41	1.31	1.35
54	BA	2284	A	C5-C4	-5.41	1.34	1.38
54	BA	2303	G	C2-N2	-5.41	1.29	1.34
54	BA	1430	G	C6-N1	-5.40	1.35	1.39
21	AA	661	G	C2-N2	-5.40	1.29	1.34
54	BA	1574	C	N3-C4	-5.40	1.30	1.33
54	BA	2267	A	C5-C4	-5.40	1.34	1.38
21	AA	408	A	C6-N1	-5.40	1.31	1.35
21	AA	687	A	C6-N1	-5.40	1.31	1.35
54	BA	130	C	C4-N4	-5.40	1.29	1.33
54	BA	1265	A	C6-N1	-5.40	1.31	1.35
54	BA	1343	G	C2-N2	-5.40	1.29	1.34
21	AA	1513	A	C5-C4	-5.40	1.34	1.38
54	BA	418	C	C4-N4	-5.40	1.29	1.33
21	AA	509	A	C6-N6	-5.40	1.29	1.33
54	BA	254	G	O3'-P	-5.40	1.54	1.61
21	AA	141	G	C6-N1	-5.40	1.35	1.39
54	BA	1336	A	C6-N6	-5.40	1.29	1.33
21	AA	26	A	C5-C4	-5.39	1.34	1.38
54	BA	218	A	C5-C4	-5.39	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1368	G	C6-N1	-5.39	1.35	1.39
54	BA	2027	G	C2-N2	-5.39	1.29	1.34
21	AA	217	C	C4-N4	-5.39	1.29	1.33
21	AA	1401	G	N1-C2	-5.39	1.33	1.37
54	BA	796	C	N3-C4	-5.39	1.30	1.33
55	BB	26	C	N3-C4	-5.39	1.30	1.33
21	AA	227	G	C2-N2	-5.39	1.29	1.34
21	AA	425	G	C2-N2	-5.39	1.29	1.34
54	BA	225	C	C4-N4	-5.39	1.29	1.33
54	BA	2341	G	C6-N1	-5.39	1.35	1.39
54	BA	2380	C	N3-C4	-5.39	1.30	1.33
21	AA	791	G	C4'-O4'	-5.39	1.38	1.45
24	A3	76	C	C4-N4	-5.39	1.29	1.33
23	A2	91	A	C6-N6	-5.39	1.29	1.33
54	BA	2174	C	N3-C4	-5.39	1.30	1.33
54	BA	8	C	N3-C4	-5.38	1.30	1.33
54	BA	1809	A	C6-N1	-5.38	1.31	1.35
54	BA	2829	A	C5-C4	-5.38	1.34	1.38
54	BA	267	C	C4-N4	-5.38	1.29	1.33
54	BA	1088	A	C6-N1	-5.38	1.31	1.35
54	BA	1757	A	C6-N1	-5.38	1.31	1.35
54	BA	2734	A	C5-C4	-5.38	1.34	1.38
21	AA	1172	C	N3-C4	-5.38	1.30	1.33
54	BA	933	A	C6-N6	-5.38	1.29	1.33
54	BA	1241	A	C6-N6	-5.38	1.29	1.33
54	BA	409	G	C2-N2	-5.38	1.29	1.34
54	BA	2658	C	C4-N4	-5.38	1.29	1.33
21	AA	402	G	N1-C2	-5.38	1.33	1.37
54	BA	544	C	N3-C4	-5.38	1.30	1.33
54	BA	2230	G	C2-N2	-5.38	1.29	1.34
21	AA	1069	C	N3-C4	-5.38	1.30	1.33
54	BA	2367	G	C6-N1	-5.38	1.35	1.39
21	AA	1434	A	C5-C4	-5.38	1.34	1.38
54	BA	274	C	C4-N4	-5.38	1.29	1.33
54	BA	1776	G	C2-N2	-5.38	1.29	1.34
54	BA	2389	G	C6-N1	-5.38	1.35	1.39
54	BA	2611	C	N3-C4	-5.38	1.30	1.33
54	BA	2670	A	C5-C4	-5.38	1.34	1.38
54	BA	2679	A	C6-N1	-5.38	1.31	1.35
55	BB	17	C	N3-C4	-5.38	1.30	1.33
21	AA	1488	G	C6-N1	-5.37	1.35	1.39
54	BA	354	A	C5-C4	-5.37	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	995	C	C4-N4	-5.37	1.29	1.33
54	BA	2128	G	C2-N2	-5.37	1.29	1.34
54	BA	2227	A	C5-C4	-5.37	1.34	1.38
21	AA	1374	A	C5-C4	-5.37	1.34	1.38
54	BA	273	G	C2-N2	-5.37	1.29	1.34
54	BA	400	G	C2-N2	-5.37	1.29	1.34
54	BA	1064	C	N3-C4	-5.37	1.30	1.33
54	BA	1697	G	C2-N2	-5.37	1.29	1.34
54	BA	2391	G	C2-N2	-5.37	1.29	1.34
21	AA	380	G	C2-N2	-5.37	1.29	1.34
54	BA	1792	G	N1-C2	-5.37	1.33	1.37
54	BA	2294	G	C2-N2	-5.37	1.29	1.34
54	BA	2515	C	C4-N4	-5.37	1.29	1.33
24	A3	7	G	N1-C2	-5.37	1.33	1.37
21	AA	1508	A	C5-C4	-5.36	1.34	1.38
55	BB	36	C	C4-N4	-5.36	1.29	1.33
21	AA	573	A	C4'-O4'	-5.36	1.38	1.45
21	AA	874	G	N1-C2	-5.36	1.33	1.37
21	AA	276	G	C2-N2	-5.36	1.29	1.34
21	AA	931	C	C4-N4	-5.36	1.29	1.33
54	BA	2311	A	C6-N1	-5.36	1.31	1.35
21	AA	1254	A	O3'-P	-5.36	1.54	1.61
21	AA	1336	C	N3-C4	-5.36	1.30	1.33
54	BA	342	A	C6-N6	-5.36	1.29	1.33
54	BA	136	G	N1-C2	-5.36	1.33	1.37
54	BA	1620	G	C2-N2	-5.36	1.29	1.34
54	BA	1984	G	C2-N2	-5.36	1.29	1.34
54	BA	2342	C	C4-N4	-5.36	1.29	1.33
21	AA	228	A	C6-N6	-5.35	1.29	1.33
54	BA	487	C	C4-N4	-5.35	1.29	1.33
54	BA	1608	A	C6-N1	-5.35	1.31	1.35
54	BA	2781	A	C6-N6	-5.35	1.29	1.33
54	BA	223	A	C6-N6	-5.35	1.29	1.33
21	AA	462	G	C6-N1	-5.35	1.35	1.39
54	BA	1014	A	O3'-P	-5.35	1.54	1.61
54	BA	2280	G	C2-N2	-5.35	1.29	1.34
54	BA	2801	G	C6-N1	-5.35	1.35	1.39
21	AA	247	G	C6-N1	-5.35	1.35	1.39
21	AA	324	G	N1-C2	-5.35	1.33	1.37
21	AA	352	C	N3-C4	-5.35	1.30	1.33
54	BA	914	G	N1-C2	-5.35	1.33	1.37
54	BA	1034	G	C2-N2	-5.35	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2199	A	C6-N6	-5.35	1.29	1.33
54	BA	2686	G	C2-N2	-5.35	1.29	1.34
54	BA	1092	C	C4-N4	-5.35	1.29	1.33
54	BA	1353	A	C6-N1	-5.35	1.31	1.35
21	AA	872	A	C5-C4	-5.34	1.35	1.38
21	AA	1191	A	C5-C4	-5.34	1.35	1.38
54	BA	2024	G	N1-C2	-5.34	1.33	1.37
24	A3	29	C	C4-N4	-5.34	1.29	1.33
54	BA	910	A	C6-N1	-5.34	1.31	1.35
54	BA	1676	A	C8-N7	-5.34	1.27	1.31
21	AA	664	G	C6-N1	-5.34	1.35	1.39
54	BA	297	G	N1-C2	-5.34	1.33	1.37
54	BA	1557	C	C4-N4	-5.34	1.29	1.33
54	BA	2061	G	C6-N1	-5.34	1.35	1.39
54	BA	2846	G	C6-N1	-5.34	1.35	1.39
54	BA	2170	A	C5-C4	-5.34	1.35	1.38
54	BA	2862	G	C2-N2	-5.34	1.29	1.34
24	A3	1	C	N3-C4	-5.33	1.30	1.33
54	BA	1241	A	C5-C4	-5.33	1.35	1.38
55	BB	81	G	C2-N2	-5.33	1.29	1.34
21	AA	1158	C	C4-N4	-5.33	1.29	1.33
21	AA	1422	G	C6-N1	-5.33	1.35	1.39
54	BA	1567	G	O3'-P	-5.33	1.54	1.61
54	BA	1785	A	C6-N6	-5.33	1.29	1.33
54	BA	2230	G	N1-C2	-5.33	1.33	1.37
21	AA	93	U	C4'-O4'	-5.33	1.38	1.45
54	BA	2089	C	C4-N4	-5.33	1.29	1.33
21	AA	1225	A	C6-N1	-5.33	1.31	1.35
21	AA	191	G	C2-N2	-5.33	1.29	1.34
54	BA	1572	A	C5-C4	-5.33	1.35	1.38
54	BA	2420	C	C4-N4	-5.33	1.29	1.33
54	BA	297	G	C2-N2	-5.32	1.29	1.34
54	BA	1124	G	C2-N2	-5.32	1.29	1.34
54	BA	1364	G	N1-C2	-5.32	1.33	1.37
54	BA	1726	C	C4-N4	-5.32	1.29	1.33
54	BA	2831	G	C2-N2	-5.32	1.29	1.34
21	AA	331	G	C2-N2	-5.32	1.29	1.34
21	AA	576	C	O3'-P	-5.32	1.54	1.61
54	BA	604	G	C6-N1	-5.32	1.35	1.39
21	AA	780	A	C6-N6	-5.32	1.29	1.33
54	BA	446	G	N1-C2	-5.32	1.33	1.37
54	BA	873	C	C4-N4	-5.32	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	676	A	C5-C4	-5.32	1.35	1.38
54	BA	2545	G	C2-N2	-5.32	1.29	1.34
21	AA	162	A	C6-N6	-5.32	1.29	1.33
24	A3	77	A	C5-C4	-5.32	1.35	1.38
54	BA	2812	G	C2-N2	-5.32	1.29	1.34
54	BA	2722	G	N1-C2	-5.32	1.33	1.37
21	AA	1105	A	C5-C4	-5.31	1.35	1.38
54	BA	294	A	C5-C4	-5.31	1.35	1.38
21	AA	305	G	N1-C2	-5.31	1.33	1.37
54	BA	1920	C	C4-N4	-5.31	1.29	1.33
54	BA	1099	G	C2-N2	-5.31	1.29	1.34
54	BA	1633	G	N1-C2	-5.31	1.33	1.37
54	BA	232	G	C2-N2	-5.31	1.29	1.34
54	BA	279	A	C6-N1	-5.31	1.31	1.35
54	BA	294	A	C6-N6	-5.31	1.29	1.33
54	BA	1093	G	C2-N2	-5.31	1.29	1.34
55	BB	21	G	C2-N2	-5.31	1.29	1.34
21	AA	858	G	C2-N2	-5.31	1.29	1.34
21	AA	1105	A	C6-N6	-5.31	1.29	1.33
54	BA	1363	C	C4-N4	-5.31	1.29	1.33
21	AA	425	G	C6-N1	-5.30	1.35	1.39
54	BA	188	G	N1-C2	-5.30	1.33	1.37
54	BA	2887	A	C5-C4	-5.30	1.35	1.38
21	AA	860	A	C6-N6	-5.30	1.29	1.33
21	AA	1523	G	N1-C2	-5.30	1.33	1.37
54	BA	1232	G	C2-N2	-5.30	1.29	1.34
21	AA	522	C	N3-C4	-5.30	1.30	1.33
21	AA	826	C	C4-N4	-5.30	1.29	1.33
21	AA	1003	G	C2-N2	-5.30	1.29	1.34
54	BA	1278	C	C4-N4	-5.30	1.29	1.33
54	BA	2212	A	C6-N6	-5.30	1.29	1.33
54	BA	2592	G	C8-N7	-5.30	1.27	1.30
21	AA	175	C	N3-C4	-5.30	1.30	1.33
21	AA	1187	G	C6-N1	-5.30	1.35	1.39
54	BA	2440	C	C4-N4	-5.30	1.29	1.33
54	BA	341	C	N3-C4	-5.29	1.30	1.33
54	BA	2114	A	C5-C4	-5.29	1.35	1.38
21	AA	356	A	C6-N6	-5.29	1.29	1.33
21	AA	860	A	C5-C4	-5.29	1.35	1.38
21	AA	861	G	C2-N2	-5.29	1.29	1.34
54	BA	640	C	N3-C4	-5.29	1.30	1.33
54	BA	1479	G	C2-N2	-5.29	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1493	C	C4-N4	-5.29	1.29	1.33
54	BA	2749	A	C5-C4	-5.29	1.35	1.38
21	AA	370	C	C4-N4	-5.29	1.29	1.33
21	AA	525	C	C4-N4	-5.29	1.29	1.33
54	BA	429	A	C6-N1	-5.29	1.31	1.35
54	BA	1654	A	C5-C4	-5.29	1.35	1.38
54	BA	2055	C	N3-C4	-5.29	1.30	1.33
21	AA	1429	A	C5'-C4'	5.29	1.57	1.51
54	BA	101	A	C6-N1	-5.29	1.31	1.35
54	BA	2738	A	C6-N6	-5.29	1.29	1.33
21	AA	510	A	C5-C4	-5.29	1.35	1.38
24	A3	71	G	C6-N1	-5.29	1.35	1.39
54	BA	333	G	C2-N2	-5.29	1.29	1.34
54	BA	2652	C	C4-N4	-5.29	1.29	1.33
21	AA	1217	C	C4-N4	-5.29	1.29	1.33
54	BA	269	C	N3-C4	-5.29	1.30	1.33
54	BA	712	G	N1-C2	-5.29	1.33	1.37
54	BA	1429	G	C2-N2	-5.29	1.29	1.34
54	BA	1435	G	C2-N2	-5.29	1.29	1.34
54	BA	2598	A	C6-N1	-5.29	1.31	1.35
54	BA	2819	G	N1-C2	-5.29	1.33	1.37
21	AA	530	G	N1-C2	-5.28	1.33	1.37
21	AA	797	C	C4-N4	-5.28	1.29	1.33
54	BA	579	G	O3'-P	-5.28	1.54	1.61
54	BA	681	G	N1-C2	-5.28	1.33	1.37
54	BA	1256	G	C2-N2	-5.28	1.29	1.34
54	BA	1810	A	C6-N1	-5.28	1.31	1.35
54	BA	2829	A	C6-N6	-5.28	1.29	1.33
55	BB	73	A	C6-N6	-5.28	1.29	1.33
22	A1	15	G	C2-N2	-5.28	1.29	1.34
54	BA	520	G	C2-N2	-5.28	1.29	1.34
54	BA	2501	C	O3'-P	-5.28	1.54	1.61
22	A1	75	C	C4-N4	-5.28	1.29	1.33
54	BA	354	A	C6-N6	-5.28	1.29	1.33
54	BA	1766	G	N1-C2	-5.28	1.33	1.37
21	AA	881	G	N1-C2	-5.27	1.33	1.37
21	AA	1385	G	C2-N2	-5.27	1.29	1.34
54	BA	1724	G	C6-N1	-5.27	1.35	1.39
54	BA	2049	G	C6-N1	-5.27	1.35	1.39
54	BA	2124	G	C2-N2	-5.27	1.29	1.34
21	AA	807	A	C4'-C3'	-5.27	1.47	1.52
21	AA	1423	G	N1-C2	-5.27	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	937	C	C4-N4	-5.27	1.29	1.33
54	BA	1981	A	C5-C4	-5.27	1.35	1.38
55	BB	35	C	C4-N4	-5.27	1.29	1.33
21	AA	57	G	N1-C2	-5.27	1.33	1.37
54	BA	805	G	C2-N2	-5.27	1.29	1.34
54	BA	1236	G	C2-N2	-5.27	1.29	1.34
54	BA	381	G	C2-N2	-5.27	1.29	1.34
54	BA	1118	C	C4-N4	-5.27	1.29	1.33
54	BA	2716	C	N3-C4	-5.27	1.30	1.33
21	AA	230	G	C2-N2	-5.27	1.29	1.34
21	AA	1080	A	C6-N1	-5.27	1.31	1.35
54	BA	1135	C	O3'-P	-5.27	1.54	1.61
54	BA	1420	A	C6-N6	-5.27	1.29	1.33
21	AA	1358	U	C4'-O4'	-5.26	1.38	1.45
21	AA	1405	G	C6-N1	-5.26	1.35	1.39
54	BA	1571	A	C5-C4	-5.26	1.35	1.38
21	AA	115	G	N1-C2	-5.26	1.33	1.37
21	AA	149	A	C6-N6	-5.26	1.29	1.33
21	AA	888	G	C4'-O4'	-5.26	1.38	1.45
54	BA	577	G	C2-N2	-5.26	1.29	1.34
54	BA	2036	C	C4-N4	-5.26	1.29	1.33
21	AA	958	A	C6-N6	-5.26	1.29	1.33
54	BA	529	A	C6-N6	-5.26	1.29	1.33
54	BA	740	C	N3-C4	-5.26	1.30	1.33
54	BA	1785	A	C5-C4	-5.26	1.35	1.38
54	BA	2383	G	C2-N2	-5.26	1.29	1.34
21	AA	413	G	C2-N2	-5.26	1.29	1.34
21	AA	604	G	C6-N1	-5.26	1.35	1.39
54	BA	177	G	C2-N2	-5.26	1.29	1.34
54	BA	2124	G	N1-C2	-5.26	1.33	1.37
54	BA	2744	G	N1-C2	-5.26	1.33	1.37
21	AA	128	G	C2-N2	-5.25	1.29	1.34
21	AA	444	G	C6-N1	-5.25	1.35	1.39
54	BA	2825	G	N1-C2	-5.25	1.33	1.37
21	AA	362	G	C2-N2	-5.25	1.29	1.34
21	AA	1362	A	C6-N1	-5.25	1.31	1.35
54	BA	1631	G	C2-N2	-5.25	1.29	1.34
54	BA	1819	A	C6-N6	-5.25	1.29	1.33
54	BA	2032	G	C6-N1	-5.25	1.35	1.39
55	BB	98	G	C6-N1	-5.25	1.35	1.39
21	AA	1204	A	C5-C4	-5.25	1.35	1.38
21	AA	1467	C	N3-C4	-5.25	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1519	A	C6-N6	-5.25	1.29	1.33
54	BA	739	A	C6-N1	-5.25	1.31	1.35
21	AA	925	G	C2-N2	-5.25	1.29	1.34
54	BA	143	C	N3-C4	-5.25	1.30	1.33
54	BA	250	G	C2-N2	-5.25	1.29	1.34
54	BA	1045	C	C4-N4	-5.25	1.29	1.33
54	BA	1248	G	C2-N2	-5.25	1.29	1.34
54	BA	1611	C	C4-N4	-5.25	1.29	1.33
21	AA	446	G	N1-C2	-5.25	1.33	1.37
21	AA	502	A	C4'-O4'	-5.25	1.38	1.45
54	BA	376	G	C2-N2	-5.25	1.29	1.34
54	BA	1399	C	C4-N4	-5.25	1.29	1.33
54	BA	2097	A	C5-C4	-5.25	1.35	1.38
54	BA	35	G	C2-N2	-5.25	1.29	1.34
54	BA	528	A	C6-N6	-5.25	1.29	1.33
54	BA	2037	A	C6-N1	-5.25	1.31	1.35
21	AA	310	G	C2-N2	-5.24	1.29	1.34
21	AA	903	G	O3'-P	-5.24	1.54	1.61
54	BA	1607	C	N3-C4	-5.24	1.30	1.33
54	BA	2830	C	C4-N4	-5.24	1.29	1.33
55	BB	76	G	N1-C2	-5.24	1.33	1.37
21	AA	918	A	C6-N1	-5.24	1.31	1.35
24	A3	7	G	C2-N2	-5.24	1.29	1.34
54	BA	656	G	C2-N2	-5.24	1.29	1.34
54	BA	930	G	C2-N2	-5.24	1.29	1.34
54	BA	1615	C	C4-N4	-5.24	1.29	1.33
54	BA	2314	A	C6-N1	-5.24	1.31	1.35
21	AA	1200	C	N3-C4	-5.24	1.30	1.33
54	BA	442	G	C6-N1	-5.24	1.35	1.39
54	BA	2156	G	C2-N2	-5.24	1.29	1.34
21	AA	746	A	C6-N1	-5.24	1.31	1.35
54	BA	1380	G	N1-C2	-5.24	1.33	1.37
54	BA	1616	A	C6-N1	-5.24	1.31	1.35
54	BA	1974	C	C4-N4	-5.24	1.29	1.33
21	AA	1092	A	N9-C4	-5.23	1.34	1.37
21	AA	147	G	C2-N2	-5.23	1.29	1.34
54	BA	64	A	C5-C4	-5.23	1.35	1.38
55	BB	2	G	N1-C2	-5.23	1.33	1.37
21	AA	318	G	N1-C2	-5.23	1.33	1.37
54	BA	711	G	C2-N2	-5.23	1.29	1.34
54	BA	1464	G	C2-N2	-5.23	1.29	1.34
54	BA	1068	G	N1-C2	-5.23	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1533	C	C4-N4	-5.23	1.29	1.33
21	AA	1204	A	C6-N6	-5.22	1.29	1.33
54	BA	1369	G	N1-C2	-5.22	1.33	1.37
54	BA	1489	C	C4-N4	-5.22	1.29	1.33
54	BA	1772	A	C6-N6	-5.22	1.29	1.33
54	BA	2803	G	N1-C2	-5.22	1.33	1.37
21	AA	1095	U	C4'-O4'	-5.22	1.38	1.45
54	BA	1702	G	C6-N1	-5.22	1.35	1.39
54	BA	2757	A	C6-N6	-5.22	1.29	1.33
54	BA	1220	G	C6-N1	-5.22	1.35	1.39
54	BA	1257	C	N3-C4	-5.22	1.30	1.33
21	AA	542	G	C2-N2	-5.22	1.29	1.34
21	AA	974	A	C6-N1	-5.22	1.31	1.35
54	BA	1207	C	N3-C4	-5.22	1.30	1.33
54	BA	1549	A	C6-N6	-5.22	1.29	1.33
54	BA	1724	G	C2-N2	-5.22	1.29	1.34
54	BA	1823	G	N1-C2	-5.22	1.33	1.37
54	BA	680	C	C4-N4	-5.22	1.29	1.33
54	BA	1073	A	C6-N6	-5.22	1.29	1.33
21	AA	260	G	O3'-P	-5.22	1.54	1.61
21	AA	880	C	C4-N4	-5.22	1.29	1.33
21	AA	906	A	C4'-O4'	-5.22	1.38	1.45
21	AA	953	G	C2-N2	-5.22	1.29	1.34
21	AA	969	A	C5-C4	-5.22	1.35	1.38
21	AA	1392	G	N1-C2	-5.22	1.33	1.37
54	BA	220	G	C6-N1	-5.22	1.35	1.39
54	BA	1665	A	C5-C4	-5.22	1.35	1.38
21	AA	204	G	N1-C2	-5.21	1.33	1.37
54	BA	346	A	C5-C4	-5.21	1.35	1.38
54	BA	673	C	N3-C4	-5.21	1.30	1.33
54	BA	2239	G	C6-N1	-5.21	1.35	1.39
54	BA	2663	G	C6-N1	-5.21	1.35	1.39
21	AA	474	G	C2-N2	-5.21	1.29	1.34
54	BA	2619	C	N3-C4	-5.21	1.30	1.33
21	AA	1209	C	N3-C4	-5.21	1.30	1.33
54	BA	1059	G	C2-N2	-5.21	1.29	1.34
21	AA	220	G	C2-N2	-5.21	1.29	1.34
21	AA	1448	C	C4-C5	-5.21	1.38	1.43
54	BA	229	C	C4-N4	-5.21	1.29	1.33
55	BB	15	A	C6-N6	-5.21	1.29	1.33
21	AA	845	A	C5-C4	-5.21	1.35	1.38
54	BA	1333	G	C2-N2	-5.21	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1572	A	C6-N6	-5.21	1.29	1.33
54	BA	2096	C	N3-C4	-5.21	1.30	1.33
21	AA	1514	G	N1-C2	-5.21	1.33	1.37
54	BA	627	A	C5-C4	-5.21	1.35	1.38
54	BA	760	G	C2-N2	-5.21	1.29	1.34
54	BA	1649	G	O3'-P	-5.21	1.54	1.61
54	BA	2610	C	C4-N4	-5.21	1.29	1.33
21	AA	252	U	C4'-O4'	-5.20	1.38	1.45
21	AA	312	C	N3-C4	-5.20	1.30	1.33
21	AA	506	G	C6-N1	-5.20	1.35	1.39
21	AA	624	C	N3-C4	-5.20	1.30	1.33
21	AA	1134	G	N1-C2	-5.20	1.33	1.37
54	BA	1538	G	C2-N2	-5.20	1.29	1.34
21	AA	958	A	C5-C4	-5.20	1.35	1.38
54	BA	739	A	C5-C4	-5.20	1.35	1.38
21	AA	580	C	C4-N4	-5.20	1.29	1.33
54	BA	1783	A	C5-C4	-5.20	1.35	1.38
54	BA	1826	G	C6-N1	-5.20	1.35	1.39
54	BA	2030	A	C6-N6	-5.20	1.29	1.33
54	BA	2575	C	C4-N4	-5.20	1.29	1.33
21	AA	971	G	C2-N2	-5.20	1.29	1.34
21	AA	991	U	C4'-O4'	-5.20	1.38	1.45
54	BA	1049	C	C4-N4	-5.20	1.29	1.33
54	BA	2279	G	C2-N2	-5.20	1.29	1.34
54	BA	1477	A	C6-N6	-5.20	1.29	1.33
54	BA	2295	C	C4-N4	-5.20	1.29	1.33
21	AA	378	G	N1-C2	-5.20	1.33	1.37
21	AA	755	G	C2-N2	-5.20	1.29	1.34
54	BA	183	C	N3-C4	-5.20	1.30	1.33
54	BA	348	A	C5-C4	-5.20	1.35	1.38
54	BA	620	G	C6-N1	-5.20	1.35	1.39
54	BA	2287	A	C6-N6	-5.20	1.29	1.33
54	BA	1667	G	C6-N1	-5.19	1.35	1.39
21	AA	823	C	C4-N4	-5.19	1.29	1.33
54	BA	186	G	C2-N2	-5.19	1.29	1.34
54	BA	1544	A	C6-N1	-5.19	1.31	1.35
54	BA	2200	C	N3-C4	-5.19	1.30	1.33
21	AA	488	C	N3-C4	-5.19	1.30	1.33
21	AA	869	G	C6-N1	-5.19	1.35	1.39
54	BA	792	A	C5-C4	-5.19	1.35	1.38
21	AA	377	G	C2-N2	-5.19	1.29	1.34
21	AA	1064	G	C2-N2	-5.19	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	687	A	C5-C4	-5.19	1.35	1.38
54	BA	81	G	C2-N2	-5.19	1.29	1.34
54	BA	1009	A	C6-N1	-5.19	1.31	1.35
54	BA	2731	G	C6-N1	-5.19	1.35	1.39
55	BB	54	G	N1-C2	-5.19	1.33	1.37
21	AA	853	C	N3-C4	-5.18	1.30	1.33
21	AA	890	G	C2-N2	-5.18	1.29	1.34
21	AA	993	G	C2-N2	-5.18	1.29	1.34
21	AA	1055	A	C6-N1	-5.18	1.31	1.35
54	BA	1658	C	C4-N4	-5.18	1.29	1.33
21	AA	406	G	C2-N2	-5.18	1.29	1.34
21	AA	925	G	N1-C2	-5.18	1.33	1.37
21	AA	1241	G	C4'-O4'	-5.18	1.38	1.45
54	BA	302	C	N3-C4	-5.18	1.30	1.33
54	BA	1368	G	C2-N2	-5.18	1.29	1.34
54	BA	159	G	N1-C2	-5.18	1.33	1.37
54	BA	1252	G	C6-N1	-5.18	1.35	1.39
54	BA	1675	C	C4-N4	-5.18	1.29	1.33
55	BB	85	G	C6-N1	-5.18	1.35	1.39
54	BA	277	G	C2-N2	-5.18	1.29	1.34
54	BA	1519	G	C6-N1	-5.18	1.35	1.39
54	BA	2776	A	C5-C4	-5.18	1.35	1.38
54	BA	1	G	C2-N2	-5.18	1.29	1.34
54	BA	2216	G	N1-C2	-5.18	1.33	1.37
21	AA	21	G	N1-C2	-5.18	1.33	1.37
21	AA	780	A	C5-C4	-5.18	1.35	1.38
21	AA	1152	A	C6-N6	-5.18	1.29	1.33
54	BA	584	C	C4-N4	-5.18	1.29	1.33
54	BA	1042	G	C2-N2	-5.18	1.29	1.34
54	BA	2294	G	C6-N1	-5.18	1.35	1.39
54	BA	2750	A	C6-N1	-5.18	1.31	1.35
54	BA	2834	G	C2-N2	-5.18	1.29	1.34
21	AA	295	C	N3-C4	-5.17	1.30	1.33
54	BA	2588	G	C2-N2	-5.17	1.29	1.34
54	BA	152	A	C6-N1	-5.17	1.31	1.35
54	BA	648	G	N1-C2	-5.17	1.33	1.37
54	BA	1480	C	N3-C4	-5.17	1.30	1.33
54	BA	2895	G	N1-C2	-5.17	1.33	1.37
21	AA	1214	C	C2'-C1'	-5.17	1.47	1.53
54	BA	1616	A	C5-C4	-5.17	1.35	1.38
54	BA	2788	C	N3-C4	-5.17	1.30	1.33
54	BA	2716	C	C4-N4	-5.17	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	668	G	C4'-C3'	-5.17	1.47	1.52
21	AA	1416	G	C6-N1	-5.17	1.35	1.39
22	A1	40	G	C2-N2	-5.17	1.29	1.34
54	BA	340	A	C6-N1	-5.17	1.31	1.35
54	BA	492	A	C6-N1	-5.17	1.31	1.35
54	BA	736	C	C4-N4	-5.17	1.29	1.33
54	BA	1072	C	N3-C4	-5.17	1.30	1.33
54	BA	1385	A	C5-C4	-5.17	1.35	1.38
54	BA	1566	A	C5-C4	-5.17	1.35	1.38
54	BA	1585	C	C4-N4	-5.17	1.29	1.33
21	AA	518	C	C4-N4	-5.17	1.29	1.33
54	BA	447	A	C6-N6	-5.17	1.29	1.33
54	BA	1516	G	C2-N2	-5.17	1.29	1.34
54	BA	1524	G	N1-C2	-5.17	1.33	1.37
54	BA	2361	G	C6-N1	-5.17	1.35	1.39
21	AA	104	G	C2-N2	-5.17	1.29	1.34
21	AA	382	A	C6-N6	-5.17	1.29	1.33
21	AA	658	C	C4'-O4'	-5.17	1.38	1.45
54	BA	323	C	C4-N4	-5.16	1.29	1.33
54	BA	654	A	C6-N6	-5.16	1.29	1.33
21	AA	774	G	C4'-O4'	-5.16	1.38	1.45
21	AA	1163	A	C5-C4	-5.16	1.35	1.38
21	AA	125	U	C4'-O4'	-5.16	1.38	1.45
21	AA	244	U	C2'-C1'	-5.16	1.47	1.53
54	BA	1702	G	C2-N2	-5.16	1.29	1.34
54	BA	2049	G	C2-N2	-5.16	1.29	1.34
21	AA	507	C	N3-C4	-5.16	1.30	1.33
21	AA	1098	C	N3-C4	-5.16	1.30	1.33
21	AA	1336	C	C2'-C1'	-5.16	1.47	1.53
54	BA	1450	G	C2-N2	-5.16	1.29	1.34
54	BA	2802	G	C6-N1	-5.16	1.35	1.39
54	BA	1025	G	O3'-P	-5.16	1.54	1.61
54	BA	1112	G	C6-N1	-5.16	1.35	1.39
54	BA	2709	G	N1-C2	-5.16	1.33	1.37
21	AA	40	C	N3-C4	-5.15	1.30	1.33
54	BA	526	A	C6-N1	-5.15	1.31	1.35
54	BA	2705	A	C5-C4	-5.15	1.35	1.38
21	AA	171	A	C6-N1	-5.15	1.31	1.35
21	AA	477	C	C4-N4	-5.15	1.29	1.33
21	AA	1274	A	C6-N1	-5.15	1.31	1.35
24	A3	52	C	C4-N4	-5.15	1.29	1.33
21	AA	186	C	N3-C4	-5.15	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	575	G	N1-C2	-5.15	1.33	1.37
54	BA	220	G	C2-N2	-5.15	1.29	1.34
54	BA	853	C	N3-C4	-5.15	1.30	1.33
21	AA	444	G	N1-C2	-5.15	1.33	1.37
21	AA	779	C	C4-N4	-5.15	1.29	1.33
21	AA	808	C	C4'-C3'	-5.15	1.47	1.52
21	AA	1429	A	C6-N6	-5.15	1.29	1.33
21	AA	1497	G	N1-C2	-5.15	1.33	1.37
54	BA	342	A	C5-C4	-5.14	1.35	1.38
54	BA	800	A	N9-C4	-5.14	1.34	1.37
54	BA	2107	G	C2-N2	-5.14	1.29	1.34
54	BA	2446	G	C2-N2	-5.14	1.29	1.34
21	AA	205	A	C6-N6	-5.14	1.29	1.33
21	AA	350	G	N1-C2	-5.14	1.33	1.37
54	BA	2255	G	N1-C2	-5.14	1.33	1.37
54	BA	2598	A	C5-C4	-5.14	1.35	1.38
54	BA	792	A	C6-N6	-5.14	1.29	1.33
13	AN	69	ARG	CZ-NH2	-5.14	1.26	1.33
21	AA	785	G	N1-C2	-5.14	1.33	1.37
21	AA	1525	G	C2-N2	-5.14	1.29	1.34
54	BA	359	G	C2-N2	-5.14	1.29	1.34
54	BA	2290	G	N1-C2	-5.14	1.33	1.37
54	BA	2328	A	C6-N1	-5.14	1.31	1.35
54	BA	2376	A	C5-C4	-5.14	1.35	1.38
54	BA	231	A	C6-N1	-5.14	1.31	1.35
54	BA	2165	C	C4-N4	-5.14	1.29	1.33
21	AA	1104	G	N1-C2	-5.14	1.33	1.37
54	BA	749	A	C5-C4	-5.14	1.35	1.38
54	BA	1455	G	N1-C2	-5.13	1.33	1.37
54	BA	2664	G	N1-C2	-5.13	1.33	1.37
21	AA	852	G	C6-N1	-5.13	1.35	1.39
21	AA	1153	G	N1-C2	-5.13	1.33	1.37
55	BB	76	G	C2-N2	-5.13	1.29	1.34
21	AA	284	C	C4-N4	-5.13	1.29	1.33
21	AA	418	C	C4'-O4'	-5.13	1.38	1.45
21	AA	1439	G	C2-N2	-5.13	1.29	1.34
24	A3	29	C	C4'-O4'	-5.13	1.38	1.45
54	BA	1050	A	O3'-P	-5.13	1.54	1.61
54	BA	1246	A	O3'-P	-5.13	1.54	1.61
21	AA	156	C	C4-N4	-5.13	1.29	1.33
54	BA	685	A	C6-N1	-5.13	1.31	1.35
54	BA	2168	G	C2-N2	-5.13	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BB	112	G	N1-C2	-5.13	1.33	1.37
21	AA	149	A	C5-C4	-5.13	1.35	1.38
21	AA	236	A	C6-N1	-5.13	1.31	1.35
54	BA	1567	G	N1-C2	-5.13	1.33	1.37
54	BA	1598	A	C6-N6	-5.13	1.29	1.33
21	AA	1074	G	C2-N2	-5.13	1.29	1.34
22	A1	27	C	C4-N4	-5.13	1.29	1.33
54	BA	809	G	C6-N1	-5.13	1.35	1.39
54	BA	844	A	C6-N1	-5.13	1.31	1.35
21	AA	50	A	C6-N1	-5.12	1.31	1.35
21	AA	178	C	C4-N4	-5.12	1.29	1.33
21	AA	1184	G	C2-N2	-5.12	1.29	1.34
54	BA	1128	G	C2-N2	-5.12	1.29	1.34
54	BA	1338	G	C2-N2	-5.12	1.29	1.34
54	BA	1490	A	C6-N1	-5.12	1.31	1.35
54	BA	1972	G	C2-N2	-5.12	1.29	1.34
21	AA	113	G	C6-N1	-5.12	1.35	1.39
54	BA	413	C	C4-N4	-5.12	1.29	1.33
54	BA	2284	A	C6-N6	-5.12	1.29	1.33
54	BA	2669	G	C2-N2	-5.12	1.29	1.34
21	AA	457	G	C6-N1	-5.12	1.35	1.39
54	BA	1632	A	C5-C4	-5.12	1.35	1.38
22	A1	38	A	C5-C4	-5.12	1.35	1.38
54	BA	1732	C	N3-C4	-5.12	1.30	1.33
54	BA	2513	A	C6-N1	-5.12	1.31	1.35
21	AA	159	G	N1-C2	-5.12	1.33	1.37
54	BA	2300	C	C4-N4	-5.12	1.29	1.33
21	AA	161	A	C6-N6	-5.12	1.29	1.33
21	AA	521	G	C6-N1	-5.12	1.35	1.39
21	AA	876	C	C4-N4	-5.12	1.29	1.33
21	AA	1162	C	N3-C4	-5.12	1.30	1.33
21	AA	1468	A	C5-C4	-5.12	1.35	1.38
54	BA	537	G	C6-N1	-5.12	1.35	1.39
54	BA	1933	G	C2-N2	-5.12	1.29	1.34
54	BA	2044	C	N3-C4	-5.12	1.30	1.33
21	AA	741	G	C2-N2	-5.11	1.29	1.34
21	AA	1382	C	C4-N4	-5.11	1.29	1.33
54	BA	1766	G	C2-N2	-5.11	1.29	1.34
54	BA	2114	A	C6-N6	-5.11	1.29	1.33
21	AA	919	A	C5-C4	-5.11	1.35	1.38
54	BA	51	G	C6-N1	-5.11	1.35	1.39
54	BA	1684	G	C6-N1	-5.11	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1545	A	C6-N6	-5.11	1.29	1.33
54	BA	2436	G	N1-C2	-5.11	1.33	1.37
21	AA	877	G	C2-N2	-5.11	1.29	1.34
54	BA	1211	C	C4-N4	-5.11	1.29	1.33
54	BA	144	A	C5-C4	-5.11	1.35	1.38
54	BA	1900	A	C5-C4	-5.11	1.35	1.38
54	BA	1974	C	N3-C4	-5.11	1.30	1.33
54	BA	2774	C	N3-C4	-5.11	1.30	1.33
54	BA	24	G	C6-N1	-5.11	1.35	1.39
54	BA	797	G	N1-C2	-5.11	1.33	1.37
54	BA	1783	A	C6-N6	-5.11	1.29	1.33
54	BA	2012	G	C6-N1	-5.11	1.35	1.39
54	BA	1085	A	C5-C4	-5.10	1.35	1.38
21	AA	602	A	C4'-O4'	-5.10	1.39	1.45
21	AA	859	G	C2-N2	-5.10	1.29	1.34
21	AA	1039	G	C2-N2	-5.10	1.29	1.34
21	AA	382	A	C6-N1	-5.10	1.31	1.35
21	AA	685	G	C6-N1	-5.10	1.35	1.39
21	AA	1457	G	C2-N2	-5.10	1.29	1.34
21	AA	589	U	C4'-O4'	-5.10	1.39	1.45
21	AA	1417	G	N1-C2	-5.10	1.33	1.37
21	AA	1518	A	C6-N1	-5.10	1.31	1.35
24	A3	57	C	C4-N4	-5.10	1.29	1.33
54	BA	23	G	C2-N2	-5.10	1.29	1.34
54	BA	2325	G	N1-C2	-5.10	1.33	1.37
54	BA	2681	C	N3-C4	-5.10	1.30	1.33
21	AA	1179	A	C4'-O4'	-5.10	1.39	1.45
54	BA	1702	G	N1-C2	-5.10	1.33	1.37
54	BA	1776	G	C6-N1	-5.10	1.35	1.39
54	BA	2429	G	C2-N2	-5.10	1.29	1.34
55	BB	59	A	C6-N1	-5.10	1.31	1.35
54	BA	24	G	C2-N2	-5.10	1.29	1.34
54	BA	2024	G	C2-N2	-5.10	1.29	1.34
21	AA	705	G	C2-N2	-5.09	1.29	1.34
21	AA	1352	C	C4-N4	-5.09	1.29	1.33
54	BA	346	A	C6-N1	-5.09	1.31	1.35
54	BA	2805	C	C4-N4	-5.09	1.29	1.33
21	AA	461	A	C6-N1	-5.09	1.31	1.35
21	AA	862	C	N3-C4	-5.09	1.30	1.33
54	BA	2002	G	C2-N2	-5.09	1.29	1.34
21	AA	745	G	C2-N2	-5.09	1.29	1.34
21	AA	1002	G	C2-N2	-5.09	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1591	A	C6-N1	-5.09	1.31	1.35
54	BA	2307	G	N1-C2	-5.09	1.33	1.37
21	AA	384	G	C2-N2	-5.09	1.29	1.34
21	AA	1114	C	N3-C4	-5.09	1.30	1.33
54	BA	1118	C	N3-C4	-5.09	1.30	1.33
54	BA	1750	G	C2-N2	-5.09	1.29	1.34
54	BA	2216	G	C6-N1	-5.09	1.35	1.39
55	BB	12	C	N3-C4	-5.09	1.30	1.33
54	BA	1804	C	C4-N4	-5.09	1.29	1.33
54	BA	2373	G	C6-N1	-5.09	1.35	1.39
21	AA	917	G	C2-N2	-5.09	1.29	1.34
54	BA	1679	A	C6-N6	-5.09	1.29	1.33
21	AA	932	C	C4-N4	-5.08	1.29	1.33
21	AA	47	C	N3-C4	-5.08	1.30	1.33
21	AA	873	A	C6-N6	-5.08	1.29	1.33
21	AA	1170	A	C5-C4	-5.08	1.35	1.38
54	BA	2071	A	C6-N1	-5.08	1.31	1.35
21	AA	132	C	C4-N4	-5.08	1.29	1.33
54	BA	1053	C	C4-N4	-5.08	1.29	1.33
54	BA	2718	G	C8-N7	-5.08	1.27	1.30
54	BA	2437	G	N1-C2	-5.08	1.33	1.37
21	AA	364	A	C6-N6	-5.08	1.29	1.33
21	AA	497	G	N1-C2	-5.08	1.33	1.37
21	AA	1234	C	C4-N4	-5.08	1.29	1.33
54	BA	1988	G	N1-C2	-5.08	1.33	1.37
54	BA	2634	A	C6-N1	-5.08	1.31	1.35
54	BA	2900	A	C6-N6	-5.08	1.29	1.33
21	AA	1027	C	O3'-P	-5.08	1.55	1.61
54	BA	1522	A	C6-N1	-5.08	1.31	1.35
54	BA	1708	C	C4-N4	-5.08	1.29	1.33
21	AA	177	G	N1-C2	-5.08	1.33	1.37
21	AA	178	C	C4-C5	-5.08	1.38	1.43
21	AA	557	G	C2-N2	-5.08	1.29	1.34
54	BA	249	C	C4-N4	-5.08	1.29	1.33
54	BA	389	G	C2-N2	-5.08	1.29	1.34
54	BA	1233	C	N3-C4	-5.08	1.30	1.33
54	BA	1566	A	C6-N1	-5.08	1.31	1.35
54	BA	1638	C	C4-N4	-5.08	1.29	1.33
55	BB	73	A	C5-C4	-5.08	1.35	1.38
21	AA	491	G	N1-C2	-5.07	1.33	1.37
54	BA	1403	A	C5-C4	-5.07	1.35	1.38
54	BA	1461	C	C4-N4	-5.07	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1902	C	C4-N4	-5.07	1.29	1.33
54	BA	1948	G	C8-N7	-5.07	1.27	1.30
54	BA	2890	G	N1-C2	-5.07	1.33	1.37
21	AA	396	C	C4-N4	-5.07	1.29	1.33
21	AA	1493	A	C6-N6	-5.07	1.29	1.33
54	BA	1999	C	C4-N4	-5.07	1.29	1.33
54	BA	2749	A	C6-N1	-5.07	1.31	1.35
54	BA	287	G	N1-C2	-5.07	1.33	1.37
54	BA	1427	A	C6-N6	-5.07	1.29	1.33
54	BA	2738	A	C6-N1	-5.07	1.32	1.35
21	AA	1047	G	C6-N1	-5.07	1.36	1.39
54	BA	245	G	O3'-P	-5.07	1.55	1.61
54	BA	432	A	C6-N6	-5.07	1.29	1.33
21	AA	243	A	C6-N1	-5.07	1.32	1.35
21	AA	513	C	C4-N4	-5.07	1.29	1.33
21	AA	584	G	C2-N2	-5.07	1.29	1.34
54	BA	35	G	C6-N1	-5.07	1.36	1.39
54	BA	528	A	C5-C4	-5.07	1.35	1.38
54	BA	1264	A	C6-N6	-5.07	1.29	1.33
54	BA	1828	G	N1-C2	-5.07	1.33	1.37
55	BB	118	C	N3-C4	-5.07	1.30	1.33
21	AA	18	C	C4-N4	-5.07	1.29	1.33
21	AA	97	G	N1-C2	-5.07	1.33	1.37
21	AA	134	G	C2-N2	-5.07	1.29	1.34
21	AA	349	A	C6-N6	-5.07	1.29	1.33
54	BA	705	A	C6-N1	-5.07	1.32	1.35
54	BA	1547	C	N3-C4	-5.07	1.30	1.33
54	BA	1797	G	C6-N1	-5.07	1.36	1.39
54	BA	2235	G	C2-N2	-5.07	1.29	1.34
21	AA	436	C	C4-N4	-5.06	1.29	1.33
54	BA	740	C	C4-N4	-5.06	1.29	1.33
21	AA	1281	C	C4-N4	-5.06	1.29	1.33
21	AA	1389	C	C4-N4	-5.06	1.29	1.33
54	BA	784	G	C6-N1	-5.06	1.36	1.39
21	AA	172	A	C5-C4	-5.06	1.35	1.38
54	BA	1831	G	C2-N2	-5.06	1.29	1.34
21	AA	424	G	C2-N2	-5.06	1.29	1.34
54	BA	944	C	N3-C4	-5.06	1.30	1.33
54	BA	1575	C	N3-C4	-5.06	1.30	1.33
54	BA	2033	A	C6-N1	-5.06	1.32	1.35
54	BA	2280	G	C6-N1	-5.06	1.36	1.39
21	AA	109	A	C6-N1	-5.05	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	818	G	O3'-P	-5.05	1.55	1.61
54	BA	1664	A	C6-N6	-5.05	1.29	1.33
54	BA	2872	A	N1-C2	-5.05	1.29	1.34
21	AA	126	G	C2-N2	-5.05	1.29	1.34
23	A2	80	C	C4-N4	-5.05	1.29	1.33
54	BA	532	A	C6-N6	-5.05	1.29	1.33
54	BA	1879	C	N3-C4	-5.05	1.30	1.33
54	BA	2171	A	C6-N6	-5.05	1.29	1.33
54	BA	190	A	C6-N1	-5.05	1.32	1.35
54	BA	2173	A	C6-N1	-5.05	1.32	1.35
21	AA	1350	A	C6-N6	-5.05	1.29	1.33
54	BA	268	C	N3-C4	-5.05	1.30	1.33
54	BA	836	G	C2-N2	-5.05	1.29	1.34
54	BA	1167	C	N3-C4	-5.05	1.30	1.33
54	BA	2579	C	N3-C4	-5.05	1.30	1.33
54	BA	2802	G	N1-C2	-5.05	1.33	1.37
21	AA	1353	G	C2-N2	-5.05	1.29	1.34
54	BA	1718	G	C6-N1	-5.05	1.36	1.39
54	BA	2386	A	C6-N6	-5.05	1.29	1.33
54	BA	2545	G	C6-N1	-5.05	1.36	1.39
21	AA	128	G	C6-N1	-5.05	1.36	1.39
54	BA	132	G	C2-N2	-5.05	1.29	1.34
54	BA	751	A	C5-C4	-5.05	1.35	1.38
54	BA	2157	G	C2-N2	-5.05	1.29	1.34
54	BA	2462	C	C4-N4	-5.05	1.29	1.33
54	BA	2064	C	C4-N4	-5.04	1.29	1.33
54	BA	2816	G	C2-N2	-5.04	1.29	1.34
21	AA	634	C	C4-N4	-5.04	1.29	1.33
21	AA	764	C	C4-N4	-5.04	1.29	1.33
21	AA	373	A	C6-N6	-5.04	1.29	1.33
21	AA	995	C	C4'-C3'	-5.04	1.47	1.52
21	AA	1181	G	C6-N1	-5.04	1.36	1.39
54	BA	477	A	C6-N1	-5.04	1.32	1.35
54	BA	610	C	N3-C4	-5.04	1.30	1.33
21	AA	1526	G	C6-N1	-5.04	1.36	1.39
54	BA	1518	C	C4-N4	-5.04	1.29	1.33
54	BA	1577	C	C4-N4	-5.04	1.29	1.33
21	AA	172	A	C6-N6	-5.04	1.29	1.33
23	A2	91	A	C5-C4	-5.04	1.35	1.38
54	BA	2316	G	C2-N2	-5.04	1.29	1.34
55	BB	86	G	C6-N1	-5.04	1.36	1.39
21	AA	142	G	N1-C2	-5.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	942	G	C2-N2	-5.04	1.29	1.34
21	AA	95	C	N3-C4	-5.04	1.30	1.33
21	AA	1366	C	C4-N4	-5.04	1.29	1.33
21	AA	433	G	C2-N2	-5.03	1.29	1.34
21	AA	1082	A	C5-C4	-5.03	1.35	1.38
54	BA	1048	A	C6-N1	-5.03	1.32	1.35
54	BA	2242	G	N1-C2	-5.03	1.33	1.37
54	BA	5	A	C5-C4	-5.03	1.35	1.38
54	BA	35	G	N1-C2	-5.03	1.33	1.37
54	BA	1420	A	C5-C4	-5.03	1.35	1.38
54	BA	2136	G	O3'-P	-5.03	1.55	1.61
21	AA	566	G	C6-N1	-5.03	1.36	1.39
21	AA	1368	A	C6-N6	-5.03	1.29	1.33
54	BA	438	G	N1-C2	-5.03	1.33	1.37
54	BA	911	A	C5-C4	-5.03	1.35	1.38
54	BA	2694	G	N1-C2	-5.03	1.33	1.37
21	AA	1002	G	C6-N1	-5.03	1.36	1.39
21	AA	1330	U	C4'-O4'	-5.03	1.39	1.45
54	BA	2433	A	C5-C4	-5.03	1.35	1.38
21	AA	1038	C	C4'-O4'	-5.03	1.39	1.45
21	AA	1503	A	C6-N1	-5.03	1.32	1.35
54	BA	89	A	C6-N1	-5.03	1.32	1.35
54	BA	1098	A	C6-N6	-5.03	1.29	1.33
54	BA	1831	G	N1-C2	-5.03	1.33	1.37
54	BA	2212	A	C5-C4	-5.03	1.35	1.38
21	AA	48	C	N3-C4	-5.02	1.30	1.33
21	AA	626	G	C2-N2	-5.02	1.29	1.34
54	BA	911	A	C6-N6	-5.02	1.29	1.33
21	AA	26	A	C6-N6	-5.02	1.29	1.33
21	AA	129	A	C5-C4	-5.02	1.35	1.38
54	BA	655	A	C6-N6	-5.02	1.29	1.33
54	BA	2567	G	O3'-P	-5.02	1.55	1.61
54	BA	2686	G	C6-N1	-5.02	1.36	1.39
54	BA	2753	A	N9-C4	-5.02	1.34	1.37
21	AA	270	A	C4'-O4'	-5.02	1.39	1.45
21	AA	391	G	N1-C2	-5.02	1.33	1.37
21	AA	572	A	C4'-O4'	-5.02	1.39	1.45
21	AA	824	G	C6-N1	-5.02	1.36	1.39
21	AA	1112	C	C4-N4	-5.02	1.29	1.33
54	BA	986	C	C4-N4	-5.02	1.29	1.33
54	BA	2733	A	C5-C4	-5.02	1.35	1.38
21	AA	1059	C	C4-N4	-5.02	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1317	C	N3-C4	-5.02	1.30	1.33
54	BA	764	A	C6-N1	-5.02	1.32	1.35
54	BA	1469	A	C6-N1	-5.02	1.32	1.35
54	BA	411	G	C6-N1	-5.02	1.36	1.39
54	BA	2024	G	C6-N1	-5.02	1.36	1.39
54	BA	9	G	C2-N2	-5.01	1.29	1.34
54	BA	336	C	N3-C4	-5.01	1.30	1.33
54	BA	490	C	N3-C4	-5.01	1.30	1.33
54	BA	1317	G	C6-N1	-5.01	1.36	1.39
21	AA	833	G	C2-N2	-5.01	1.29	1.34
54	BA	1037	G	C2-N2	-5.01	1.29	1.34
54	BA	2406	A	C6-N1	-5.01	1.32	1.35
21	AA	288	A	C5-C4	-5.01	1.35	1.38
21	AA	492	C	C4-N4	-5.01	1.29	1.33
21	AA	1454	G	C4'-O4'	-5.01	1.39	1.45
54	BA	2432	A	C6-N1	-5.01	1.32	1.35
21	AA	1499	A	C6-N1	-5.01	1.32	1.35
21	AA	1533	C	C4-N4	-5.01	1.29	1.33
54	BA	270	A	C5-C4	-5.01	1.35	1.38
54	BA	318	C	C4-N4	-5.01	1.29	1.33
54	BA	1089	A	C6-N6	-5.01	1.29	1.33
54	BA	2750	A	C5-C4	-5.01	1.35	1.38
55	BB	68	C	C4-N4	-5.01	1.29	1.33
21	AA	962	C	C4-N4	-5.01	1.29	1.33
54	BA	2862	G	C6-N1	-5.01	1.36	1.39
21	AA	1048	G	C2-N2	-5.01	1.29	1.34
21	AA	1403	C	N3-C4	-5.01	1.30	1.33
54	BA	1698	A	C6-N6	-5.01	1.29	1.33
54	BA	1893	C	O3'-P	-5.01	1.55	1.61
54	BA	2087	G	C2-N2	-5.01	1.29	1.34
55	BB	16	G	C6-N1	-5.01	1.36	1.39
54	BA	1434	A	C5-C4	-5.00	1.35	1.38
54	BA	1721	G	C2-N2	-5.00	1.29	1.34
54	BA	716	A	C6-N6	-5.00	1.29	1.33
54	BA	1746	A	C6-N1	-5.00	1.32	1.35
54	BA	2381	A	C6-N6	-5.00	1.29	1.33
21	AA	745	G	C4'-O4'	-5.00	1.39	1.45
54	BA	2335	A	C4'-O4'	-5.00	1.39	1.45
54	BA	2569	G	C2-N2	-5.00	1.29	1.34

All (8646) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2510	C	N3-C2-O2	-15.56	111.01	121.90
54	BA	975	A	N1-C6-N6	-13.84	110.30	118.60
54	BA	479	A	N1-C6-N6	-13.45	110.53	118.60
21	AA	412	A	N1-C6-N6	-12.78	110.93	118.60
54	BA	900	A	N1-C6-N6	-12.71	110.97	118.60
54	BA	2062	A	N1-C6-N6	-12.44	111.14	118.60
21	AA	172	A	N1-C6-N6	-12.39	111.17	118.60
23	A2	91	A	N1-C6-N6	-12.35	111.19	118.60
54	BA	2433	A	N1-C6-N6	-12.34	111.19	118.60
54	BA	2198	A	N1-C6-N6	-12.33	111.20	118.60
21	AA	845	A	N1-C6-N6	-12.29	111.23	118.60
21	AA	665	A	N1-C6-N6	-12.21	111.28	118.60
21	AA	1117	A	N1-C6-N6	-12.15	111.31	118.60
21	AA	676	A	N1-C6-N6	-12.11	111.33	118.60
55	BB	94	A	N1-C6-N6	-12.04	111.37	118.60
54	BA	1073	A	N1-C6-N6	-12.01	111.39	118.60
25	BC	176	ARG	NE-CZ-NH1	11.98	126.29	120.30
21	AA	364	A	N1-C6-N6	-11.94	111.44	118.60
21	AA	1188	A	N1-C6-N6	-11.92	111.45	118.60
21	AA	792	A	N1-C6-N6	-11.85	111.49	118.60
21	AA	1150	A	N1-C6-N6	-11.84	111.49	118.60
54	BA	910	A	N1-C6-N6	-11.82	111.50	118.60
54	BA	1359	A	N1-C6-N6	-11.82	111.51	118.60
54	BA	761	A	N1-C6-N6	-11.80	111.52	118.60
22	A1	66	A	N1-C6-N6	-11.78	111.53	118.60
21	AA	547	A	N1-C6-N6	-11.78	111.53	118.60
54	BA	1821	A	N1-C6-N6	-11.77	111.54	118.60
54	BA	371	A	N1-C6-N6	-11.77	111.54	118.60
54	BA	932	U	O4'-C1'-N1	11.77	117.62	108.20
54	BA	1970	A	N1-C6-N6	-11.77	111.54	118.60
54	BA	1404	C	N3-C2-O2	-11.75	113.68	121.90
54	BA	323	C	O4'-C1'-N1	11.74	117.59	108.20
21	AA	825	A	N1-C6-N6	-11.74	111.56	118.60
54	BA	931	U	O4'-C1'-N1	11.73	117.58	108.20
21	AA	493	A	N1-C6-N6	-11.67	111.60	118.60
54	BA	1021	A	N1-C6-N6	-11.67	111.60	118.60
54	BA	643	A	O4'-C1'-N9	11.65	117.52	108.20
54	BA	1552	A	N1-C6-N6	-11.62	111.63	118.60
21	AA	1042	A	N1-C6-N6	-11.58	111.65	118.60
54	BA	1641	A	N1-C6-N6	-11.58	111.65	118.60
54	BA	19	A	N1-C6-N6	-11.55	111.67	118.60
54	BA	2288	A	N1-C6-N6	-11.54	111.68	118.60
55	BB	34	A	N1-C6-N6	-11.51	111.70	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2872	A	N1-C6-N6	-11.48	111.71	118.60
54	BA	1142	A	N1-C6-N6	-11.46	111.73	118.60
13	AN	63	ARG	NE-CZ-NH1	11.43	126.02	120.30
54	BA	2090	A	N1-C6-N6	-11.43	111.74	118.60
54	BA	982	C	N3-C2-O2	-11.41	113.91	121.90
21	AA	510	A	N1-C6-N6	-11.41	111.75	118.60
54	BA	631	A	N1-C6-N6	-11.39	111.77	118.60
54	BA	2311	A	N1-C6-N6	-11.39	111.77	118.60
54	BA	1008	A	N1-C6-N6	-11.38	111.77	118.60
21	AA	914	A	N1-C6-N6	-11.38	111.77	118.60
54	BA	2426	A	N1-C6-N6	-11.37	111.78	118.60
13	AN	69	ARG	NE-CZ-NH1	11.36	125.98	120.30
54	BA	706	A	N1-C6-N6	-11.28	111.83	118.60
21	AA	382	A	N1-C6-N6	-11.28	111.83	118.60
54	BA	1545	A	N1-C6-N6	-11.27	111.84	118.60
21	AA	1285	A	N1-C6-N6	-11.24	111.86	118.60
21	AA	560	A	N1-C6-N6	-11.21	111.88	118.60
54	BA	825	A	N1-C6-N6	-11.20	111.88	118.60
54	BA	582	A	N1-C6-N6	-11.18	111.89	118.60
21	AA	152	A	N1-C6-N6	-11.16	111.90	118.60
54	BA	1404	C	N1-C2-O2	11.14	125.58	118.90
54	BA	2060	A	N1-C6-N6	-11.13	111.92	118.60
54	BA	497	A	N1-C6-N6	-11.13	111.92	118.60
54	BA	1133	A	N1-C6-N6	-11.13	111.92	118.60
54	BA	2823	A	N1-C6-N6	-11.13	111.92	118.60
21	AA	520	A	N1-C6-N6	-11.12	111.93	118.60
54	BA	1746	A	N1-C6-N6	-11.11	111.93	118.60
21	AA	1251	A	N1-C6-N6	-11.09	111.95	118.60
54	BA	1328	A	N1-C6-N6	-11.08	111.95	118.60
54	BA	750	A	N1-C6-N6	-11.08	111.95	118.60
21	AA	1197	A	N1-C6-N6	-11.07	111.96	118.60
54	BA	1505	A	N1-C6-N6	-11.06	111.96	118.60
21	AA	622	A	N1-C6-N6	-11.06	111.96	118.60
54	BA	347	A	N1-C6-N6	-11.03	111.98	118.60
24	A3	77	A	N1-C6-N6	-11.03	111.98	118.60
21	AA	1502	A	N1-C6-N6	-11.02	111.99	118.60
54	BA	2810	A	N1-C6-N6	-11.02	111.99	118.60
21	AA	1429	A	N1-C6-N6	-10.99	112.01	118.60
54	BA	2411	A	N1-C6-N6	-10.99	112.00	118.60
54	BA	2406	A	N1-C6-N6	-10.98	112.01	118.60
54	BA	161	A	N1-C6-N6	-10.97	112.02	118.60
46	BX	44	ARG	NE-CZ-NH1	10.96	125.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	821	A	N1-C6-N6	-10.95	112.03	118.60
21	AA	468	A	N1-C6-N6	-10.93	112.05	118.60
21	AA	181	A	N1-C6-N6	-10.92	112.05	118.60
21	AA	363	A	N1-C6-N6	-10.90	112.06	118.60
54	BA	529	A	N1-C6-N6	-10.89	112.07	118.60
21	AA	179	A	N1-C6-N6	-10.88	112.07	118.60
54	BA	1490	A	N1-C6-N6	-10.88	112.07	118.60
54	BA	384	A	N1-C6-N6	-10.88	112.07	118.60
54	BA	1759	A	N1-C6-N6	-10.88	112.07	118.60
54	BA	10	A	N1-C6-N6	-10.87	112.08	118.60
54	BA	2147	A	N1-C6-N6	-10.86	112.08	118.60
21	AA	1105	A	N1-C6-N6	-10.86	112.09	118.60
54	BA	217	A	N1-C6-N6	-10.84	112.09	118.60
54	BA	346	A	N1-C6-N6	-10.83	112.10	118.60
54	BA	1385	A	N1-C6-N6	-10.83	112.10	118.60
21	AA	523	A	N1-C6-N6	-10.82	112.11	118.60
54	BA	752	A	O4'-C1'-N9	10.82	116.86	108.20
54	BA	2598	A	N1-C6-N6	-10.82	112.11	118.60
54	BA	2267	A	N1-C6-N6	-10.81	112.11	118.60
17	AR	56	ARG	NE-CZ-NH1	10.80	125.70	120.30
21	AA	1288	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	279	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	1260	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	1420	A	N1-C6-N6	-10.80	112.12	118.60
21	AA	546	A	N1-C6-N6	-10.79	112.12	118.60
54	BA	2850	A	N1-C6-N6	-10.79	112.12	118.60
15	AP	25	ARG	NE-CZ-NH1	10.78	125.69	120.30
21	AA	356	A	N1-C6-N6	-10.78	112.13	118.60
54	BA	1098	A	N1-C6-N6	-10.78	112.13	118.60
54	BA	2439	A	N1-C6-N6	-10.77	112.14	118.60
54	BA	2381	A	N1-C6-N6	-10.77	112.14	118.60
21	AA	171	A	N1-C6-N6	-10.76	112.15	118.60
21	AA	1238	A	N1-C6-N6	-10.75	112.15	118.60
54	BA	2900	A	N1-C6-N6	-10.75	112.15	118.60
21	AA	366	A	N1-C6-N6	-10.74	112.15	118.60
21	AA	563	A	N1-C6-N6	-10.74	112.16	118.60
54	BA	2142	A	N1-C6-N6	-10.74	112.16	118.60
21	AA	109	A	N1-C6-N6	-10.73	112.16	118.60
21	AA	681	A	N1-C6-N6	-10.73	112.16	118.60
54	BA	504	A	N1-C6-N6	-10.73	112.16	118.60
21	AA	1374	A	N1-C6-N6	-10.72	112.17	118.60
54	BA	676	A	N1-C6-N6	-10.71	112.17	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	861	A	N1-C6-N6	-10.71	112.17	118.60
54	BA	528	A	N1-C6-N6	-10.70	112.18	118.60
54	BA	983	A	N1-C6-N6	-10.69	112.19	118.60
21	AA	1225	A	N1-C6-N6	-10.68	112.19	118.60
38	BP	100	ARG	NE-CZ-NH1	10.68	125.64	120.30
54	BA	1566	A	N1-C6-N6	-10.65	112.21	118.60
24	A3	60	A	N1-C6-N6	-10.65	112.21	118.60
21	AA	1151	A	N1-C6-N6	-10.65	112.21	118.60
21	AA	1441	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	2734	A	N1-C6-N6	-10.65	112.21	118.60
36	BN	64	ARG	NE-CZ-NH1	10.62	125.61	120.30
54	BA	223	A	N1-C6-N6	-10.61	112.23	118.60
54	BA	1808	A	N1-C6-N6	-10.61	112.23	118.60
54	BA	1652	A	N1-C6-N6	-10.61	112.24	118.60
21	AA	1518	A	N1-C6-N6	-10.60	112.24	118.60
21	AA	509	A	N1-C6-N6	-10.59	112.25	118.60
54	BA	614	A	N1-C6-N6	-10.59	112.25	118.60
54	BA	1916	A	N1-C6-N6	-10.59	112.25	118.60
21	AA	1468	A	N1-C6-N6	-10.59	112.25	118.60
21	AA	766	A	N1-C6-N6	-10.57	112.26	118.60
54	BA	2031	A	N1-C6-N6	-10.57	112.26	118.60
54	BA	715	A	N1-C6-N6	-10.57	112.26	118.60
54	BA	1327	A	N1-C6-N6	-10.55	112.27	118.60
55	BB	15	A	N1-C6-N6	-10.55	112.27	118.60
21	AA	383	A	N1-C6-N6	-10.54	112.27	118.60
54	BA	2751	G	O4'-C1'-N9	10.54	116.63	108.20
3	AD	110	ARG	NE-CZ-NH1	10.53	125.56	120.30
11	AL	30	ARG	NE-CZ-NH1	10.51	125.56	120.30
21	AA	1434	A	N1-C6-N6	-10.48	112.31	118.60
54	BA	1129	A	N1-C6-N6	-10.48	112.31	118.60
54	BA	172	A	N1-C6-N6	-10.47	112.32	118.60
21	AA	696	A	N1-C6-N6	-10.47	112.32	118.60
54	BA	94	A	N1-C6-N6	-10.46	112.32	118.60
21	AA	162	A	N1-C6-N6	-10.44	112.34	118.60
24	A3	73	A	C5-C6-N1	10.44	122.92	117.70
54	BA	1773	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	1535	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	1966	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	2080	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	1614	A	N1-C6-N6	-10.43	112.34	118.60
21	AA	807	A	N1-C6-N6	-10.42	112.35	118.60
54	BA	1365	A	N1-C6-N6	-10.41	112.35	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	91	A	O4'-C1'-N9	10.41	116.53	108.20
54	BA	144	A	N1-C6-N6	-10.41	112.35	118.60
54	BA	2274	A	N1-C6-N6	-10.41	112.35	118.60
54	BA	2307	G	O4'-C1'-N9	10.41	116.53	108.20
21	AA	1022	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	1711	A	N1-C6-N6	-10.39	112.36	118.60
54	BA	1134	A	N1-C6-N6	-10.39	112.37	118.60
54	BA	2358	A	N1-C6-N6	-10.39	112.37	118.60
54	BA	1276	A	N1-C6-N6	-10.39	112.37	118.60
54	BA	127	A	N1-C6-N6	-10.38	112.37	118.60
4	AE	28	ARG	NE-CZ-NH1	10.38	125.49	120.30
54	BA	2451	A	N1-C6-N6	-10.37	112.38	118.60
54	BA	1847	A	O4'-C1'-N9	10.37	116.50	108.20
54	BA	352	A	N1-C6-N6	-10.37	112.38	118.60
54	BA	2721	A	N1-C6-N6	-10.37	112.38	118.60
21	AA	873	A	N1-C6-N6	-10.36	112.38	118.60
3	AD	62	ARG	NE-CZ-NH1	10.34	125.47	120.30
6	AG	69	ARG	NE-CZ-NH1	10.33	125.47	120.30
21	AA	1191	A	N1-C6-N6	-10.33	112.40	118.60
54	BA	1981	A	N1-C6-N6	-10.32	112.41	118.60
54	BA	2158	A	N1-C6-N6	-10.32	112.41	118.60
54	BA	1654	A	N1-C6-N6	-10.32	112.41	118.60
21	AA	243	A	N1-C6-N6	-10.31	112.41	118.60
54	BA	1088	A	N1-C6-N6	-10.31	112.41	118.60
19	AT	73	ARG	NE-CZ-NH1	10.31	125.45	120.30
54	BA	556	A	N1-C6-N6	-10.30	112.42	118.60
54	BA	2639	A	N1-C6-N6	-10.30	112.42	118.60
21	AA	1318	A	N1-C6-N6	-10.30	112.42	118.60
54	BA	1679	A	N1-C6-N6	-10.29	112.42	118.60
21	AA	845	A	C5-C6-N1	10.28	122.84	117.70
21	AA	704	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	996	A	N1-C6-N6	-10.26	112.44	118.60
21	AA	329	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	661	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	2381	A	C4-C5-C6	-10.25	111.88	117.00
21	AA	937	A	N1-C6-N6	-10.24	112.45	118.60
54	BA	2726	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	1036	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	1167	A	N1-C6-N6	-10.23	112.46	118.60
54	BA	653	U	O4'-C1'-N1	10.23	116.38	108.20
54	BA	526	A	N1-C6-N6	-10.22	112.47	118.60
54	BA	270	A	N1-C6-N6	-10.22	112.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	130	A	N1-C6-N6	-10.22	112.47	118.60
54	BA	739	A	N1-C6-N6	-10.21	112.47	118.60
54	BA	2654	A	N1-C6-N6	-10.21	112.47	118.60
21	AA	1362	A	N1-C6-N6	-10.21	112.47	118.60
21	AA	1152	A	N1-C6-N6	-10.21	112.48	118.60
21	AA	495	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	480	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	2666	C	O4'-C1'-N1	10.19	116.35	108.20
54	BA	1969	A	N1-C6-N6	-10.19	112.49	118.60
26	BD	83	ARG	NE-CZ-NH1	10.19	125.39	120.30
54	BA	2873	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	515	A	N1-C6-N6	-10.18	112.49	118.60
21	AA	576	C	N3-C2-O2	-10.18	114.78	121.90
54	BA	877	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	1854	A	N1-C6-N6	-10.17	112.50	118.60
21	AA	162	A	C4-C5-C6	-10.17	111.92	117.00
54	BA	1241	A	N1-C6-N6	-10.16	112.50	118.60
21	AA	573	A	N1-C6-N6	-10.14	112.52	118.60
54	BA	280	U	O4'-C1'-N1	10.14	116.31	108.20
55	BB	29	A	N1-C6-N6	-10.13	112.52	118.60
54	BA	265	A	N1-C6-N6	-10.13	112.52	118.60
21	AA	251	G	O4'-C1'-N9	10.11	116.28	108.20
54	BA	1900	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	949	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	735	A	N1-C6-N6	-10.09	112.55	118.60
21	AA	353	A	C5-C6-N1	10.08	122.74	117.70
47	BY	23	ARG	NE-CZ-NH1	10.07	125.34	120.30
54	BA	945	A	N1-C6-N6	-10.07	112.56	118.60
21	AA	1508	A	N1-C6-N6	-10.06	112.56	118.60
54	BA	2386	A	N1-C6-N6	-10.06	112.56	118.60
21	AA	1324	A	N1-C6-N6	-10.06	112.57	118.60
21	AA	1346	A	C5-C6-N1	10.05	122.72	117.70
54	BA	1678	A	N1-C6-N6	-10.04	112.58	118.60
22	A1	41	A	N1-C6-N6	-10.04	112.58	118.60
54	BA	439	A	N1-C6-N6	-10.04	112.58	118.60
54	BA	1810	A	N1-C6-N6	-10.04	112.58	118.60
54	BA	160	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	227	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	447	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	2227	A	N1-C6-N6	-10.03	112.58	118.60
27	BE	114	ARG	NE-CZ-NH1	10.02	125.31	120.30
54	BA	1927	A	N1-C6-N6	-9.99	112.60	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	131	A	N1-C6-N6	-9.99	112.61	118.60
54	BA	1809	A	N1-C6-N6	-9.99	112.61	118.60
54	BA	1204	A	C5-C6-N1	9.98	122.69	117.70
54	BA	1819	A	C5-C6-N1	9.98	122.69	117.70
54	BA	42	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	71	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	1758	U	O4'-C1'-N1	9.97	116.18	108.20
54	BA	1819	A	N1-C6-N6	-9.97	112.62	118.60
21	AA	959	A	N1-C6-N6	-9.97	112.62	118.60
21	AA	781	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	507	A	N1-C6-N6	-9.96	112.62	118.60
54	BA	2761	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	161	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	2503	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	468	A	C5-C6-N1	9.95	122.67	117.70
21	AA	382	A	C5-C6-N1	9.93	122.67	117.70
34	BL	41	ARG	NE-CZ-NH1	9.93	125.27	120.30
21	AA	892	A	N1-C6-N6	-9.93	112.64	118.60
54	BA	1147	A	N1-C6-N6	-9.92	112.64	118.60
54	BA	2590	A	N1-C6-N6	-9.92	112.65	118.60
21	AA	51	A	N1-C6-N6	-9.92	112.65	118.60
21	AA	1428	A	N1-C6-N6	-9.92	112.65	118.60
21	AA	892	A	C4-C5-C6	-9.91	112.04	117.00
21	AA	1269	A	N1-C6-N6	-9.91	112.65	118.60
21	AA	935	A	N1-C6-N6	-9.91	112.66	118.60
35	BM	6	ARG	NE-CZ-NH1	9.91	125.25	120.30
54	BA	1987	A	N1-C6-N6	-9.91	112.66	118.60
21	AA	958	A	N1-C6-N6	-9.89	112.66	118.60
23	A2	91	A	C5-C6-N1	9.89	122.64	117.70
21	AA	32	A	N1-C6-N6	-9.88	112.67	118.60
55	BB	46	A	N1-C6-N6	-9.88	112.67	118.60
3	AD	164	ARG	NE-CZ-NH1	9.87	125.24	120.30
54	BA	374	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	1772	A	C5-C6-N1	9.87	122.64	117.70
54	BA	2030	A	N1-C6-N6	-9.87	112.68	118.60
21	AA	1252	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	1847	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	2850	A	O4'-C1'-N9	9.86	116.09	108.20
54	BA	2670	A	N1-C6-N6	-9.86	112.68	118.60
21	AA	665	A	C5-C6-N1	9.86	122.63	117.70
54	BA	412	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	2482	A	N1-C6-N6	-9.85	112.69	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	872	A	N1-C6-N6	-9.85	112.69	118.60
36	BN	30	ARG	NE-CZ-NH1	9.85	125.22	120.30
54	BA	527	C	N3-C2-O2	-9.85	115.01	121.90
21	AA	1534	A	C1'-O4'-C4'	-9.85	102.02	109.90
21	AA	1534	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	83	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	101	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	2634	A	N1-C6-N6	-9.84	112.70	118.60
21	AA	607	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	2419	U	O4'-C1'-N1	9.84	116.07	108.20
54	BA	49	A	N1-C6-N6	-9.83	112.70	118.60
21	AA	196	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	2530	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	368	A	N1-C6-N6	-9.82	112.71	118.60
21	AA	1340	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	2872	A	C5-C6-N1	9.81	122.61	117.70
54	BA	2781	A	C4-C5-C6	-9.81	112.10	117.00
13	AN	85	ARG	NE-CZ-NH1	9.80	125.20	120.30
21	AA	608	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	161	A	C5-C6-N1	9.80	122.60	117.70
21	AA	687	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	608	A	C5-C6-N1	9.80	122.60	117.70
54	BA	793	A	N1-C6-N6	-9.79	112.72	118.60
54	BA	1757	A	N1-C6-N6	-9.79	112.73	118.60
54	BA	2281	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	2176	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	2469	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	478	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	1528	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	1772	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	478	A	N1-C6-N6	-9.76	112.74	118.60
21	AA	907	A	N1-C6-N6	-9.76	112.74	118.60
12	AM	106	ARG	NE-CZ-NH1	9.76	125.18	120.30
54	BA	1353	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	1073	A	C5-C6-N1	9.74	122.57	117.70
55	BB	101	A	N1-C6-N6	-9.74	112.75	118.60
54	BA	529	A	C5-C6-N1	9.74	122.57	117.70
54	BA	1009	A	N1-C6-N6	-9.74	112.76	118.60
54	BA	1603	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	574	A	N1-C6-N6	-9.73	112.76	118.60
21	AA	728	A	C5-C6-N1	9.72	122.56	117.70
21	AA	1289	A	N1-C6-N6	-9.71	112.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	627	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	2792	A	N1-C6-N6	-9.70	112.78	118.60
21	AA	313	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1143	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	878	A	N1-C6-N6	-9.69	112.78	118.60
21	AA	460	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	241	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	670	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	1559	U	O4'-C1'-N1	9.68	115.94	108.20
54	BA	633	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	498	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	1211	C	O4'-C1'-N1	9.66	115.93	108.20
54	BA	1057	A	N1-C6-N6	-9.66	112.80	118.60
21	AA	919	A	N1-C6-N6	-9.65	112.81	118.60
24	A3	44	A	N1-C6-N6	-9.65	112.81	118.60
54	BA	428	A	N1-C6-N6	-9.64	112.82	118.60
21	AA	964	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	2170	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	1987	A	C5-C6-N1	9.63	122.51	117.70
21	AA	784	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	982	C	N1-C2-O2	9.62	124.67	118.90
54	BA	1593	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	1084	A	C5-C6-N1	9.60	122.50	117.70
54	BA	207	A	N1-C6-N6	-9.60	112.84	118.60
21	AA	1336	C	N3-C2-O2	-9.59	115.19	121.90
21	AA	1180	A	N1-C6-N6	-9.59	112.85	118.60
21	AA	1410	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	300	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	2126	A	O4'-C1'-N9	9.59	115.87	108.20
54	BA	196	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	498	A	C5-C6-N1	9.58	122.49	117.70
54	BA	430	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	1428	A	C5-C6-N1	9.57	122.49	117.70
6	AG	95	ARG	NE-CZ-NH1	9.57	125.09	120.30
54	BA	233	A	N1-C6-N6	-9.57	112.86	118.60
21	AA	364	A	C5-C6-N1	9.57	122.48	117.70
21	AA	1357	A	C4-C5-C6	-9.56	112.22	117.00
54	BA	2358	A	C5-C6-N1	9.56	122.48	117.70
54	BA	457	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	1404	C	O4'-C1'-N1	9.56	115.85	108.20
21	AA	353	A	N1-C6-N6	-9.55	112.87	118.60
55	BB	52	A	N1-C6-N6	-9.55	112.87	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	299	A	C5-C6-N1	9.55	122.47	117.70
54	BA	2882	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	2108	A	N1-C6-N6	-9.54	112.87	118.60
54	BA	2453	A	N1-C6-N6	-9.54	112.87	118.60
54	BA	1413	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	1630	A	N1-C6-N6	-9.54	112.88	118.60
8	AI	105	ARG	NE-CZ-NH1	9.53	125.06	120.30
21	AA	749	A	N1-C6-N6	-9.52	112.89	118.60
22	A1	38	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	1532	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	896	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	792	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	1772	A	C4-C5-C6	-9.50	112.25	117.00
54	BA	1713	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	1616	A	N1-C6-N6	-9.49	112.90	118.60
54	BA	2733	A	N1-C6-N6	-9.49	112.91	118.60
40	BR	79	ARG	NE-CZ-NH1	9.49	125.04	120.30
54	BA	792	A	C5-C6-N1	9.49	122.44	117.70
21	AA	451	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	563	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	1274	A	C5-C6-N1	9.48	122.44	117.70
21	AA	675	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	423	A	C5-C6-N1	9.47	122.44	117.70
54	BA	2309	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	767	A	N1-C6-N6	-9.47	112.92	118.60
20	AU	17	ARG	NE-CZ-NH1	9.47	125.03	120.30
54	BA	103	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	499	A	N1-C6-N6	-9.47	112.92	118.60
38	BP	88	ARG	NE-CZ-NH1	9.46	125.03	120.30
54	BA	846	U	O4'-C1'-N1	9.46	115.77	108.20
54	BA	432	A	N1-C6-N6	-9.45	112.93	118.60
4	AE	53	ARG	NE-CZ-NH1	9.45	125.03	120.30
54	BA	1427	A	C5-C6-N1	9.45	122.43	117.70
53	B4	36	ARG	NE-CZ-NH1	9.45	125.03	120.30
21	AA	349	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	923	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	599	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1609	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	246	A	N1-C6-N6	-9.44	112.93	118.60
54	BA	2587	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1340	U	O4'-C1'-N1	9.44	115.75	108.20
54	BA	2174	C	N3-C2-O2	-9.44	115.29	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	415	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	915	A	C5-C6-N1	9.44	122.42	117.70
21	AA	1519	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	2734	A	C5-C6-N1	9.43	122.42	117.70
54	BA	1084	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	1477	A	C5-C6-N1	9.43	122.41	117.70
54	BA	1626	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	190	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	872	A	C5-C6-N1	9.42	122.41	117.70
54	BA	668	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	2851	A	C5-C6-N1	9.42	122.41	117.70
54	BA	2886	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	2176	A	C4-C5-C6	-9.41	112.29	117.00
54	BA	176	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	356	A	C5-C6-N1	9.41	122.40	117.70
54	BA	592	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	1476	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	2267	A	C5-C6-N1	9.39	122.40	117.70
54	BA	470	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	250	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	2369	A	C5-C6-N1	9.38	122.39	117.70
21	AA	1145	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	2273	A	N1-C6-N6	-9.38	112.97	118.60
21	AA	371	A	N1-C6-N6	-9.37	112.98	118.60
21	AA	1171	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	2009	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	716	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1347	A	N1-C6-N6	-9.37	112.98	118.60
21	AA	26	A	C5-C6-N1	9.37	122.38	117.70
54	BA	44	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	2750	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1434	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	322	A	C5-C6-N1	9.36	122.38	117.70
21	AA	1219	A	N1-C6-N6	-9.36	112.99	118.60
22	A1	66	A	C5-C6-N1	9.35	122.38	117.70
13	AN	24	ARG	NE-CZ-NH1	9.35	124.97	120.30
54	BA	1046	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	218	A	N1-C6-N6	-9.34	112.99	118.60
54	BA	167	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	941	A	N1-C6-N6	-9.33	113.00	118.60
21	AA	397	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	1264	A	N1-C6-N6	-9.33	113.00	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2749	A	N1-C6-N6	-9.32	113.00	118.60
21	AA	819	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	1357	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	1901	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	1044	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	927	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	1513	A	C5-C6-N1	9.31	122.36	117.70
21	AA	143	A	N1-C6-N6	-9.31	113.01	118.60
54	BA	655	A	C5-C6-N1	9.31	122.36	117.70
21	AA	510	A	C5-C6-N1	9.31	122.35	117.70
54	BA	2800	A	N1-C6-N6	-9.31	113.02	118.60
55	BB	39	A	N1-C6-N6	-9.31	113.02	118.60
8	AI	122	ARG	NE-CZ-NH2	9.31	124.95	120.30
21	AA	300	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	1598	A	C5-C6-N1	9.30	122.35	117.70
42	BT	77	ARG	NE-CZ-NH1	9.30	124.95	120.30
54	BA	613	A	N1-C6-N6	-9.30	113.02	118.60
21	AA	383	A	C5-C6-N1	9.30	122.35	117.70
54	BA	1204	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	2886	A	O4'-C1'-N9	9.30	115.64	108.20
54	BA	456	C	N3-C2-O2	-9.30	115.39	121.90
21	AA	579	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	873	A	C5-C6-N1	9.29	122.34	117.70
54	BA	1434	A	C5-C6-N1	9.29	122.34	117.70
38	BP	20	ARG	NE-CZ-NH1	9.28	124.94	120.30
54	BA	125	A	C5-C6-N1	9.28	122.34	117.70
54	BA	693	A	N1-C6-N6	-9.28	113.03	118.60
21	AA	205	A	C5-C6-N1	9.28	122.34	117.70
39	BQ	91	ARG	NE-CZ-NH1	9.27	124.94	120.30
54	BA	2602	A	C5-C6-N1	9.27	122.33	117.70
54	BA	2227	A	C5-C6-N1	9.27	122.33	117.70
54	BA	354	A	N1-C6-N6	-9.26	113.04	118.60
54	BA	1610	A	N1-C6-N6	-9.26	113.04	118.60
54	BA	2614	A	C5-C6-N1	9.26	122.33	117.70
54	BA	477	A	N1-C6-N6	-9.26	113.04	118.60
54	BA	2322	A	C4-C5-C6	-9.26	112.37	117.00
21	AA	414	A	N1-C6-N6	-9.25	113.05	118.60
34	BL	18	ARG	NE-CZ-NH1	9.25	124.92	120.30
54	BA	346	A	C5-C6-N1	9.24	122.32	117.70
21	AA	493	A	C5-C6-N1	9.24	122.32	117.70
18	AS	77	ARG	NE-CZ-NH1	9.23	124.92	120.30
54	BA	1549	A	N1-C6-N6	-9.23	113.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1937	A	N1-C6-N6	-9.23	113.06	118.60
23	A2	79	A	N1-C6-N6	-9.23	113.06	118.60
54	BA	2705	A	C5-C6-N1	9.23	122.31	117.70
55	BB	15	A	C5-C6-N1	9.23	122.31	117.70
40	BR	21	ARG	NE-CZ-NH1	9.22	124.91	120.30
48	BZ	37	ARG	NE-CZ-NH1	9.22	124.91	120.30
54	BA	721	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	1803	A	N1-C6-N6	-9.22	113.07	118.60
21	AA	1375	A	C5-C6-N1	9.21	122.31	117.70
54	BA	2119	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	973	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	382	A	N1-C6-N6	-9.21	113.08	118.60
54	BA	979	A	N1-C6-N6	-9.21	113.08	118.60
54	BA	2675	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	1513	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	2450	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	63	A	C5-C6-N1	9.19	122.29	117.70
54	BA	1630	A	C5-C6-N1	9.19	122.30	117.70
21	AA	553	A	C5-C6-N1	9.19	122.29	117.70
21	AA	1285	A	C5-C6-N1	9.19	122.29	117.70
54	BA	2308	G	O4'-C1'-N9	9.19	115.55	108.20
21	AA	1299	A	C5-C6-N1	9.18	122.29	117.70
54	BA	1236	G	O4'-C1'-N9	9.18	115.55	108.20
54	BA	2090	A	C4-C5-C6	-9.18	112.41	117.00
21	AA	1170	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	911	A	C5-C6-N1	9.18	122.29	117.70
54	BA	1262	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	513	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	1247	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	509	A	C5-C6-N1	9.17	122.28	117.70
54	BA	2060	A	C5-C6-N1	9.17	122.28	117.70
54	BA	490	C	N3-C2-O2	-9.17	115.48	121.90
54	BA	1853	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	2030	A	C5-C6-N1	9.16	122.28	117.70
21	AA	1360	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	244	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	1090	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	330	A	O4'-C1'-N9	9.15	115.52	108.20
54	BA	743	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2173	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2211	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2825	G	O4'-C1'-N9	9.15	115.52	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1655	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	1170	A	C5-C6-N1	9.14	122.27	117.70
33	BK	78	ARG	NE-CZ-NH1	9.14	124.87	120.30
21	AA	1346	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	502	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	626	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	1280	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	1858	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	2090	A	C5-C6-N1	9.13	122.27	117.70
21	AA	931	C	N3-C2-O2	-9.13	115.51	121.90
42	BT	69	ARG	NE-CZ-NH1	9.13	124.86	120.30
54	BA	91	A	N1-C6-N6	-9.13	113.12	118.60
18	AS	80	ARG	NE-CZ-NH1	9.12	124.86	120.30
21	AA	371	A	C5-C6-N1	9.12	122.26	117.70
54	BA	990	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	928	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	483	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	441	A	C5-C6-N1	9.11	122.26	117.70
54	BA	1014	A	N1-C6-N6	-9.11	113.13	118.60
14	AO	76	ARG	NE-CZ-NH1	9.11	124.86	120.30
54	BA	654	A	C5-C6-N1	9.11	122.25	117.70
54	BA	920	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	943	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	1027	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	1637	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	2766	A	N1-C6-N6	-9.11	113.14	118.60
21	AA	958	A	C5-C6-N1	9.10	122.25	117.70
21	AA	1031	C	N3-C2-O2	-9.10	115.53	121.90
24	A3	73	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	905	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	1780	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	104	A	C5-C6-N1	9.10	122.25	117.70
54	BA	42	A	C4-C5-C6	-9.10	112.45	117.00
21	AA	155	A	N1-C6-N6	-9.09	113.14	118.60
21	AA	199	A	N1-C6-N6	-9.09	113.14	118.60
37	BO	33	ARG	NE-CZ-NH2	9.09	124.84	120.30
21	AA	298	A	C4-C5-C6	-9.08	112.46	117.00
21	AA	1216	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	1385	A	C5-C6-N1	9.08	122.24	117.70
21	AA	1418	A	C5-C6-N1	9.08	122.24	117.70
54	BA	546	U	O4'-C1'-N1	9.08	115.47	108.20
54	BA	2386	A	C4-C5-C6	-9.08	112.46	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1287	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	432	A	C5-C6-N1	9.08	122.24	117.70
21	AA	1169	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	192	A	N1-C6-N6	-9.07	113.16	118.60
38	BP	38	ARG	NE-CZ-NH1	9.07	124.84	120.30
54	BA	205	G	O4'-C1'-N9	9.07	115.46	108.20
54	BA	1932	A	C5-C6-N1	9.07	122.24	117.70
54	BA	2199	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	313	A	C4-C5-C6	-9.07	112.47	117.00
54	BA	1395	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	2284	A	C5-C6-N1	9.07	122.23	117.70
54	BA	1890	A	N1-C6-N6	-9.06	113.16	118.60
54	BA	959	A	N1-C6-N6	-9.06	113.16	118.60
54	BA	270	A	C5-C6-N1	9.06	122.23	117.70
54	BA	1085	A	C5-C6-N1	9.06	122.23	117.70
21	AA	408	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	718	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	1378	A	N1-C6-N6	-9.06	113.17	118.60
21	AA	913	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	2560	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1900	A	C5-C6-N1	9.05	122.23	117.70
54	BA	2665	A	N1-C6-N6	-9.05	113.17	118.60
21	AA	712	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	2154	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	28	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	104	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	804	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	1427	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	1509	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	1580	A	N1-C6-N6	-9.04	113.18	118.60
21	AA	279	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	1089	A	C5-C6-N1	9.04	122.22	117.70
37	BO	102	ARG	NE-CZ-NH1	9.03	124.82	120.30
54	BA	2887	A	C5-C6-N1	9.03	122.22	117.70
21	AA	228	A	C5-C6-N1	9.03	122.21	117.70
54	BA	2899	A	N1-C6-N6	-9.03	113.19	118.60
54	BA	1960	A	N1-C6-N6	-9.02	113.19	118.60
21	AA	44	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	896	A	C5-C6-N1	9.01	122.21	117.70
54	BA	2283	C	O4'-C1'-N1	9.01	115.41	108.20
21	AA	1021	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	56	A	C4-C5-C6	-9.01	112.49	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	423	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	2534	A	N1-C6-N6	-9.01	113.20	118.60
21	AA	695	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	915	A	C4-C5-C6	-9.00	112.50	117.00
21	AA	1337	G	C1'-O4'-C4'	-9.00	102.70	109.90
54	BA	218	A	C5-C6-N1	9.00	122.20	117.70
21	AA	181	A	C5-C6-N1	9.00	122.20	117.70
21	AA	906	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	1142	A	C5-C6-N1	9.00	122.20	117.70
21	AA	900	A	N1-C6-N6	-8.99	113.20	118.60
21	AA	949	A	C5-C6-N1	8.99	122.20	117.70
21	AA	1152	A	C5-C6-N1	8.99	122.20	117.70
54	BA	348	A	N1-C6-N6	-8.99	113.20	118.60
54	BA	1918	A	N1-C6-N6	-8.99	113.20	118.60
54	BA	1808	A	C5-C6-N1	8.99	122.19	117.70
54	BA	2241	A	N1-C6-N6	-8.99	113.21	118.60
55	BB	59	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	1275	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	1700	A	C5-C6-N1	8.98	122.19	117.70
54	BA	2542	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2739	U	O4'-C1'-N1	8.98	115.38	108.20
54	BA	2781	A	C5-C6-N1	8.98	122.19	117.70
21	AA	1109	C	N3-C2-O2	-8.97	115.62	121.90
54	BA	2392	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	1163	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	1346	A	C4-C5-C6	-8.96	112.52	117.00
54	BA	1570	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1275	A	C5-C6-N1	8.96	122.18	117.70
54	BA	2706	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	635	A	N1-C6-N6	-8.96	113.23	118.60
21	AA	715	A	N1-C6-N6	-8.96	113.23	118.60
21	AA	101	A	N1-C6-N6	-8.96	113.23	118.60
21	AA	889	A	N1-C6-N6	-8.96	113.23	118.60
54	BA	2346	A	N1-C6-N6	-8.96	113.23	118.60
21	AA	938	A	N1-C6-N6	-8.95	113.23	118.60
21	AA	649	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	2740	A	N1-C6-N6	-8.95	113.23	118.60
21	AA	72	A	N1-C6-N6	-8.94	113.23	118.60
21	AA	238	A	N1-C6-N6	-8.95	113.23	118.60
21	AA	546	A	C5-C6-N1	8.94	122.17	117.70
30	BH	27	ARG	NE-CZ-NH1	8.94	124.77	120.30
21	AA	129	A	N1-C6-N6	-8.94	113.24	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2868	A	N1-C6-N6	-8.94	113.24	118.60
21	AA	1508	A	C5-C6-N1	8.93	122.17	117.70
21	AA	1519	A	C5-C6-N1	8.93	122.17	117.70
25	BC	237	ARG	NE-CZ-NH1	8.93	124.77	120.30
54	BA	14	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	433	C	N3-C2-O2	-8.93	115.65	121.90
54	BA	1494	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	479	A	C5-C6-N1	8.93	122.16	117.70
21	AA	1117	A	C5-C6-N1	8.93	122.16	117.70
54	BA	2114	A	C5-C6-N1	8.92	122.16	117.70
54	BA	2510	C	N1-C2-O2	8.92	124.25	118.90
21	AA	129	A	C5-C6-N1	8.92	122.16	117.70
21	AA	192	A	C5-C6-N1	8.92	122.16	117.70
21	AA	1231	G	C1'-O4'-C4'	-8.92	102.77	109.90
54	BA	1302	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	1783	A	N1-C6-N6	-8.92	113.25	118.60
25	BC	216	ARG	NE-CZ-NH1	8.91	124.76	120.30
54	BA	2171	A	C5-C6-N1	8.91	122.16	117.70
54	BA	155	A	C5-C6-N1	8.91	122.16	117.70
54	BA	2814	A	C5-C6-N1	8.91	122.15	117.70
21	AA	1429	A	C4-C5-C6	-8.91	112.55	117.00
54	BA	675	A	N1-C6-N6	-8.91	113.26	118.60
21	AA	415	A	N1-C6-N6	-8.90	113.26	118.60
33	BK	31	ARG	NE-CZ-NH1	8.90	124.75	120.30
54	BA	1783	A	C5-C6-N1	8.90	122.15	117.70
22	A1	38	A	C5-C6-N1	8.90	122.15	117.70
54	BA	111	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	204	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1287	A	N1-C6-N6	-8.89	113.26	118.60
34	BL	78	ARG	NE-CZ-NH1	8.89	124.75	120.30
54	BA	63	A	N1-C6-N6	-8.89	113.26	118.60
24	A3	22	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	65	A	C5-C6-N1	8.89	122.14	117.70
21	AA	969	A	C5-C6-N1	8.89	122.14	117.70
54	BA	752	A	C5-C6-N1	8.89	122.14	117.70
54	BA	2058	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	994	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	1784	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	56	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	1552	A	O4'-C1'-N9	8.88	115.30	108.20
54	BA	1654	A	C5-C6-N1	8.87	122.14	117.70
21	AA	74	A	C5-C6-N1	8.87	122.13	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	223	A	C5-C6-N1	8.87	122.13	117.70
54	BA	1322	A	C5-C6-N1	8.86	122.13	117.70
21	AA	959	A	C5-C6-N1	8.86	122.13	117.70
36	BN	45	ARG	NE-CZ-NH1	8.86	124.73	120.30
21	AA	1110	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	2322	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	1264	A	C4-C5-C6	-8.86	112.57	117.00
54	BA	1701	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	2227	A	C4-C5-C6	-8.86	112.57	117.00
54	BA	645	C	N3-C2-O2	-8.86	115.70	121.90
54	BA	2799	A	N1-C6-N6	-8.86	113.29	118.60
21	AA	1111	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	1020	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	1431	A	N1-C6-N6	-8.85	113.29	118.60
42	BT	3	ARG	NE-CZ-NH1	8.85	124.72	120.30
54	BA	1336	A	C5-C6-N1	8.85	122.13	117.70
54	BA	2734	A	C4-C5-C6	-8.85	112.58	117.00
54	BA	5	A	C5-C6-N1	8.85	122.12	117.70
11	AL	98	ARG	NE-CZ-NH1	8.85	124.72	120.30
21	AA	915	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	1264	A	C5-C6-N1	8.85	122.12	117.70
54	BA	2829	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	1885	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	2434	A	C5-C6-N1	8.85	122.12	117.70
21	AA	1368	A	C5-C6-N1	8.85	122.12	117.70
54	BA	1566	A	C5-C6-N1	8.85	122.12	117.70
21	AA	1377	A	N1-C6-N6	-8.84	113.30	118.60
24	A3	38	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	829	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	988	A	C5-C6-N1	8.84	122.12	117.70
54	BA	2781	A	N1-C6-N6	-8.84	113.30	118.60
21	AA	1500	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	984	A	N1-C6-N6	-8.83	113.30	118.60
21	AA	841	C	N1-C2-O2	8.83	124.20	118.90
54	BA	439	A	C5-C6-N1	8.83	122.11	117.70
54	BA	1111	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	2900	A	C5-C6-N1	8.83	122.11	117.70
54	BA	637	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	611	C	N3-C2-O2	-8.81	115.73	121.90
21	AA	482	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	1098	A	C5-C6-N1	8.81	122.10	117.70
21	AA	860	A	C5-C6-N1	8.80	122.10	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	911	A	N1-C6-N6	-8.81	113.32	118.60
54	BA	1969	A	C5-C6-N1	8.81	122.10	117.70
54	BA	2654	A	C4-C5-C6	-8.81	112.60	117.00
54	BA	195	A	C5-C6-N1	8.80	122.10	117.70
54	BA	1760	C	N3-C2-O2	-8.80	115.74	121.90
10	AK	52	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	AB	62	ARG	NE-CZ-NH1	8.80	124.70	120.30
21	AA	572	A	C4-C5-C6	-8.79	112.60	117.00
54	BA	616	A	N1-C6-N6	-8.79	113.32	118.60
54	BA	2376	A	C5-C6-N1	8.79	122.10	117.70
21	AA	313	A	C5-C6-N1	8.79	122.10	117.70
21	AA	345	C	O4'-C1'-N1	8.79	115.23	108.20
54	BA	532	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	1086	A	C5-C6-N1	8.79	122.10	117.70
54	BA	2635	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	1930	G	O4'-C1'-N9	8.79	115.23	108.20
54	BA	1783	A	C4-C5-C6	-8.79	112.61	117.00
54	BA	789	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	74	A	C5-C6-N1	8.78	122.09	117.70
54	BA	909	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	1203	C	N3-C2-O2	-8.77	115.76	121.90
21	AA	681	A	C5-C6-N1	8.77	122.08	117.70
21	AA	729	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	518	C	N3-C2-O2	-8.76	115.77	121.90
54	BA	1241	A	C5-C6-N1	8.76	122.08	117.70
54	BA	1754	A	N1-C6-N6	-8.76	113.34	118.60
43	BU	6	ARG	NE-CZ-NH1	8.76	124.68	120.30
54	BA	2058	A	C4-C5-C6	-8.76	112.62	117.00
17	AR	52	ARG	NE-CZ-NH2	-8.75	115.92	120.30
21	AA	162	A	C5-C6-N1	8.75	122.08	117.70
54	BA	2856	A	C5-C6-N1	8.75	122.08	117.70
2	AC	130	ARG	NE-CZ-NH1	8.75	124.67	120.30
21	AA	794	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	864	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	1889	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	2711	A	N1-C6-N6	-8.75	113.35	118.60
55	BB	109	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	1311	A	N1-C6-N6	-8.74	113.35	118.60
54	BA	1095	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	1126	A	N1-C6-N6	-8.74	113.36	118.60
21	AA	78	A	N1-C6-N6	-8.74	113.36	118.60
21	AA	373	A	C5-C6-N1	8.74	122.07	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	125	A	N1-C6-N6	-8.74	113.36	118.60
21	AA	1248	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	2813	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	64	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1551	A	C4-C5-C6	-8.73	112.64	117.00
54	BA	2829	A	C5-C6-N1	8.73	122.06	117.70
54	BA	1987	A	C4-C5-C6	-8.73	112.64	117.00
54	BA	527	C	N1-C2-O2	8.73	124.14	118.90
54	BA	2762	C	N3-C2-O2	-8.72	115.79	121.90
18	AS	54	ARG	NE-CZ-NH1	8.72	124.66	120.30
54	BA	294	A	C5-C6-N1	8.72	122.06	117.70
54	BA	2540	C	O4'-C1'-N1	8.72	115.18	108.20
21	AA	74	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	1876	A	C5-C6-N1	8.72	122.06	117.70
54	BA	718	A	C5-C6-N1	8.72	122.06	117.70
54	BA	1700	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	2439	A	C5-C6-N1	8.72	122.06	117.70
54	BA	788	A	N1-C6-N6	-8.71	113.37	118.60
21	AA	780	A	C5-C6-N1	8.71	122.06	117.70
22	A1	6	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	119	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	676	A	C5-C6-N1	8.71	122.06	117.70
21	AA	205	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	833	A	N1-C6-N6	-8.71	113.38	118.60
33	BK	108	ARG	NE-CZ-NH1	8.71	124.65	120.30
21	AA	1016	A	N1-C6-N6	-8.70	113.38	118.60
25	BC	220	ARG	NE-CZ-NH1	8.70	124.65	120.30
54	BA	1665	A	C4-C5-C6	-8.70	112.65	117.00
54	BA	1761	C	N3-C2-O2	-8.70	115.81	121.90
54	BA	2080	A	C5-C6-N1	8.70	122.05	117.70
21	AA	1170	A	C4-C5-C6	-8.70	112.65	117.00
54	BA	222	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	1156	A	N1-C6-N6	-8.70	113.38	118.60
21	AA	1082	A	C4-C5-C6	-8.70	112.65	117.00
21	AA	792	A	C4-C5-C6	-8.69	112.66	117.00
24	A3	16	C	N3-C2-O2	-8.69	115.82	121.90
36	BN	12	ARG	NE-CZ-NH2	-8.69	115.96	120.30
54	BA	587	C	N3-C2-O2	-8.69	115.82	121.90
54	BA	2654	A	C5-C6-N1	8.69	122.04	117.70
54	BA	2097	A	N1-C6-N6	-8.69	113.39	118.60
21	AA	533	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	1302	A	C5-C6-N1	8.69	122.04	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2829	A	C4-C5-C6	-8.68	112.66	117.00
21	AA	1480	A	C4-C5-C6	-8.68	112.66	117.00
54	BA	2565	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1419	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	2433	A	C5-C6-N1	8.68	122.04	117.70
21	AA	1046	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	1785	A	C5-C6-N1	8.67	122.04	117.70
21	AA	1204	A	C5-C6-N1	8.67	122.03	117.70
54	BA	1032	A	C4-C5-C6	-8.67	112.67	117.00
21	AA	1012	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	2425	A	O4'-C1'-N9	8.67	115.13	108.20
54	BA	1451	C	O4'-C1'-N1	8.66	115.13	108.20
54	BA	2856	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	1211	C	N1-C2-O2	8.66	124.10	118.90
44	BV	9	ARG	NE-CZ-NH1	8.66	124.63	120.30
54	BA	2478	A	N1-C6-N6	-8.66	113.41	118.60
54	BA	1936	A	N1-C6-N6	-8.66	113.41	118.60
2	AC	142	ARG	NE-CZ-NH1	8.65	124.63	120.30
54	BA	1366	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	1664	A	C5-C6-N1	8.65	122.03	117.70
54	BA	439	A	C4-C5-C6	-8.65	112.68	117.00
54	BA	2879	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	2468	A	C5-C6-N1	8.64	122.02	117.70
54	BA	1260	A	C4-C5-C6	-8.64	112.68	117.00
21	AA	1493	A	C5-C6-N1	8.63	122.02	117.70
54	BA	2054	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	288	A	C5-C6-N1	8.63	122.02	117.70
54	BA	532	A	C5-C6-N1	8.63	122.02	117.70
21	AA	743	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	1281	C	N3-C2-O2	-8.63	115.86	121.90
54	BA	429	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	1272	A	O4'-C1'-N9	8.63	115.11	108.20
21	AA	1337	G	O4'-C1'-N9	8.63	115.10	108.20
54	BA	1213	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	1628	G	O4'-C1'-N9	8.63	115.10	108.20
21	AA	172	A	C4-C5-C6	-8.63	112.69	117.00
8	AI	98	ARG	NE-CZ-NH1	8.62	124.61	120.30
21	AA	573	A	C4-C5-C6	-8.62	112.69	117.00
12	AM	106	ARG	NE-CZ-NH2	-8.62	115.99	120.30
21	AA	889	A	C4-C5-C6	-8.61	112.69	117.00
21	AA	1429	A	C5-C6-N1	8.61	122.01	117.70
54	BA	140	C	N3-C2-O2	-8.61	115.87	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	282	A	C5-C6-N1	8.61	122.01	117.70
54	BA	2518	A	C4-C5-C6	-8.61	112.69	117.00
21	AA	1533	C	N3-C2-O2	-8.61	115.87	121.90
54	BA	1913	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	2346	A	C5-C6-N1	8.61	122.00	117.70
54	BA	742	A	N1-C6-N6	-8.61	113.44	118.60
21	AA	1105	A	C4-C5-C6	-8.60	112.70	117.00
54	BA	2076	U	O4'-C1'-N1	8.60	115.08	108.20
54	BA	2602	A	N1-C6-N6	-8.60	113.44	118.60
24	A3	74	A	N1-C6-N6	-8.60	113.44	118.60
22	A1	73	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	676	A	C5-C6-N1	8.59	122.00	117.70
21	AA	560	A	C5-C6-N1	8.59	122.00	117.70
54	BA	1090	A	C5-C6-N1	8.59	122.00	117.70
54	BA	1420	A	C5-C6-N1	8.59	122.00	117.70
54	BA	2101	A	N1-C6-N6	-8.59	113.45	118.60
16	AQ	5	ARG	NE-CZ-NH1	8.59	124.59	120.30
21	AA	373	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	1105	A	C5-C6-N1	8.59	121.99	117.70
21	AA	236	A	N1-C6-N6	-8.58	113.45	118.60
21	AA	371	A	C4-C5-C6	-8.58	112.71	117.00
54	BA	2587	A	C5-C6-N1	8.58	121.99	117.70
54	BA	71	A	C5-C6-N1	8.57	121.99	117.70
54	BA	980	A	C5-C6-N1	8.57	121.99	117.70
54	BA	2750	A	C5-C6-N1	8.57	121.99	117.70
21	AA	1434	A	C5-C6-N1	8.57	121.98	117.70
54	BA	1047	G	O4'-C1'-N9	8.57	115.06	108.20
54	BA	1050	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	1549	A	C5-C6-N1	8.57	121.99	117.70
23	A2	80	C	N3-C2-O2	-8.57	115.90	121.90
54	BA	152	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	2238	G	O4'-C1'-N9	8.57	115.05	108.20
11	AL	120	ARG	NE-CZ-NH1	8.56	124.58	120.30
21	AA	729	A	C4-C5-C6	-8.56	112.72	117.00
54	BA	792	A	C4-C5-C6	-8.56	112.72	117.00
21	AA	160	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	750	A	C4-C5-C6	-8.56	112.72	117.00
54	BA	936	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	53	A	N1-C6-N6	-8.56	113.47	118.60
21	AA	977	A	N1-C6-N6	-8.56	113.47	118.60
21	AA	1329	A	C5-C6-N1	8.55	121.98	117.70
54	BA	1244	A	N1-C6-N6	-8.56	113.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	354	A	C5-C6-N1	8.55	121.98	117.70
54	BA	2776	A	C5-C6-N1	8.55	121.98	117.70
21	AA	223	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	308	C	N3-C2-O2	-8.55	115.91	121.90
27	BE	21	ARG	NE-CZ-NH1	8.55	124.58	120.30
54	BA	454	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	328	C	N1-C2-O2	8.55	124.03	118.90
21	AA	901	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	172	A	C5-C6-N1	8.55	121.97	117.70
21	AA	937	A	C5-C6-N1	8.54	121.97	117.70
21	AA	1468	A	C5-C6-N1	8.54	121.97	117.70
54	BA	1981	A	C5-C6-N1	8.54	121.97	117.70
54	BA	2740	A	C5-C6-N1	8.54	121.97	117.70
54	BA	42	A	C5-C6-N1	8.54	121.97	117.70
54	BA	1054	A	N1-C6-N6	-8.54	113.48	118.60
20	AU	6	ARG	NE-CZ-NH1	8.53	124.57	120.30
21	AA	694	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	119	A	C4-C5-C6	-8.53	112.73	117.00
51	B2	33	ARG	NE-CZ-NH1	8.53	124.56	120.30
14	AO	16	ARG	NE-CZ-NH1	8.53	124.56	120.30
54	BA	627	A	C5-C6-N1	8.53	121.96	117.70
2	AC	10	ARG	NE-CZ-NH1	8.52	124.56	120.30
54	BA	1872	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	221	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	582	A	C4-C5-C6	-8.52	112.74	117.00
21	AA	663	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	702	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	1411	C	N3-C2-O2	-8.52	115.94	121.90
54	BA	1359	A	C5-C6-N1	8.52	121.96	117.70
54	BA	1515	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	309	A	N1-C6-N6	-8.52	113.49	118.60
22	A1	58	A	N1-C6-N6	-8.51	113.49	118.60
44	BV	93	ARG	NE-CZ-NH1	8.51	124.56	120.30
54	BA	2088	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	2814	A	N1-C6-N6	-8.51	113.49	118.60
21	AA	349	A	C5-C6-N1	8.51	121.95	117.70
21	AA	546	A	C4-C5-C6	-8.51	112.75	117.00
54	BA	608	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	1788	C	N3-C2-O2	-8.51	115.94	121.90
55	BB	73	A	N1-C6-N6	-8.51	113.49	118.60
21	AA	780	A	N1-C6-N6	-8.51	113.50	118.60
46	BX	49	ARG	NE-CZ-NH1	8.51	124.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	510	A	C4-C5-C6	-8.51	112.75	117.00
54	BA	1634	A	N1-C6-N6	-8.51	113.50	118.60
21	AA	841	C	N3-C2-O2	-8.50	115.95	121.90
54	BA	482	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	2381	A	C5-C6-N1	8.50	121.95	117.70
54	BA	2328	A	N1-C6-N6	-8.50	113.50	118.60
13	AN	90	ARG	NE-CZ-NH1	8.50	124.55	120.30
21	AA	673	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	1342	C	N3-C2-O2	-8.50	115.95	121.90
54	BA	1969	A	C4-C5-C6	-8.50	112.75	117.00
54	BA	2432	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	33	A	N1-C6-N6	-8.49	113.50	118.60
21	AA	65	A	N1-C6-N6	-8.49	113.50	118.60
21	AA	1169	A	C5-C6-N1	8.49	121.95	117.70
54	BA	889	C	N3-C2-O2	-8.49	115.96	121.90
54	BA	1403	A	C5-C6-N1	8.49	121.95	117.70
54	BA	1876	A	N1-C6-N6	-8.49	113.50	118.60
55	BB	78	A	N1-C6-N6	-8.49	113.50	118.60
21	AA	151	A	N1-C6-N6	-8.49	113.51	118.60
54	BA	716	A	O4'-C1'-N9	8.48	114.99	108.20
54	BA	1420	A	C4-C5-C6	-8.48	112.76	117.00
54	BA	2657	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1008	A	C5-C6-N1	8.48	121.94	117.70
54	BA	2288	A	C5-C6-N1	8.48	121.94	117.70
54	BA	2448	A	C4-C5-C6	-8.48	112.76	117.00
55	BB	109	A	C4-C5-C6	-8.48	112.76	117.00
54	BA	1490	A	C5-C6-N1	8.47	121.94	117.70
54	BA	2139	U	O4'-C1'-N1	8.47	114.98	108.20
21	AA	80	A	N1-C6-N6	-8.47	113.52	118.60
21	AA	968	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	149	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	2757	A	C5-C6-N1	8.47	121.94	117.70
54	BA	2451	A	C5-C6-N1	8.47	121.94	117.70
21	AA	65	A	C4-C5-C6	-8.47	112.77	117.00
21	AA	1054	C	O4'-C1'-N1	8.46	114.97	108.20
19	AT	24	ARG	NE-CZ-NH1	8.46	124.53	120.30
21	AA	60	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	528	A	C5-C6-N1	8.46	121.93	117.70
54	BA	526	A	C5-C6-N1	8.46	121.93	117.70
21	AA	8	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	1501	C	N3-C2-O2	-8.46	115.98	121.90
54	BA	1321	A	N1-C6-N6	-8.46	113.53	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	131	A	C4-C5-C6	-8.45	112.78	117.00
32	BJ	37	ARG	NE-CZ-NH1	8.45	124.53	120.30
21	AA	303	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	2176	A	C5-C6-N1	8.45	121.92	117.70
21	AA	576	C	N1-C2-O2	8.45	123.97	118.90
54	BA	2809	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	161	A	C4-C5-C6	-8.44	112.78	117.00
54	BA	2376	A	N1-C6-N6	-8.44	113.53	118.60
21	AA	466	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	2899	A	C5-C6-N1	8.44	121.92	117.70
4	AE	149	PRO	CA-N-CD	-8.44	99.68	111.50
54	BA	94	A	C5-C6-N1	8.44	121.92	117.70
54	BA	1550	C	N3-C2-O2	-8.44	115.99	121.90
54	BA	433	C	N1-C2-O2	8.44	123.96	118.90
54	BA	866	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	795	C	N3-C2-O2	-8.44	116.00	121.90
54	BA	2435	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	1082	A	C5-C6-N1	8.43	121.92	117.70
26	BD	128	ARG	NE-CZ-NH1	8.43	124.52	120.30
21	AA	1531	A	N1-C6-N6	-8.43	113.54	118.60
21	AA	1447	A	N1-C6-N6	-8.43	113.54	118.60
32	BJ	116	ARG	NE-CZ-NH1	8.43	124.51	120.30
54	BA	764	A	N1-C6-N6	-8.43	113.55	118.60
54	BA	2518	A	C5-C6-N1	8.43	121.91	117.70
21	AA	747	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2434	A	N1-C6-N6	-8.42	113.55	118.60
43	BU	85	ARG	NE-CZ-NH1	8.42	124.51	120.30
54	BA	644	A	C5-C6-N1	8.42	121.91	117.70
21	AA	53	A	C4-C5-C6	-8.42	112.79	117.00
21	AA	7	A	C4-C5-C6	-8.41	112.79	117.00
21	AA	174	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	2851	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	498	A	C4-C5-C6	-8.41	112.80	117.00
54	BA	2199	A	C5-C6-N1	8.41	121.90	117.70
54	BA	1336	A	C4-C5-C6	-8.41	112.80	117.00
54	BA	2547	A	N1-C6-N6	-8.41	113.56	118.60
21	AA	816	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	654	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	819	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	1503	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	1366	A	C4-C5-C6	-8.40	112.80	117.00
26	BD	13	ARG	NE-CZ-NH1	8.40	124.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	756	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2191	A	N1-C6-N6	-8.40	113.56	118.60
53	B4	24	ARG	NE-CZ-NH1	8.40	124.50	120.30
54	BA	1655	A	C4-C5-C6	-8.40	112.80	117.00
54	BA	1057	A	C5-C6-N1	8.39	121.90	117.70
54	BA	1786	A	N1-C6-N6	-8.39	113.56	118.60
21	AA	743	A	C5-C6-N1	8.39	121.89	117.70
54	BA	31	C	N3-C2-O2	-8.39	116.03	121.90
54	BA	2411	A	C5-C6-N1	8.39	121.89	117.70
54	BA	716	A	C5-C6-N1	8.39	121.89	117.70
54	BA	1647	U	O4'-C1'-N1	8.39	114.91	108.20
54	BA	721	A	C4-C5-C6	-8.39	112.81	117.00
54	BA	2738	A	C5-C6-N1	8.39	121.89	117.70
21	AA	1213	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	1871	A	N1-C6-N6	-8.38	113.57	118.60
21	AA	1191	A	C5-C6-N1	8.38	121.89	117.70
54	BA	2776	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	149	A	C5-C6-N1	8.38	121.89	117.70
54	BA	1732	C	N3-C2-O2	-8.38	116.04	121.90
54	BA	1789	A	C4-C5-C6	-8.38	112.81	117.00
21	AA	279	A	C5-C6-N1	8.37	121.89	117.70
21	AA	441	A	C4-C5-C6	-8.37	112.81	117.00
54	BA	2212	A	C5-C6-N1	8.37	121.89	117.70
54	BA	2287	A	C5-C6-N1	8.37	121.89	117.70
21	AA	1480	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	77	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1522	A	N1-C6-N6	-8.37	113.58	118.60
25	BC	211	ARG	NE-CZ-NH1	8.36	124.48	120.30
21	AA	389	A	N1-C6-N6	-8.36	113.58	118.60
21	AA	932	C	N3-C2-O2	-8.36	116.05	121.90
54	BA	2700	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	1784	A	C4-C5-C6	-8.36	112.82	117.00
54	BA	1952	A	N1-C6-N6	-8.36	113.58	118.60
21	AA	1046	A	C4-C5-C6	-8.35	112.82	117.00
21	AA	1014	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	219	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	1960	A	C5-C6-N1	8.35	121.88	117.70
56	B5	71	ARG	NE-CZ-NH1	8.35	124.48	120.30
56	B5	164	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	AB	138	ARG	NE-CZ-NH1	8.35	124.47	120.30
24	A3	77	A	C5-C6-N1	8.35	121.87	117.70
54	BA	2682	A	N1-C6-N6	-8.35	113.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1299	A	N1-C6-N6	-8.35	113.59	118.60
24	A3	74	A	C5-C6-N1	8.35	121.87	117.70
54	BA	1548	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	629	A	N1-C6-N6	-8.34	113.59	118.60
20	AU	33	ARG	NE-CZ-NH1	8.34	124.47	120.30
21	AA	1274	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	1301	A	C5-C6-N1	8.34	121.87	117.70
55	BB	70	C	N3-C2-O2	-8.34	116.06	121.90
54	BA	2032	G	C8-N9-C4	-8.34	103.06	106.40
22	A1	9	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	332	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	1545	A	C5-C6-N1	8.33	121.86	117.70
21	AA	1081	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	495	A	C5-C6-N1	8.33	121.86	117.70
54	BA	1080	A	N1-C6-N6	-8.33	113.61	118.60
54	BA	1535	A	C5-C6-N1	8.33	121.86	117.70
54	BA	1650	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	528	A	C4-C5-C6	-8.32	112.84	117.00
54	BA	2165	C	N3-C2-O2	-8.32	116.07	121.90
21	AA	50	A	C5-C6-N1	8.32	121.86	117.70
54	BA	56	A	C5-C6-N1	8.32	121.86	117.70
54	BA	177	G	O4'-C1'-N9	8.32	114.86	108.20
21	AA	26	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	325	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	699	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	218	A	C4-C5-C6	-8.32	112.84	117.00
29	BG	34	ARG	NE-CZ-NH1	8.31	124.46	120.30
24	A3	75	C	N3-C2-O2	-8.31	116.08	121.90
54	BA	449	A	N1-C6-N6	-8.31	113.61	118.60
21	AA	728	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	2476	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	2766	A	C5-C6-N1	8.31	121.86	117.70
54	BA	2541	A	N1-C6-N6	-8.31	113.61	118.60
21	AA	328	C	N3-C2-O2	-8.31	116.08	121.90
21	AA	1101	A	C4-C5-C6	-8.31	112.85	117.00
54	BA	213	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	2741	A	N1-C6-N6	-8.30	113.62	118.60
55	BB	15	A	O4'-C1'-N9	8.30	114.84	108.20
21	AA	431	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	2589	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	2882	A	C4-C5-C6	-8.30	112.85	117.00
54	BA	1090	A	C4-C5-C6	-8.30	112.85	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2575	C	N3-C2-O2	-8.30	116.09	121.90
21	AA	50	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	1175	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	1913	A	C5-C6-N1	8.29	121.85	117.70
48	BZ	30	ARG	NE-CZ-NH1	8.29	124.44	120.30
54	BA	727	A	C5-C6-N1	8.29	121.85	117.70
55	BB	57	A	C5-C6-N1	8.29	121.85	117.70
21	AA	559	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	910	A	C5-C6-N1	8.29	121.84	117.70
54	BA	1698	A	C5-C6-N1	8.29	121.84	117.70
54	BA	655	A	C4-C5-C6	-8.28	112.86	117.00
54	BA	1810	A	C5-C6-N1	8.28	121.84	117.70
54	BA	2407	A	N1-C6-N6	-8.28	113.63	118.60
21	AA	10	A	C4-C5-C6	-8.28	112.86	117.00
22	A1	35	A	C4-C5-C6	-8.28	112.86	117.00
54	BA	1237	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	1801	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	1938	A	C5-C6-N1	8.28	121.84	117.70
1	AB	112	ARG	NE-CZ-NH1	8.28	124.44	120.30
21	AA	1441	A	C5-C6-N1	8.28	121.84	117.70
54	BA	497	A	C5-C6-N1	8.28	121.84	117.70
54	BA	63	A	C4-C5-C6	-8.28	112.86	117.00
54	BA	196	A	O4'-C1'-N9	8.28	114.82	108.20
54	BA	1050	A	C5-C6-N1	8.28	121.84	117.70
54	BA	1876	A	C4-C5-C6	-8.28	112.86	117.00
54	BA	979	A	C5-C6-N1	8.27	121.84	117.70
54	BA	1165	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	865	A	N1-C6-N6	-8.27	113.64	118.60
45	BW	76	ARG	NE-CZ-NH1	8.27	124.44	120.30
54	BA	2660	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	336	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	2199	A	C4-C5-C6	-8.27	112.86	117.00
28	BF	177	ARG	NE-CZ-NH2	8.27	124.43	120.30
54	BA	2184	A	N1-C6-N6	-8.27	113.64	118.60
34	BL	47	ARG	NE-CZ-NH1	8.26	124.43	120.30
54	BA	2598	A	C5-C6-N1	8.26	121.83	117.70
54	BA	1569	A	N1-C6-N6	-8.26	113.64	118.60
19	AT	9	ARG	NE-CZ-NH1	8.26	124.43	120.30
22	A1	21	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	582	A	C5-C6-N1	8.26	121.83	117.70
21	AA	356	A	C4-C5-C6	-8.26	112.87	117.00
54	BA	342	A	C5-C6-N1	8.26	121.83	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1571	A	C5-C6-N1	8.26	121.83	117.70
21	AA	1398	A	C5-C6-N1	8.26	121.83	117.70
21	AA	149	A	C5-C6-N1	8.26	121.83	117.70
54	BA	1800	C	N3-C2-O2	-8.26	116.12	121.90
54	BA	2254	C	N3-C2-O2	-8.26	116.12	121.90
21	AA	262	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	374	A	C5-C6-N1	8.25	121.83	117.70
54	BA	1762	A	C5-C6-N1	8.25	121.83	117.70
21	AA	522	C	N3-C2-O2	-8.25	116.13	121.90
54	BA	689	A	C4-C5-C6	-8.25	112.88	117.00
54	BA	1020	A	C5-C6-N1	8.25	121.82	117.70
54	BA	2635	A	C5-C6-N1	8.25	121.82	117.70
21	AA	448	A	C5-C6-N1	8.24	121.82	117.70
49	B0	15	ARG	NE-CZ-NH1	8.24	124.42	120.30
54	BA	2644	G	O4'-C1'-N9	8.24	114.80	108.20
21	AA	1204	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1285	A	C4-C5-C6	-8.24	112.88	117.00
54	BA	2810	A	C5-C6-N1	8.24	121.82	117.70
54	BA	1655	A	C5-C6-N1	8.23	121.82	117.70
21	AA	1196	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2391	G	O4'-C1'-N9	8.23	114.79	108.20
54	BA	1493	C	N3-C2-O2	-8.23	116.14	121.90
21	AA	640	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	1368	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	1936	A	C5-C6-N1	8.23	121.82	117.70
54	BA	1847	A	C5-C6-N1	8.23	121.81	117.70
54	BA	2434	A	C4-C5-C6	-8.23	112.89	117.00
54	BA	204	A	C4-C5-C6	-8.23	112.89	117.00
54	BA	2764	A	N1-C6-N6	-8.23	113.66	118.60
1	AB	224	ARG	NE-CZ-NH1	8.22	124.41	120.30
21	AA	466	A	C5-C6-N1	8.22	121.81	117.70
54	BA	1111	A	C5-C6-N1	8.22	121.81	117.70
54	BA	2566	A	C5-C6-N1	8.22	121.81	117.70
24	A3	45	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	64	A	C5-C6-N1	8.22	121.81	117.70
54	BA	2513	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1528	A	C5-C6-N1	8.22	121.81	117.70
54	BA	2418	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1088	A	C5-C6-N1	8.21	121.81	117.70
55	BB	8	C	N3-C2-O2	-8.21	116.15	121.90
21	AA	274	A	N1-C6-N6	-8.21	113.67	118.60
41	BS	18	ARG	NE-CZ-NH1	8.21	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AI	118	ARG	NE-CZ-NH1	8.21	124.40	120.30
36	BN	12	ARG	NE-CZ-NH1	8.21	124.40	120.30
21	AA	815	A	N1-C6-N6	-8.21	113.68	118.60
54	BA	715	A	C5-C6-N1	8.21	121.80	117.70
54	BA	2335	A	C5-C6-N1	8.21	121.80	117.70
21	AA	1418	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	443	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1354	A	C5-C6-N1	8.20	121.80	117.70
54	BA	2170	A	C5-C6-N1	8.20	121.80	117.70
21	AA	19	A	N1-C6-N6	-8.20	113.68	118.60
21	AA	1238	A	C5-C6-N1	8.20	121.80	117.70
54	BA	2021	C	N3-C2-O2	-8.20	116.16	121.90
54	BA	49	A	C5-C6-N1	8.20	121.80	117.70
21	AA	149	A	N1-C6-N6	-8.19	113.68	118.60
54	BA	575	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	1308	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	64	A	C4-C5-C6	-8.19	112.91	117.00
54	BA	1077	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	1533	C	N3-C2-O2	-8.19	116.17	121.90
54	BA	1953	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	1000	A	C5-C6-N1	8.18	121.79	117.70
47	BY	48	ARG	NE-CZ-NH1	8.18	124.39	120.30
54	BA	2060	A	C4-C5-C6	-8.18	112.91	117.00
54	BA	735	A	C5-C6-N1	8.17	121.79	117.70
54	BA	2407	A	C5-C6-N1	8.17	121.79	117.70
56	B5	122	ARG	NE-CZ-NH1	8.17	124.39	120.30
27	BE	49	ARG	NE-CZ-NH1	8.17	124.39	120.30
54	BA	320	A	N1-C6-N6	-8.17	113.70	118.60
13	AN	53	ARG	NE-CZ-NH1	8.17	124.38	120.30
54	BA	6	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	458	G	O4'-C1'-N9	8.17	114.73	108.20
54	BA	1899	A	N1-C6-N6	-8.17	113.70	118.60
13	AN	63	ARG	NE-CZ-NH2	-8.16	116.22	120.30
21	AA	243	A	C5-C6-N1	8.16	121.78	117.70
54	BA	1679	A	C5-C6-N1	8.16	121.78	117.70
21	AA	1030	U	O4'-C1'-N1	8.16	114.73	108.20
21	AA	228	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	1606	C	N3-C2-O2	-8.16	116.19	121.90
54	BA	2384	U	O4'-C1'-N1	8.16	114.73	108.20
12	AM	100	ARG	NE-CZ-NH1	8.16	124.38	120.30
21	AA	435	A	C5-C6-N1	8.16	121.78	117.70
21	AA	1214	C	N3-C2-O2	-8.16	116.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BN	4	ARG	NE-CZ-NH1	8.16	124.38	120.30
22	A1	60	C	N3-C2-O2	-8.15	116.19	121.90
54	BA	1451	C	N3-C2-O2	-8.15	116.19	121.90
54	BA	1367	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	1762	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	1368	A	C4-C5-C6	-8.15	112.92	117.00
54	BA	1383	A	C5-C6-N1	8.15	121.78	117.70
17	AR	52	ARG	NE-CZ-NH1	8.15	124.37	120.30
54	BA	1454	C	N3-C2-O2	-8.15	116.20	121.90
54	BA	1785	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	389	A	C4-C5-C6	-8.14	112.93	117.00
54	BA	739	A	C5-C6-N1	8.14	121.77	117.70
54	BA	1941	C	N3-C2-O2	-8.14	116.20	121.90
21	AA	784	A	C5-C6-N1	8.14	121.77	117.70
54	BA	1617	C	N3-C2-O2	-8.14	116.20	121.90
54	BA	41	C	N3-C2-O2	-8.14	116.20	121.90
54	BA	1085	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	2077	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	1552	A	C5-C6-N1	8.14	121.77	117.70
37	BO	94	ARG	NE-CZ-NH1	8.14	124.37	120.30
54	BA	5	A	C4-C5-C6	-8.13	112.93	117.00
54	BA	182	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	563	A	C5-C6-N1	8.14	121.77	117.70
54	BA	1593	A	C5-C6-N1	8.13	121.77	117.70
54	BA	2317	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	33	A	C5-C6-N1	8.13	121.77	117.70
21	AA	59	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	1483	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	2070	A	C4-C5-C6	-8.13	112.94	117.00
46	BX	73	ARG	NE-CZ-NH1	8.13	124.36	120.30
54	BA	975	A	C5-C6-N1	8.13	121.76	117.70
54	BA	1289	C	N3-C2-O2	-8.12	116.21	121.90
54	BA	2670	A	C5-C6-N1	8.12	121.76	117.70
21	AA	1433	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1067	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1630	A	C4-C5-C6	-8.12	112.94	117.00
21	AA	396	C	N3-C2-O2	-8.12	116.22	121.90
54	BA	1544	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	2063	C	N3-C2-O2	-8.12	116.22	121.90
55	BB	40	U	O4'-C1'-N1	8.12	114.70	108.20
21	AA	1110	A	C4-C5-C6	-8.12	112.94	117.00
54	BA	802	A	C5-C6-N1	8.12	121.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	877	A	C5-C6-N1	8.11	121.76	117.70
54	BA	1787	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	106	C	N3-C2-O2	-8.11	116.22	121.90
21	AA	386	C	N3-C2-O2	-8.11	116.22	121.90
2	AC	53	ARG	NE-CZ-NH1	8.11	124.36	120.30
54	BA	1001	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2736	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	572	A	C5-C6-N1	8.11	121.75	117.70
23	A2	91	A	C4-C5-C6	-8.11	112.95	117.00
54	BA	2368	C	N3-C2-O2	-8.11	116.22	121.90
54	BA	833	A	C4-C5-C6	-8.10	112.95	117.00
54	BA	323	C	N1-C2-O2	8.10	123.76	118.90
54	BA	1962	C	N3-C2-O2	-8.10	116.23	121.90
55	BB	26	C	N3-C2-O2	-8.10	116.23	121.90
10	AK	92	ARG	NE-CZ-NH1	8.10	124.35	120.30
21	AA	972	C	N3-C2-O2	-8.10	116.23	121.90
21	AA	1339	A	C4-C5-C6	-8.10	112.95	117.00
54	BA	199	A	O4'-C1'-N9	8.10	114.68	108.20
54	BA	2700	A	C4-C5-C6	-8.10	112.95	117.00
54	BA	2679	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	1257	A	N1-C6-N6	-8.10	113.74	118.60
37	BO	30	ARG	NE-CZ-NH1	8.10	124.35	120.30
54	BA	900	A	C5-C6-N1	8.10	121.75	117.70
54	BA	2297	A	N1-C6-N6	-8.10	113.74	118.60
19	AT	28	ARG	NE-CZ-NH1	8.09	124.35	120.30
54	BA	1616	A	C5-C6-N1	8.09	121.75	117.70
54	BA	142	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	2425	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	197	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	1744	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	1765	U	O4'-C1'-N1	8.09	114.67	108.20
21	AA	355	C	N3-C2-O2	-8.09	116.24	121.90
22	A1	76	A	C5-C6-N1	8.09	121.74	117.70
54	BA	2560	A	C5-C6-N1	8.09	121.74	117.70
54	BA	2835	A	N1-C6-N6	-8.09	113.75	118.60
21	AA	320	A	C4-C5-C6	-8.09	112.96	117.00
54	BA	160	A	C5-C6-N1	8.09	121.74	117.70
54	BA	422	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	1044	C	N3-C2-O2	-8.09	116.24	121.90
21	AA	195	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	821	A	C5-C6-N1	8.08	121.74	117.70
54	BA	2471	A	N1-C6-N6	-8.08	113.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	BP	92	ARG	NE-CZ-NH1	8.08	124.34	120.30
54	BA	119	A	C5-C6-N1	8.08	121.74	117.70
54	BA	222	A	C5-C6-N1	8.08	121.74	117.70
54	BA	1010	A	C5-C6-N1	8.08	121.74	117.70
54	BA	1607	C	N3-C2-O2	-8.08	116.24	121.90
54	BA	1672	A	C5-C6-N1	8.08	121.74	117.70
54	BA	1919	A	N1-C6-N6	-8.08	113.75	118.60
21	AA	250	A	C5-C6-N1	8.08	121.74	117.70
54	BA	2690	U	O4'-C1'-N1	8.08	114.66	108.20
54	BA	1433	A	C4-C5-C6	-8.07	112.96	117.00
54	BA	2453	A	C5-C6-N1	8.07	121.74	117.70
54	BA	2448	A	C5-C6-N1	8.07	121.74	117.70
21	AA	40	C	N3-C2-O2	-8.07	116.25	121.90
21	AA	1213	A	C5-C6-N1	8.07	121.74	117.70
54	BA	447	A	C5-C6-N1	8.07	121.73	117.70
54	BA	1253	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	2287	A	O4'-C1'-N9	8.07	114.66	108.20
21	AA	7	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	1322	A	N1-C6-N6	-8.07	113.76	118.60
55	BB	73	A	C5-C6-N1	8.07	121.73	117.70
54	BA	2761	A	C5-C6-N1	8.07	121.73	117.70
21	AA	919	A	C5-C6-N1	8.06	121.73	117.70
29	BG	148	ARG	NE-CZ-NH1	8.06	124.33	120.30
46	BX	2	ARG	NE-CZ-NH1	8.06	124.33	120.30
54	BA	2507	C	N3-C2-O2	-8.06	116.25	121.90
54	BA	2893	A	N1-C6-N6	-8.06	113.76	118.60
21	AA	182	A	N1-C6-N6	-8.06	113.77	118.60
21	AA	1339	A	C5-C6-N1	8.06	121.73	117.70
21	AA	1431	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	1717	A	N1-C6-N6	-8.06	113.77	118.60
54	BA	2084	C	N3-C2-O2	-8.05	116.26	121.90
49	B0	9	ARG	NE-CZ-NH2	8.05	124.33	120.30
21	AA	860	A	C4-C5-C6	-8.05	112.97	117.00
54	BA	82	U	O4'-C1'-N1	8.05	114.64	108.20
54	BA	925	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	547	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	689	A	C5-C6-N1	8.05	121.72	117.70
54	BA	1637	A	C5-C6-N1	8.05	121.72	117.70
54	BA	1089	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	742	A	C5-C6-N1	8.05	121.72	117.70
54	BA	1664	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	819	A	C5-C6-N1	8.04	121.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	984	A	C5-C6-N1	8.04	121.72	117.70
54	BA	1741	C	N3-C2-O2	-8.04	116.27	121.90
23	A2	82	A	N1-C6-N6	-8.04	113.77	118.60
21	AA	1016	A	C5-C6-N1	8.04	121.72	117.70
54	BA	282	A	C4-C5-C6	-8.04	112.98	117.00
54	BA	821	A	C4-C5-C6	-8.04	112.98	117.00
54	BA	2386	A	C5-C6-N1	8.04	121.72	117.70
21	AA	607	A	C5-C6-N1	8.04	121.72	117.70
55	BB	45	A	C5-C6-N1	8.04	121.72	117.70
21	AA	964	A	C5-C6-N1	8.03	121.72	117.70
54	BA	1572	A	C5-C6-N1	8.03	121.72	117.70
54	BA	1961	C	N3-C2-O2	-8.03	116.28	121.90
54	BA	2241	A	C5-C6-N1	8.03	121.72	117.70
21	AA	665	A	C4-C5-C6	-8.03	112.99	117.00
41	BS	11	ARG	NE-CZ-NH1	8.03	124.31	120.30
54	BA	2726	A	O4'-C1'-N9	8.03	114.62	108.20
49	B0	39	ARG	NE-CZ-NH1	8.02	124.31	120.30
54	BA	731	C	N3-C2-O2	-8.02	116.28	121.90
54	BA	829	A	C5-C6-N1	8.02	121.71	117.70
54	BA	1632	A	C5-C6-N1	8.02	121.71	117.70
1	AB	207	ARG	NE-CZ-NH2	-8.02	116.29	120.30
15	AP	8	ARG	NE-CZ-NH1	8.02	124.31	120.30
54	BA	1970	A	C5-C6-N1	8.02	121.71	117.70
54	BA	2198	A	C5-C6-N1	8.02	121.71	117.70
54	BA	204	A	C5-C6-N1	8.02	121.71	117.70
21	AA	523	A	C5-C6-N1	8.01	121.71	117.70
21	AA	790	A	N1-C6-N6	-8.01	113.79	118.60
21	AA	1112	C	N3-C2-O2	-8.01	116.29	121.90
54	BA	1084	A	C4-C5-C6	-8.01	112.99	117.00
21	AA	681	A	C4-C5-C6	-8.01	113.00	117.00
54	BA	1525	A	C4-C5-C6	-8.01	113.00	117.00
21	AA	860	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	1067	A	C5-C6-N1	8.01	121.70	117.70
54	BA	2119	A	C5-C6-N1	8.01	121.70	117.70
21	AA	792	A	C5-C6-N1	8.00	121.70	117.70
33	BK	49	ARG	NE-CZ-NH1	8.00	124.30	120.30
38	BP	108	ARG	NE-CZ-NH2	8.00	124.30	120.30
54	BA	2468	A	N1-C6-N6	-8.00	113.80	118.60
55	BB	60	C	N3-C2-O2	-8.00	116.30	121.90
54	BA	1618	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	1229	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1254	A	C5-C6-N1	8.00	121.70	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2352	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	2311	A	C5-C6-N1	8.00	121.70	117.70
54	BA	2451	A	C4-C5-C6	-8.00	113.00	117.00
21	AA	374	A	C4-C5-C6	-7.99	113.00	117.00
22	A1	58	A	C4-C5-C6	-7.99	113.00	117.00
54	BA	330	A	N1-C6-N6	-7.99	113.80	118.60
54	BA	761	A	C5-C6-N1	7.99	121.70	117.70
54	BA	1010	A	N1-C6-N6	-7.99	113.80	118.60
21	AA	1333	A	N1-C6-N6	-7.99	113.81	118.60
40	BR	68	ARG	NE-CZ-NH1	7.99	124.30	120.30
54	BA	146	A	C5-C6-N1	7.99	121.69	117.70
54	BA	1307	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	802	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	341	C	N3-C2-O2	-7.99	116.31	121.90
54	BA	1665	A	C5-C6-N1	7.99	121.69	117.70
54	BA	2856	A	C4-C5-C6	-7.99	113.00	117.00
36	BN	71	ARG	NE-CZ-NH1	7.99	124.29	120.30
21	AA	729	A	C5-C6-N1	7.99	121.69	117.70
21	AA	1413	A	C4-C5-C6	-7.99	113.01	117.00
21	AA	448	A	C4-C5-C6	-7.98	113.01	117.00
54	BA	1675	C	N3-C2-O2	-7.98	116.31	121.90
21	AA	288	A	N1-C6-N6	-7.97	113.81	118.60
54	BA	556	A	C5-C6-N1	7.97	121.69	117.70
21	AA	780	A	C4-C5-C6	-7.97	113.02	117.00
54	BA	391	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	1916	A	C5-C6-N1	7.97	121.69	117.70
21	AA	253	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	554	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	1877	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	1167	A	C5-C6-N1	7.96	121.68	117.70
54	BA	173	A	C5-C6-N1	7.96	121.68	117.70
54	BA	281	C	N3-C2-O2	-7.96	116.32	121.90
21	AA	280	C	N3-C2-O2	-7.96	116.33	121.90
54	BA	1189	A	N1-C6-N6	-7.96	113.82	118.60
21	AA	1374	A	C5-C6-N1	7.96	121.68	117.70
54	BA	750	A	C5-C6-N1	7.96	121.68	117.70
54	BA	155	A	C4-C5-C6	-7.96	113.02	117.00
45	BW	38	ARG	NE-CZ-NH1	7.96	124.28	120.30
54	BA	564	C	N3-C2-O2	-7.96	116.33	121.90
54	BA	2665	A	C5-C6-N1	7.96	121.68	117.70
54	BA	2352	A	C4-C5-C6	-7.96	113.02	117.00
12	AM	89	ARG	NE-CZ-NH1	7.95	124.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	248	C	N3-C2-O2	-7.95	116.33	121.90
54	BA	550	C	N3-C2-O2	-7.95	116.33	121.90
54	BA	2700	A	C5-C6-N1	7.95	121.68	117.70
55	BB	35	C	N3-C2-O2	-7.95	116.33	121.90
54	BA	384	A	C5-C6-N1	7.95	121.68	117.70
54	BA	2247	A	C4-C5-C6	-7.95	113.02	117.00
54	BA	94	A	C4-C5-C6	-7.95	113.03	117.00
21	AA	164	G	O4'-C1'-N9	7.95	114.56	108.20
21	AA	321	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	614	A	C5-C6-N1	7.95	121.67	117.70
54	BA	825	A	C5-C6-N1	7.95	121.67	117.70
54	BA	1268	A	C4-C5-C6	-7.95	113.03	117.00
54	BA	2824	C	N3-C2-O2	-7.95	116.34	121.90
21	AA	1339	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	718	A	C4-C5-C6	-7.95	113.03	117.00
21	AA	284	C	N3-C2-O2	-7.94	116.34	121.90
25	BC	86	ARG	NE-CZ-NH2	-7.94	116.33	120.30
53	B4	4	ARG	NE-CZ-NH1	7.94	124.27	120.30
21	AA	1349	A	N1-C6-N6	-7.94	113.83	118.60
54	BA	262	A	N1-C6-N6	-7.94	113.83	118.60
54	BA	402	A	N1-C6-N6	-7.94	113.83	118.60
54	BA	1258	U	O4'-C1'-N1	7.94	114.56	108.20
55	BB	118	C	N3-C2-O2	-7.94	116.34	121.90
54	BA	721	A	C5-C6-N1	7.94	121.67	117.70
54	BA	294	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	749	A	N1-C6-N6	-7.94	113.84	118.60
21	AA	205	A	C4-C5-C6	-7.93	113.03	117.00
21	AA	345	C	N3-C2-O2	-7.93	116.34	121.90
54	BA	2374	C	N3-C2-O2	-7.93	116.35	121.90
21	AA	305	G	N1-C6-O6	-7.93	115.14	119.90
54	BA	84	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	1439	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	2025	C	N3-C2-O2	-7.93	116.35	121.90
21	AA	1261	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	1467	C	N3-C2-O2	-7.93	116.35	121.90
54	BA	994	C	N3-C2-O2	-7.93	116.35	121.90
54	BA	1584	U	O4'-C1'-N1	7.93	114.54	108.20
21	AA	1004	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	190	A	C5-C6-N1	7.92	121.66	117.70
21	AA	539	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1791	A	C5-C6-N1	7.92	121.66	117.70
24	A3	36	A	N1-C6-N6	-7.91	113.85	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2298	A	N1-C6-N6	-7.91	113.85	118.60
7	AH	113	ARG	NE-CZ-NH1	7.91	124.25	120.30
47	BY	7	ARG	NE-CZ-NH1	7.91	124.25	120.30
54	BA	2003	A	N1-C6-N6	-7.91	113.86	118.60
21	AA	131	A	C5-C6-N1	7.91	121.65	117.70
21	AA	728	A	C4-C5-C6	-7.91	113.05	117.00
54	BA	2350	C	N3-C2-O2	-7.91	116.37	121.90
54	BA	2412	A	C5-C6-N1	7.91	121.65	117.70
54	BA	2564	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	1118	C	N3-C2-O2	-7.90	116.37	121.90
21	AA	978	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1191	A	C4-C5-C6	-7.90	113.05	117.00
21	AA	1319	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	2126	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1098	C	N3-C2-O2	-7.90	116.37	121.90
54	BA	1635	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	1686	C	N3-C2-O2	-7.90	116.37	121.90
54	BA	2342	C	N3-C2-O2	-7.90	116.37	121.90
21	AA	414	A	C5-C6-N1	7.90	121.65	117.70
54	BA	1774	C	N3-C2-O2	-7.90	116.37	121.90
54	BA	2520	C	N3-C2-O2	-7.89	116.38	121.90
55	BB	57	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	1780	A	C5-C6-N1	7.89	121.65	117.70
21	AA	309	A	N1-C6-N6	-7.89	113.87	118.60
54	BA	1996	C	N3-C2-O2	-7.89	116.38	121.90
54	BA	2740	A	C4-C5-C6	-7.89	113.06	117.00
54	BA	2780	G	O4'-C1'-N9	7.89	114.51	108.20
54	BA	145	C	N3-C2-O2	-7.89	116.38	121.90
54	BA	572	A	C5-C6-N1	7.89	121.64	117.70
21	AA	431	A	C5-C6-N1	7.89	121.64	117.70
54	BA	1211	C	N3-C2-O2	-7.89	116.38	121.90
54	BA	1353	A	C5-C6-N1	7.89	121.64	117.70
54	BA	917	A	N1-C6-N6	-7.88	113.87	118.60
21	AA	161	A	C5-C6-N1	7.88	121.64	117.70
54	BA	323	C	N3-C2-O2	-7.88	116.38	121.90
54	BA	983	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1321	A	C5-C6-N1	7.88	121.64	117.70
18	AS	36	ARG	NE-CZ-NH1	7.88	124.24	120.30
21	AA	51	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1048	A	N1-C6-N6	-7.88	113.87	118.60
19	AT	9	ARG	NE-CZ-NH2	-7.88	116.36	120.30
54	BA	751	A	C5-C6-N1	7.88	121.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2247	A	N1-C6-N6	-7.88	113.87	118.60
21	AA	448	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	2058	A	C5-C6-N1	7.88	121.64	117.70
21	AA	59	A	C4-C5-C6	-7.88	113.06	117.00
54	BA	1151	A	N1-C6-N6	-7.88	113.88	118.60
54	BA	2560	A	C4-C5-C6	-7.88	113.06	117.00
54	BA	1387	A	C5-C6-N1	7.87	121.64	117.70
21	AA	1227	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	1237	C	N3-C2-O2	-7.87	116.39	121.90
21	AA	1479	C	N3-C2-O2	-7.87	116.39	121.90
21	AA	1155	A	N1-C6-N6	-7.87	113.88	118.60
38	BP	52	ARG	NE-CZ-NH1	7.87	124.23	120.30
38	BP	52	ARG	NE-CZ-NH2	-7.87	116.37	120.30
54	BA	2452	C	N3-C2-O2	-7.87	116.39	121.90
21	AA	441	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	1508	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	1809	A	C5-C6-N1	7.86	121.63	117.70
54	BA	2435	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1009	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1254	A	C4-C5-C6	-7.86	113.07	117.00
54	BA	503	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1085	A	C4-C5-C6	-7.86	113.07	117.00
21	AA	1507	A	N1-C6-N6	-7.86	113.89	118.60
34	BL	69	ARG	NE-CZ-NH1	7.86	124.23	120.30
54	BA	1269	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	2044	C	N3-C2-O2	-7.86	116.40	121.90
54	BA	2774	C	N3-C2-O2	-7.86	116.40	121.90
11	AL	55	ARG	NE-CZ-NH1	7.85	124.23	120.30
21	AA	782	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	282	A	N1-C6-N6	-7.85	113.89	118.60
21	AA	156	C	N3-C2-O2	-7.85	116.41	121.90
27	BE	117	ARG	NE-CZ-NH1	7.85	124.22	120.30
54	BA	531	C	N3-C2-O2	-7.85	116.41	121.90
54	BA	972	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	1913	A	O4'-C1'-N9	7.85	114.48	108.20
4	AE	111	ARG	NE-CZ-NH1	7.85	124.22	120.30
54	BA	947	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	2534	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2717	C	N3-C2-O2	-7.84	116.41	121.90
24	A3	35	C	N3-C2-O2	-7.84	116.41	121.90
54	BA	1789	A	N1-C6-N6	-7.84	113.89	118.60
21	AA	98	A	C5-C6-N1	7.84	121.62	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	482	A	C5-C6-N1	7.84	121.62	117.70
54	BA	644	A	N1-C6-N6	-7.84	113.90	118.60
54	BA	671	C	N1-C2-O2	7.84	123.60	118.90
54	BA	1952	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2369	A	C4-C5-C6	-7.84	113.08	117.00
54	BA	2726	A	C5-C6-N1	7.84	121.62	117.70
54	BA	191	A	C5-C6-N1	7.84	121.62	117.70
54	BA	429	A	C5-C6-N1	7.84	121.62	117.70
54	BA	1366	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2666	C	N3-C2-O2	-7.83	116.42	121.90
21	AA	298	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1453	A	C5-C6-N1	7.83	121.62	117.70
54	BA	1966	A	C5-C6-N1	7.83	121.62	117.70
21	AA	1375	A	C4-C5-C6	-7.83	113.08	117.00
54	BA	2266	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	1519	A	C4-C5-C6	-7.83	113.09	117.00
54	BA	208	C	N3-C2-O2	-7.83	116.42	121.90
54	BA	457	A	C5-C6-N1	7.83	121.61	117.70
54	BA	1284	A	C5-C6-N1	7.83	121.61	117.70
21	AA	160	A	C5-C6-N1	7.82	121.61	117.70
21	AA	573	A	C5-C6-N1	7.82	121.61	117.70
54	BA	353	C	N3-C2-O2	-7.82	116.43	121.90
54	BA	1226	A	C5-C6-N1	7.82	121.61	117.70
21	AA	907	A	C5-C6-N1	7.82	121.61	117.70
21	AA	171	A	C5-C6-N1	7.82	121.61	117.70
21	AA	1256	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1784	A	C5-C6-N1	7.82	121.61	117.70
21	AA	98	A	C4-C5-C6	-7.82	113.09	117.00
21	AA	983	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	1866	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	988	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	1244	A	C5-C6-N1	7.81	121.61	117.70
21	AA	985	C	N3-C2-O2	-7.81	116.43	121.90
54	BA	1942	C	N3-C2-O2	-7.81	116.43	121.90
54	BA	1870	C	N3-C2-O2	-7.81	116.43	121.90
54	BA	2503	A	O4'-C1'-N9	7.81	114.45	108.20
21	AA	48	C	N3-C2-O2	-7.81	116.44	121.90
21	AA	1250	A	C5-C6-N1	7.81	121.60	117.70
54	BA	1749	A	C4-C5-C6	-7.81	113.10	117.00
21	AA	1163	A	C5-C6-N1	7.80	121.60	117.70
21	AA	279	A	C4-C5-C6	-7.80	113.10	117.00
21	AA	188	C	N3-C2-O2	-7.80	116.44	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	502	A	C4-C5-C6	-7.80	113.10	117.00
21	AA	1129	C	N3-C2-O2	-7.80	116.44	121.90
21	AA	655	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	781	A	C5-C6-N1	7.80	121.60	117.70
54	BA	146	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	1503	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	2556	C	N3-C2-O2	-7.80	116.44	121.90
3	AD	61	ARG	NE-CZ-NH1	7.79	124.20	120.30
54	BA	1067	A	C4-C5-C6	-7.79	113.10	117.00
22	A1	35	A	C5-C6-N1	7.79	121.60	117.70
54	BA	1128	G	O4'-C1'-N9	7.79	114.43	108.20
54	BA	155	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	899	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	1877	A	C4-C5-C6	-7.79	113.11	117.00
21	AA	194	C	N3-C2-O2	-7.79	116.45	121.90
21	AA	1364	U	O4'-C1'-N1	7.79	114.43	108.20
54	BA	794	A	C4-C5-C6	-7.79	113.11	117.00
54	BA	358	U	O4'-C1'-N1	7.79	114.43	108.20
21	AA	60	A	C5-C6-N1	7.79	121.59	117.70
54	BA	1827	U	O4'-C1'-N1	7.79	114.43	108.20
54	BA	2711	A	C4-C5-C6	-7.79	113.11	117.00
21	AA	1398	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	322	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	899	A	C5-C6-N1	7.78	121.59	117.70
54	BA	928	A	C5-C6-N1	7.78	121.59	117.70
54	BA	2887	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	889	A	C5-C6-N1	7.78	121.59	117.70
54	BA	173	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	2749	A	C5-C6-N1	7.78	121.59	117.70
54	BA	1351	C	O4'-C1'-N1	7.78	114.42	108.20
54	BA	456	C	N1-C2-O2	7.78	123.56	118.90
54	BA	2778	A	C5-C6-N1	7.78	121.59	117.70
28	BF	70	ARG	NE-CZ-NH1	7.77	124.19	120.30
54	BA	1899	A	C5-C6-N1	7.77	121.59	117.70
54	BA	2572	A	C4-C5-C6	-7.77	113.11	117.00
54	BA	1274	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	1265	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	1284	A	N1-C6-N6	-7.77	113.94	118.60
21	AA	66	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	2699	C	N3-C2-O2	-7.77	116.46	121.90
54	BA	294	A	C4-C5-C6	-7.76	113.12	117.00
54	BA	538	A	N1-C6-N6	-7.76	113.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2080	A	C4-C5-C6	-7.76	113.12	117.00
54	BA	541	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	794	A	C5-C6-N1	7.76	121.58	117.70
24	A3	73	A	C4-C5-C6	-7.76	113.12	117.00
54	BA	479	A	C4-C5-C6	-7.76	113.12	117.00
54	BA	671	C	N3-C2-O2	-7.76	116.47	121.90
54	BA	787	C	N3-C2-O2	-7.76	116.47	121.90
54	BA	943	A	C5-C6-N1	7.76	121.58	117.70
54	BA	1470	A	N1-C6-N6	-7.76	113.94	118.60
21	AA	1287	A	C5-C6-N1	7.76	121.58	117.70
21	AA	539	A	C5-C6-N1	7.76	121.58	117.70
54	BA	947	A	C5-C6-N1	7.76	121.58	117.70
54	BA	1711	A	C5-C6-N1	7.76	121.58	117.70
54	BA	603	A	C5-C6-N1	7.75	121.58	117.70
54	BA	794	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	475	C	N3-C2-O2	-7.75	116.47	121.90
21	AA	482	A	C5-C6-N1	7.75	121.58	117.70
33	BK	64	ARG	NE-CZ-NH1	7.75	124.17	120.30
54	BA	265	A	C5-C6-N1	7.75	121.58	117.70
21	AA	10	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	143	A	C5-C6-N1	7.75	121.57	117.70
21	AA	1396	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	861	A	C5-C6-N1	7.75	121.58	117.70
55	BB	89	U	O4'-C1'-N1	7.75	114.40	108.20
21	AA	435	A	C4-C5-C6	-7.75	113.13	117.00
54	BA	165	A	C4-C5-C6	-7.75	113.13	117.00
54	BA	2126	A	C5-C6-N1	7.75	121.57	117.70
54	BA	2208	C	N3-C2-O2	-7.75	116.48	121.90
54	BA	2655	G	O4'-C1'-N9	7.75	114.40	108.20
54	BA	2777	G	C8-N9-C4	-7.75	103.30	106.40
21	AA	909	A	N1-C6-N6	-7.75	113.95	118.60
50	B1	27	ARG	NE-CZ-NH1	7.75	124.17	120.30
18	AS	54	ARG	NE-CZ-NH2	-7.74	116.43	120.30
39	BQ	27	ARG	NE-CZ-NH1	7.74	124.17	120.30
54	BA	764	A	C5-C6-N1	7.74	121.57	117.70
21	AA	1367	C	N3-C2-O2	-7.74	116.48	121.90
54	BA	2591	C	N3-C2-O2	-7.74	116.48	121.90
54	BA	272	A	N1-C6-N6	-7.74	113.95	118.60
54	BA	368	A	C5-C6-N1	7.73	121.57	117.70
54	BA	2268	A	C5-C6-N1	7.73	121.57	117.70
21	AA	223	A	C4-C5-C6	-7.73	113.13	117.00
21	AA	451	A	C5-C6-N1	7.73	121.56	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2453	A	C4-C5-C6	-7.73	113.14	117.00
54	BA	544	C	N3-C2-O2	-7.73	116.49	121.90
21	AA	880	C	N3-C2-O2	-7.73	116.49	121.90
21	AA	1518	A	C5-C6-N1	7.73	121.56	117.70
27	BE	44	ARG	NE-CZ-NH1	7.73	124.16	120.30
36	BN	46	ARG	NE-CZ-NH1	7.73	124.16	120.30
54	BA	2705	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	2738	A	N1-C6-N6	-7.73	113.96	118.60
14	AO	57	ARG	NE-CZ-NH1	7.72	124.16	120.30
54	BA	226	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	1213	A	C5-C6-N1	7.72	121.56	117.70
5	AF	24	ARG	NE-CZ-NH1	7.72	124.16	120.30
6	AG	4	ARG	NE-CZ-NH1	7.72	124.16	120.30
15	AP	14	ARG	NE-CZ-NH1	7.72	124.16	120.30
54	BA	1785	A	C4-C5-C6	-7.72	113.14	117.00
55	BB	78	A	C4-C5-C6	-7.72	113.14	117.00
54	BA	655	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	768	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	1375	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	1754	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1103	A	C5-C6-N1	7.71	121.56	117.70
21	AA	609	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	1046	A	C5-C6-N1	7.71	121.56	117.70
9	AJ	37	ARG	NE-CZ-NH1	7.71	124.15	120.30
54	BA	1274	A	C4-C5-C6	-7.71	113.15	117.00
54	BA	2723	C	N3-C2-O2	-7.71	116.50	121.90
6	AG	77	ARG	NE-CZ-NH1	7.71	124.15	120.30
21	AA	186	C	N3-C2-O2	-7.71	116.51	121.90
54	BA	457	A	C4-C5-C6	-7.71	113.15	117.00
54	BA	477	A	C5-C6-N1	7.71	121.55	117.70
54	BA	960	A	N1-C6-N6	-7.71	113.98	118.60
54	BA	1885	A	C5-C6-N1	7.71	121.55	117.70
21	AA	336	A	C5-C6-N1	7.70	121.55	117.70
21	AA	622	A	C5-C6-N1	7.70	121.55	117.70
21	AA	1254	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	1414	C	N3-C2-O2	-7.70	116.51	121.90
54	BA	2448	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	933	A	C5-C6-N1	7.70	121.55	117.70
54	BA	800	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	1049	U	O4'-C1'-N1	7.70	114.36	108.20
54	BA	383	C	O4'-C1'-N1	7.70	114.36	108.20
54	BA	982	C	C2-N1-C1'	7.70	127.27	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1912	A	C5-C6-N1	7.70	121.55	117.70
54	BA	2900	A	C4-C5-C6	-7.70	113.15	117.00
24	A3	62	C	N3-C2-O2	-7.70	116.51	121.90
19	AT	23	ARG	NE-CZ-NH1	7.69	124.15	120.30
21	AA	918	A	N1-C6-N6	-7.69	113.98	118.60
21	AA	1252	A	C5-C6-N1	7.69	121.55	117.70
45	BW	40	ARG	NE-CZ-NH1	7.69	124.14	120.30
54	BA	453	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	2169	A	N1-C6-N6	-7.69	113.99	118.60
21	AA	55	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	1054	A	C5-C6-N1	7.69	121.54	117.70
54	BA	337	C	N3-C2-O2	-7.68	116.52	121.90
54	BA	286	U	O4'-C1'-N1	7.68	114.35	108.20
54	BA	1230	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	2314	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	2461	A	C5-C6-N1	7.68	121.54	117.70
21	AA	210	C	N3-C2-O2	-7.68	116.52	121.90
21	AA	1288	A	C5-C6-N1	7.68	121.54	117.70
21	AA	1394	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	704	G	C8-N9-C4	-7.68	103.33	106.40
54	BA	1102	C	N3-C2-O2	-7.68	116.53	121.90
21	AA	977	A	C4-C5-C6	-7.68	113.16	117.00
54	BA	2733	A	C5-C6-N1	7.68	121.54	117.70
3	AD	43	ARG	NE-CZ-NH1	7.67	124.14	120.30
21	AA	143	A	C4-C5-C6	-7.67	113.16	117.00
54	BA	2134	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	2882	A	C5-C6-N1	7.67	121.54	117.70
21	AA	1231	G	O4'-C1'-N9	7.67	114.34	108.20
21	AA	1136	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	2450	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1127	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	1508	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1736	U	O4'-C1'-N1	7.67	114.33	108.20
54	BA	1848	A	N1-C6-N6	-7.67	114.00	118.60
50	B1	5	ARG	NE-CZ-NH1	7.67	124.13	120.30
54	BA	693	A	C5-C6-N1	7.67	121.53	117.70
54	BA	918	A	C5-C6-N1	7.67	121.53	117.70
54	BA	631	A	C5-C6-N1	7.66	121.53	117.70
21	AA	737	C	N3-C2-O2	-7.66	116.54	121.90
24	A3	1	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	2377	A	C5-C6-N1	7.66	121.53	117.70
21	AA	1329	A	N1-C6-N6	-7.66	114.00	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	101	A	C5-C6-N1	7.66	121.53	117.70
24	A3	67	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	1632	A	N1-C6-N6	-7.66	114.01	118.60
25	BC	86	ARG	NE-CZ-NH1	7.66	124.13	120.30
54	BA	1363	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	2284	A	C4-C5-C6	-7.66	113.17	117.00
14	AO	53	ARG	NE-CZ-NH1	7.65	124.13	120.30
21	AA	182	A	C4-C5-C6	-7.65	113.17	117.00
54	BA	1352	U	O4'-C1'-N1	7.65	114.32	108.20
54	BA	1805	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	6	A	C4-C5-C6	-7.64	113.18	117.00
54	BA	2540	C	C1'-O4'-C4'	-7.64	103.79	109.90
21	AA	1213	A	C4-C5-C6	-7.64	113.18	117.00
54	BA	83	A	C5-C6-N1	7.64	121.52	117.70
54	BA	471	A	C5-C6-N1	7.63	121.52	117.70
54	BA	492	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	752	A	N1-C6-N6	-7.63	114.02	118.60
21	AA	345	C	N1-C2-O2	7.63	123.48	118.90
54	BA	144	A	C5-C6-N1	7.63	121.51	117.70
21	AA	892	A	C5-C6-N1	7.63	121.51	117.70
54	BA	1362	C	N3-C2-O2	-7.63	116.56	121.90
54	BA	1854	A	C4-C5-C6	-7.63	113.19	117.00
54	BA	984	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	1403	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	2270	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	596	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	2610	C	N3-C2-O2	-7.62	116.57	121.90
55	BB	30	C	N3-C2-O2	-7.62	116.57	121.90
54	BA	1537	G	N3-C4-C5	-7.62	124.79	128.60
21	AA	116	A	C5-C6-N1	7.62	121.51	117.70
22	A1	26	A	C5-C6-N1	7.62	121.51	117.70
32	BJ	27	ARG	NE-CZ-NH1	7.62	124.11	120.30
36	BN	86	ARG	NE-CZ-NH1	7.62	124.11	120.30
54	BA	172	A	C5-C6-N1	7.62	121.51	117.70
54	BA	802	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	1387	A	C4-C5-C6	-7.62	113.19	117.00
21	AA	924	C	N3-C2-O2	-7.61	116.57	121.90
21	AA	1509	C	N3-C2-O2	-7.61	116.57	121.90
54	BA	1548	A	C5-C6-N1	7.61	121.51	117.70
21	AA	602	A	N1-C6-N6	-7.61	114.03	118.60
21	AA	554	A	C4-C5-C6	-7.61	113.19	117.00
54	BA	129	C	N3-C2-O2	-7.61	116.57	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	231	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	571	U	O4'-C1'-N1	7.61	114.29	108.20
54	BA	2025	C	N1-C2-O2	7.61	123.47	118.90
21	AA	1197	A	C5-C6-N1	7.61	121.50	117.70
55	BB	58	A	C4-C5-C6	-7.61	113.20	117.00
21	AA	1071	C	N3-C2-O2	-7.60	116.58	121.90
54	BA	2432	A	O4'-C1'-N9	7.60	114.28	108.20
21	AA	766	A	C5-C6-N1	7.60	121.50	117.70
21	AA	535	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	2541	A	C5-C6-N1	7.60	121.50	117.70
23	A2	82	A	C5-C6-N1	7.60	121.50	117.70
54	BA	1434	A	C4-C5-C6	-7.60	113.20	117.00
15	AP	28	ARG	NE-CZ-NH1	7.60	124.10	120.30
21	AA	974	A	N1-C6-N6	-7.59	114.04	118.60
21	AA	1081	A	C5-C6-N1	7.59	121.50	117.70
54	BA	127	A	C5-C6-N1	7.59	121.50	117.70
21	AA	10	A	C5-C6-N1	7.59	121.50	117.70
54	BA	213	A	C5-C6-N1	7.59	121.50	117.70
54	BA	217	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1000	A	N1-C6-N6	-7.59	114.05	118.60
21	AA	1250	A	N1-C6-N6	-7.59	114.05	118.60
37	BO	16	ARG	NE-CZ-NH1	7.59	124.09	120.30
54	BA	316	C	N3-C2-O2	-7.59	116.59	121.90
54	BA	2860	A	N1-C6-N6	-7.59	114.05	118.60
21	AA	600	A	N1-C6-N6	-7.59	114.05	118.60
21	AA	148	G	C5-C6-N1	7.59	115.29	111.50
54	BA	730	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	2278	A	C4-C5-C6	-7.59	113.21	117.00
54	BA	2332	C	N3-C2-O2	-7.59	116.59	121.90
21	AA	1082	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	2073	C	N3-C2-O2	-7.58	116.59	121.90
54	BA	2145	C	O4'-C1'-N1	7.58	114.27	108.20
21	AA	440	C	N3-C2-O2	-7.58	116.59	121.90
21	AA	1350	A	C5-C6-N1	7.58	121.49	117.70
40	BR	78	ARG	NE-CZ-NH2	7.58	124.09	120.30
54	BA	2070	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	1822	C	N3-C2-O2	-7.58	116.59	121.90
54	BA	2377	A	C4-C5-C6	-7.58	113.21	117.00
43	BU	5	ARG	NE-CZ-NH1	7.58	124.09	120.30
54	BA	911	A	C4-C5-C6	-7.58	113.21	117.00
21	AA	109	A	C5-C6-N1	7.57	121.49	117.70
21	AA	648	A	N1-C6-N6	-7.57	114.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2687	U	O4'-C1'-N1	7.57	114.26	108.20
21	AA	16	A	C5-C6-N1	7.57	121.49	117.70
21	AA	233	C	N3-C2-O2	-7.57	116.60	121.90
54	BA	1302	A	C4-C5-C6	-7.57	113.21	117.00
21	AA	430	A	N1-C6-N6	-7.57	114.06	118.60
21	AA	487	A	C4-C5-C6	-7.57	113.22	117.00
21	AA	196	A	C5-C6-N1	7.57	121.48	117.70
21	AA	819	A	C5-C6-N1	7.57	121.48	117.70
8	AI	11	ARG	NE-CZ-NH1	7.56	124.08	120.30
54	BA	806	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	1070	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	793	A	C5-C6-N1	7.56	121.48	117.70
54	BA	1808	A	C4-C5-C6	-7.56	113.22	117.00
21	AA	47	C	N3-C2-O2	-7.56	116.61	121.90
21	AA	1317	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	300	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2346	A	C4-C5-C6	-7.56	113.22	117.00
2	AC	155	ARG	NE-CZ-NH1	7.56	124.08	120.30
7	AH	12	ARG	NE-CZ-NH1	7.56	124.08	120.30
54	BA	10	A	C5-C6-N1	7.56	121.48	117.70
54	BA	241	A	C5-C6-N1	7.56	121.48	117.70
3	AD	13	ARG	NE-CZ-NH1	7.55	124.08	120.30
55	BB	57	A	C4-C5-C6	-7.55	113.22	117.00
8	AI	84	ARG	NE-CZ-NH1	7.55	124.08	120.30
54	BA	109	C	N3-C2-O2	-7.55	116.61	121.90
54	BA	960	A	C5-C6-N1	7.55	121.48	117.70
55	BB	24	G	N3-C4-C5	-7.55	124.82	128.60
55	BB	3	C	N3-C2-O2	-7.55	116.61	121.90
21	AA	938	A	C4-C5-C6	-7.55	113.23	117.00
54	BA	1072	C	N3-C2-O2	-7.55	116.62	121.90
54	BA	2112	G	C8-N9-C4	-7.55	103.38	106.40
54	BA	2727	A	C5-C6-N1	7.55	121.47	117.70
21	AA	1030	U	C1'-O4'-C4'	-7.54	103.86	109.90
54	BA	886	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	2586	U	O4'-C1'-N1	7.54	114.23	108.20
54	BA	300	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	2809	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1562	U	O4'-C1'-N1	7.54	114.23	108.20
54	BA	131	A	C5-C6-N1	7.54	121.47	117.70
54	BA	443	A	C5-C6-N1	7.54	121.47	117.70
54	BA	644	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	1596	A	C5-C6-N1	7.54	121.47	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1749	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	2134	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	722	A	C5-C6-N1	7.53	121.47	117.70
54	BA	1996	C	N1-C2-O2	7.53	123.42	118.90
55	BB	53	A	C5-C6-N1	7.53	121.47	117.70
54	BA	227	A	C5-C6-N1	7.53	121.47	117.70
16	AQ	39	ARG	NE-CZ-NH1	7.53	124.06	120.30
21	AA	859	G	N1-C6-O6	-7.53	115.38	119.90
54	BA	348	A	C5-C6-N1	7.53	121.46	117.70
54	BA	783	A	N1-C6-N6	-7.53	114.08	118.60
21	AA	28	A	C4-C5-C6	-7.53	113.24	117.00
21	AA	490	C	N3-C2-O2	-7.53	116.63	121.90
54	BA	325	G	O4'-C1'-N9	7.53	114.22	108.20
54	BA	2872	A	C4-C5-C6	-7.52	113.24	117.00
3	AD	153	ARG	NE-CZ-NH1	7.52	124.06	120.30
54	BA	945	A	C5-C6-N1	7.52	121.46	117.70
22	A1	75	C	C1'-O4'-C4'	-7.52	103.89	109.90
24	A3	58	A	C5-C6-N1	7.52	121.46	117.70
54	BA	609	A	C4-C5-C6	-7.52	113.24	117.00
54	BA	749	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1597	A	N1-C6-N6	-7.52	114.09	118.60
21	AA	98	A	N1-C6-N6	-7.52	114.09	118.60
23	A2	79	A	C5-C6-N1	7.52	121.46	117.70
54	BA	275	C	N3-C2-O2	-7.52	116.64	121.90
54	BA	2013	A	C5-C6-N1	7.52	121.46	117.70
2	AC	135	ARG	NE-CZ-NH1	7.52	124.06	120.30
21	AA	1337	G	N3-C4-C5	-7.52	124.84	128.60
21	AA	1210	C	N3-C2-O2	-7.51	116.64	121.90
54	BA	1248	G	O4'-C1'-N9	7.51	114.21	108.20
21	AA	1480	A	C5-C6-N1	7.51	121.45	117.70
54	BA	2742	G	O4'-C1'-N9	7.51	114.21	108.20
54	BA	277	G	N3-C4-C5	-7.51	124.85	128.60
55	BB	17	C	O4'-C1'-N1	7.51	114.21	108.20
54	BA	2764	A	C4-C5-C6	-7.51	113.25	117.00
21	AA	994	A	C5-C6-N1	7.50	121.45	117.70
39	BQ	69	ARG	NE-CZ-NH1	7.50	124.05	120.30
54	BA	1504	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	2459	A	N1-C6-N6	-7.50	114.10	118.60
55	BB	37	C	N3-C2-O2	-7.50	116.65	121.90
26	BD	59	ARG	NE-CZ-NH1	7.50	124.05	120.30
55	BB	109	A	C5-C6-N1	7.50	121.45	117.70
24	A3	45	A	C5-C6-N1	7.50	121.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	23	A	C5-C6-N1	7.50	121.45	117.70
27	BE	79	ARG	NE-CZ-NH1	7.50	124.05	120.30
54	BA	632	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	1610	A	O4'-C1'-N9	7.50	114.20	108.20
54	BA	2335	A	C4-C5-C6	-7.50	113.25	117.00
54	BA	946	C	N3-C2-O2	-7.50	116.65	121.90
54	BA	1575	C	N3-C2-O2	-7.50	116.65	121.90
54	BA	1744	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2380	C	N3-C2-O2	-7.50	116.65	121.90
21	AA	906	A	C4-C5-C6	-7.50	113.25	117.00
54	BA	2003	A	C5-C6-N1	7.50	121.45	117.70
21	AA	167	A	C4-C5-C6	-7.49	113.25	117.00
21	AA	1493	A	C4-C5-C6	-7.49	113.25	117.00
22	A1	9	A	C5-C6-N1	7.49	121.44	117.70
54	BA	502	A	C5-C6-N1	7.49	121.44	117.70
54	BA	515	A	C5-C6-N1	7.49	121.44	117.70
54	BA	1731	G	O4'-C1'-N9	7.49	114.19	108.20
54	BA	2666	C	N1-C2-O2	7.49	123.39	118.90
55	BB	45	A	N1-C6-N6	-7.49	114.11	118.60
24	A3	17	C	N3-C2-O2	-7.49	116.66	121.90
54	BA	654	A	C4-C5-C6	-7.49	113.26	117.00
54	BA	961	C	N3-C2-O2	-7.49	116.66	121.90
54	BA	1871	A	C5-C6-N1	7.49	121.44	117.70
54	BA	2160	C	N3-C2-O2	-7.49	116.66	121.90
21	AA	6	G	N3-C4-C5	-7.48	124.86	128.60
21	AA	152	A	C5-C6-N1	7.48	121.44	117.70
24	A3	59	A	C5-C6-N1	7.48	121.44	117.70
54	BA	996	A	C4-C5-C6	-7.48	113.26	117.00
14	AO	63	ARG	NE-CZ-NH1	7.48	124.04	120.30
21	AA	189	A	C4-C5-C6	-7.48	113.26	117.00
54	BA	460	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	1144	A	C5-C6-N1	7.48	121.44	117.70
54	BA	2212	A	C4-C5-C6	-7.48	113.26	117.00
21	AA	149	A	C4-C5-C6	-7.48	113.26	117.00
21	AA	1176	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	457	A	O4'-C1'-N9	7.48	114.18	108.20
54	BA	2211	A	C5-C6-N1	7.48	121.44	117.70
21	AA	366	A	P-O3'-C3'	7.48	128.67	119.70
51	B2	28	ARG	NE-CZ-NH1	7.47	124.04	120.30
54	BA	1001	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1143	A	C5-C6-N1	7.47	121.44	117.70
54	BA	378	C	N3-C2-O2	-7.47	116.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	501	C	N3-C2-O2	-7.47	116.67	121.90
21	AA	432	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	1805	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1382	G	N3-C4-C5	-7.47	124.87	128.60
54	BA	1590	A	C4-C5-C6	-7.46	113.27	117.00
21	AA	340	U	O4'-C1'-N1	7.46	114.17	108.20
54	BA	1991	U	O4'-C1'-N1	7.46	114.17	108.20
54	BA	1874	C	O4'-C1'-N1	7.46	114.17	108.20
54	BA	2727	A	N1-C6-N6	-7.46	114.12	118.60
54	BA	941	A	C5-C6-N1	7.46	121.43	117.70
54	BA	2496	C	N3-C2-O2	-7.46	116.68	121.90
21	AA	840	C	N3-C2-O2	-7.46	116.68	121.90
21	AA	461	A	N1-C6-N6	-7.46	114.13	118.60
24	A3	57	C	N3-C2-O2	-7.46	116.68	121.90
54	BA	849	A	C5-C6-N1	7.46	121.43	117.70
21	AA	811	C	N3-C2-O2	-7.46	116.68	121.90
21	AA	967	C	N3-C2-O2	-7.46	116.68	121.90
54	BA	2406	A	C5-C6-N1	7.46	121.43	117.70
21	AA	465	A	O4'-C1'-N9	7.45	114.16	108.20
54	BA	959	A	C5-C6-N1	7.45	121.43	117.70
54	BA	1178	C	N3-C2-O2	-7.45	116.68	121.90
54	BA	1268	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1494	A	C5-C6-N1	7.45	121.42	117.70
54	BA	2362	C	N3-C2-O2	-7.45	116.69	121.90
54	BA	2818	U	O4'-C1'-N1	7.45	114.16	108.20
25	BC	181	ARG	NE-CZ-NH1	7.45	124.02	120.30
54	BA	2284	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	1180	A	C4-C5-C6	-7.45	113.28	117.00
54	BA	789	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1571	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	1826	G	O4'-C1'-N9	7.45	114.16	108.20
21	AA	572	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	1447	C	N3-C2-O2	-7.45	116.69	121.90
54	BA	2619	C	N3-C2-O2	-7.45	116.69	121.90
54	BA	1698	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	528	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	383	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	1054	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	2268	A	N1-C6-N6	-7.44	114.14	118.60
21	AA	864	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	362	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	2317	A	C5-C6-N1	7.44	121.42	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1288	G	O4'-C1'-N9	7.44	114.15	108.20
54	BA	2753	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	415	A	C5-C6-N1	7.44	121.42	117.70
54	BA	126	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	1328	A	C5-C6-N1	7.44	121.42	117.70
21	AA	465	A	N1-C6-N6	-7.43	114.14	118.60
32	BJ	13	ARG	NE-CZ-NH1	7.43	124.02	120.30
54	BA	740	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	2827	C	O4'-C1'-N1	7.43	114.15	108.20
21	AA	393	A	C4-C5-C6	-7.43	113.28	117.00
21	AA	1246	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	893	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	1069	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	1872	A	C5-C6-N1	7.43	121.42	117.70
21	AA	221	C	N3-C2-O2	-7.43	116.70	121.90
21	AA	1320	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	1427	A	C4-C5-C6	-7.43	113.29	117.00
54	BA	2600	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	2692	G	N3-C4-C5	-7.43	124.89	128.60
5	AF	2	ARG	NE-CZ-NH1	7.43	124.01	120.30
11	AL	82	ARG	NE-CZ-NH1	7.43	124.01	120.30
21	AA	1446	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	470	A	C5-C6-N1	7.43	121.41	117.70
54	BA	1646	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	103	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1144	A	N1-C6-N6	-7.42	114.14	118.60
54	BA	2014	A	N1-C6-N6	-7.42	114.14	118.60
54	BA	2510	C	C2-N3-C4	-7.42	116.19	119.90
21	AA	130	A	C5-C6-N1	7.42	121.41	117.70
21	AA	938	A	C5-C6-N1	7.42	121.41	117.70
21	AA	329	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1021	A	C4-C5-C6	-7.42	113.29	117.00
54	BA	2015	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	489	C	N3-C2-O2	-7.42	116.71	121.90
54	BA	1320	C	N3-C2-O2	-7.42	116.71	121.90
54	BA	1532	A	C5-C6-N1	7.42	121.41	117.70
54	BA	861	A	C4-C5-C6	-7.42	113.29	117.00
10	AK	36	ARG	NE-CZ-NH1	7.42	124.01	120.30
21	AA	456	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	74	A	C4-C5-C6	-7.41	113.30	117.00
21	AA	485	U	O4'-C1'-N1	7.41	114.13	108.20
21	AA	1216	A	C5-C6-N1	7.41	121.40	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2443	C	N3-C2-O2	-7.41	116.72	121.90
21	AA	1169	A	C4-C5-C6	-7.40	113.30	117.00
21	AA	59	A	C5-C6-N1	7.40	121.40	117.70
54	BA	513	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1027	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	1285	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1700	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	1780	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	2273	A	C4-C5-C6	-7.40	113.30	117.00
3	AD	153	ARG	NE-CZ-NH2	-7.40	116.60	120.30
21	AA	977	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2274	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2378	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	1214	C	N1-C2-O2	7.40	123.34	118.90
54	BA	1365	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1480	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	58	C	N3-C2-O2	-7.39	116.72	121.90
54	BA	2164	C	N3-C2-O2	-7.39	116.72	121.90
6	AG	94	ARG	NE-CZ-NH1	7.39	124.00	120.30
21	AA	962	C	N3-C2-O2	-7.39	116.73	121.90
43	BU	93	ARG	NE-CZ-NH1	7.39	124.00	120.30
21	AA	246	A	C5-C6-N1	7.39	121.39	117.70
22	A1	71	C	N3-C2-O2	-7.39	116.73	121.90
54	BA	1640	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	2006	C	N3-C2-O2	-7.39	116.73	121.90
54	BA	2789	C	O4'-C1'-N1	7.39	114.11	108.20
54	BA	710	U	O4'-C1'-N1	7.39	114.11	108.20
21	AA	1462	C	N3-C2-O2	-7.39	116.73	121.90
54	BA	302	C	N3-C2-O2	-7.39	116.73	121.90
54	BA	487	C	N3-C2-O2	-7.39	116.73	121.90
54	BA	1384	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	1932	A	C4-C5-C6	-7.39	113.31	117.00
21	AA	1158	C	N3-C2-O2	-7.38	116.73	121.90
21	AA	1322	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	1735	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	611	C	N3-C2-O2	-7.38	116.74	121.90
54	BA	2426	A	C5-C6-N1	7.38	121.39	117.70
54	BA	933	A	C4-C5-C6	-7.38	113.31	117.00
21	AA	1102	A	N1-C6-N6	-7.37	114.17	118.60
54	BA	719	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	1431	A	C5-C6-N1	7.37	121.39	117.70
54	BA	2614	A	N1-C6-N6	-7.37	114.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	705	G	N1-C6-O6	-7.37	115.48	119.90
22	A1	27	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	139	A	N1-C6-N6	-7.37	114.18	118.60
21	AA	167	A	N1-C6-N6	-7.37	114.18	118.60
21	AA	1100	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	401	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	2823	A	C5-C6-N1	7.37	121.38	117.70
54	BA	980	A	C4-C5-C6	-7.37	113.32	117.00
21	AA	1363	A	C4-C5-C6	-7.37	113.32	117.00
54	BA	342	A	C4-C5-C6	-7.37	113.32	117.00
21	AA	130	A	C4-C5-C6	-7.36	113.32	117.00
21	AA	1012	A	C5-C6-N1	7.36	121.38	117.70
55	BB	45	A	C4-C5-C6	-7.36	113.32	117.00
54	BA	279	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1433	A	C5-C6-N1	7.36	121.38	117.70
54	BA	76	C	N3-C2-O2	-7.36	116.75	121.90
21	AA	306	A	N1-C6-N6	-7.36	114.19	118.60
21	AA	932	C	C1'-O4'-C4'	-7.36	104.01	109.90
21	AA	1046	A	C5-C6-N1	7.36	121.38	117.70
37	BO	25	ARG	NE-CZ-NH1	7.36	123.98	120.30
54	BA	431	U	O4'-C1'-N1	7.36	114.09	108.20
54	BA	599	A	C4-C5-C6	-7.36	113.32	117.00
54	BA	1550	C	N1-C2-O2	7.36	123.31	118.90
54	BA	1771	C	O4'-C1'-N1	7.36	114.09	108.20
54	BA	2094	A	C4-C5-C6	-7.36	113.32	117.00
55	BB	36	C	N3-C2-O2	-7.36	116.75	121.90
21	AA	6	G	N1-C6-O6	-7.36	115.49	119.90
21	AA	1350	A	N1-C6-N6	-7.36	114.19	118.60
54	BA	717	C	N3-C2-O2	-7.36	116.75	121.90
54	BA	419	U	O4'-C1'-N1	7.35	114.08	108.20
54	BA	751	A	C4-C5-C6	-7.35	113.32	117.00
21	AA	642	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	900	A	C5-C6-N1	7.35	121.37	117.70
54	BA	572	A	C4-C5-C6	-7.35	113.33	117.00
54	BA	2517	C	O4'-C1'-N1	7.35	114.08	108.20
39	BQ	12	ARG	NE-CZ-NH2	7.35	123.97	120.30
54	BA	2051	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	156	A	C4-C5-C6	-7.34	113.33	117.00
54	BA	2531	A	N1-C6-N6	-7.34	114.19	118.60
54	BA	2516	A	N1-C6-N6	-7.34	114.19	118.60
21	AA	487	A	N1-C6-N6	-7.34	114.20	118.60
21	AA	794	A	C5-C6-N1	7.34	121.37	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	833	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1786	A	C5-C6-N1	7.34	121.37	117.70
54	BA	756	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2556	C	O4'-C1'-N1	7.34	114.07	108.20
21	AA	753	A	C5-C6-N1	7.34	121.37	117.70
21	AA	779	C	N3-C2-O2	-7.34	116.77	121.90
21	AA	839	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	670	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1804	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	2054	A	C5-C6-N1	7.34	121.37	117.70
21	AA	949	A	C4-C5-C6	-7.33	113.33	117.00
54	BA	146	A	C4-C5-C6	-7.33	113.33	117.00
54	BA	514	A	C5-C6-N1	7.33	121.37	117.70
54	BA	2226	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	2510	C	N1-C2-N3	7.33	124.33	119.20
54	BA	2860	A	C4-C5-C6	-7.33	113.33	117.00
21	AA	608	A	C4-C5-C6	-7.33	113.33	117.00
21	AA	914	A	C5-C6-N1	7.33	121.37	117.70
54	BA	1801	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2222	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	621	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	173	A	C4-C5-C6	-7.33	113.34	117.00
25	BC	132	ARG	NE-CZ-NH1	7.32	123.96	120.30
54	BA	1454	C	N1-C2-O2	7.32	123.29	118.90
54	BA	1998	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	1137	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	324	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1977	A	C4-C5-C6	-7.32	113.34	117.00
21	AA	640	A	C5-C6-N1	7.32	121.36	117.70
21	AA	913	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2062	A	C5-C6-N1	7.32	121.36	117.70
21	AA	1377	A	C4-C5-C6	-7.31	113.34	117.00
54	BA	295	G	C8-N9-C4	-7.31	103.47	106.40
54	BA	1534	U	O4'-C1'-N1	7.31	114.05	108.20
54	BA	2704	C	N3-C2-O2	-7.31	116.78	121.90
21	AA	344	A	C5-C6-N1	7.31	121.35	117.70
21	AA	1158	C	N1-C2-O2	7.31	123.28	118.90
21	AA	1403	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	1938	A	C1'-O4'-C4'	-7.31	104.05	109.90
54	BA	2564	A	C4-C5-C6	-7.31	113.35	117.00
54	BA	675	A	C5-C6-N1	7.30	121.35	117.70
54	BA	229	C	O4'-C1'-N1	7.30	114.04	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1226	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	2135	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	74	A	C4-C5-C6	-7.30	113.35	117.00
22	A1	66	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	240	C	N3-C2-O2	-7.30	116.79	121.90
54	BA	1354	A	C4-C5-C6	-7.30	113.35	117.00
21	AA	156	C	O4'-C1'-N1	7.29	114.03	108.20
54	BA	165	A	N1-C6-N6	-7.29	114.22	118.60
54	BA	595	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	2748	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	1201	A	C4-C5-C6	-7.29	113.35	117.00
54	BA	9	G	N1-C6-O6	-7.29	115.53	119.90
54	BA	430	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1999	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	2590	A	C5-C6-N1	7.29	121.34	117.70
5	AF	79	ARG	NE-CZ-NH1	7.29	123.94	120.30
21	AA	848	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	1336	A	N1-C6-N6	-7.29	114.23	118.60
21	AA	1520	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	896	A	O4'-C1'-N9	7.29	114.03	108.20
54	BA	13	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	508	A	C4-C5-C6	-7.29	113.36	117.00
54	BA	973	A	C5-C6-N1	7.29	121.34	117.70
54	BA	2635	A	C4-C5-C6	-7.29	113.36	117.00
54	BA	2660	A	O4'-C1'-N9	7.29	114.03	108.20
54	BA	2755	C	N3-C2-O2	-7.29	116.80	121.90
21	AA	262	A	C5-C6-N1	7.28	121.34	117.70
21	AA	370	C	N3-C2-O2	-7.28	116.80	121.90
22	A1	69	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	1103	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	1606	C	N1-C2-O2	7.28	123.27	118.90
21	AA	197	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	2287	A	C4-C5-C6	-7.28	113.36	117.00
24	A3	39	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1769	U	C4'-C3'-C2'	-7.28	95.32	102.60
21	AA	853	C	N3-C2-O2	-7.28	116.81	121.90
21	AA	1245	C	N3-C2-O2	-7.28	116.80	121.90
21	AA	1318	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1221	C	N3-C2-O2	-7.28	116.80	121.90
54	BA	2459	A	C5-C6-N1	7.28	121.34	117.70
43	BU	21	ARG	NE-CZ-NH1	7.28	123.94	120.30
54	BA	1459	G	O4'-C1'-N9	7.28	114.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	19	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1952	A	C4-C5-C6	-7.28	113.36	117.00
21	AA	1469	C	N3-C2-O2	-7.27	116.81	121.90
21	AA	1226	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	116	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	920	A	C4-C5-C6	-7.27	113.36	117.00
21	AA	907	A	C4-C5-C6	-7.27	113.36	117.00
54	BA	753	A	C4-C5-C6	-7.27	113.36	117.00
54	BA	1986	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	2452	C	N1-C2-O2	7.27	123.26	118.90
21	AA	1225	A	C5-C6-N1	7.27	121.33	117.70
34	BL	33	ARG	NE-CZ-NH1	7.27	123.93	120.30
54	BA	783	A	C5-C6-N1	7.27	121.33	117.70
21	AA	1267	C	N3-C2-O2	-7.26	116.81	121.90
54	BA	1641	A	C5-C6-N1	7.26	121.33	117.70
56	B5	134	ARG	NE-CZ-NH1	7.26	123.93	120.30
54	BA	192	C	N1-C2-O2	7.26	123.25	118.90
54	BA	1070	A	C4-C5-C6	-7.26	113.37	117.00
54	BA	71	A	C4-C5-C6	-7.26	113.37	117.00
21	AA	1408	A	C4-C5-C6	-7.26	113.37	117.00
54	BA	480	A	C5-C6-N1	7.26	121.33	117.70
22	A1	56	C	N3-C2-O2	-7.25	116.82	121.90
54	BA	2760	C	N3-C2-O2	-7.25	116.82	121.90
11	AL	85	ARG	NE-CZ-NH1	7.25	123.93	120.30
21	AA	1319	A	C5-C6-N1	7.25	121.33	117.70
54	BA	1746	A	C5-C6-N1	7.25	121.33	117.70
54	BA	1796	U	O4'-C1'-N1	7.25	114.00	108.20
54	BA	1900	A	C4-C5-C6	-7.25	113.37	117.00
25	BC	213	ARG	NE-CZ-NH1	7.25	123.92	120.30
54	BA	1134	A	C5-C6-N1	7.25	121.33	117.70
21	AA	1398	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	108	G	N1-C6-O6	-7.25	115.55	119.90
54	BA	478	A	C5-C6-N1	7.25	121.32	117.70
54	BA	722	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	2050	C	N3-C2-O2	-7.25	116.83	121.90
21	AA	1254	A	C5-C6-N1	7.25	121.32	117.70
24	A3	60	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1879	C	N3-C2-O2	-7.25	116.83	121.90
21	AA	1031	C	N1-C2-O2	7.24	123.25	118.90
27	BE	49	ARG	NE-CZ-NH2	-7.24	116.68	120.30
39	BQ	50	ARG	NE-CZ-NH2	7.24	123.92	120.30
54	BA	2794	C	N3-C2-O2	-7.24	116.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	983	A	C5-C6-N1	7.24	121.32	117.70
21	AA	1101	A	C5-C6-N1	7.24	121.32	117.70
54	BA	742	A	C4-C5-C6	-7.24	113.38	117.00
54	BA	2310	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	2266	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2708	G	O4'-C1'-N9	7.24	113.99	108.20
42	BT	76	ARG	NE-CZ-NH1	7.24	123.92	120.30
54	BA	340	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	1142	A	C4-C5-C6	-7.24	113.38	117.00
54	BA	1561	C	N3-C2-O2	-7.23	116.84	121.90
21	AA	298	A	C5-C6-N1	7.23	121.32	117.70
21	AA	478	A	C5-C6-N1	7.23	121.32	117.70
21	AA	583	A	N1-C6-N6	-7.23	114.26	118.60
36	BN	118	ARG	NE-CZ-NH1	7.23	123.92	120.30
54	BA	1496	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	1650	A	C5-C6-N1	7.23	121.32	117.70
21	AA	1413	A	C5-C6-N1	7.23	121.31	117.70
54	BA	1419	A	C5-C6-N1	7.23	121.31	117.70
54	BA	1757	A	C5-C6-N1	7.23	121.32	117.70
54	BA	1789	A	C5-C6-N1	7.23	121.31	117.70
20	AU	20	ARG	NE-CZ-NH1	7.23	123.91	120.30
21	AA	583	A	C5-C6-N1	7.23	121.31	117.70
54	BA	475	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	2880	C	N3-C2-O2	-7.23	116.84	121.90
6	AG	110	ARG	NE-CZ-NH1	7.23	123.91	120.30
21	AA	28	A	N1-C6-N6	-7.23	114.27	118.60
35	BM	50	ARG	NE-CZ-NH1	7.23	123.91	120.30
54	BA	590	A	C5-C6-N1	7.22	121.31	117.70
54	BA	915	C	N3-C2-O2	-7.22	116.84	121.90
54	BA	990	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2089	C	N3-C2-O2	-7.22	116.84	121.90
54	BA	1230	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	52	A	C5-C6-N1	7.22	121.31	117.70
54	BA	581	C	O4'-C1'-N1	7.22	113.97	108.20
54	BA	2283	C	N3-C2-O2	-7.22	116.85	121.90
54	BA	849	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	2264	C	N3-C2-O2	-7.22	116.85	121.90
21	AA	435	A	N1-C6-N6	-7.21	114.27	118.60
29	BG	169	ARG	NE-CZ-NH1	7.21	123.91	120.30
54	BA	1260	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2851	A	C4-C5-C6	-7.21	113.39	117.00
21	AA	263	A	N1-C6-N6	-7.21	114.27	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1357	A	C5-C6-N1	7.21	121.31	117.70
54	BA	184	C	N3-C2-O2	-7.21	116.85	121.90
21	AA	767	A	C5-C6-N1	7.21	121.31	117.70
22	A1	14	A	N1-C6-N6	-7.21	114.27	118.60
22	A1	16	C	N3-C2-O2	-7.21	116.85	121.90
51	B2	3	ARG	NE-CZ-NH2	7.21	123.91	120.30
21	AA	946	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1947	C	N3-C2-O2	-7.21	116.85	121.90
21	AA	716	A	C4-C5-C6	-7.21	113.39	117.00
54	BA	391	A	C5-C6-N1	7.21	121.30	117.70
54	BA	1773	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2287	A	N1-C6-N6	-7.21	114.28	118.60
54	BA	2717	C	N3-C4-C5	7.21	124.78	121.90
54	BA	1238	G	C5-C6-N1	7.21	115.10	111.50
54	BA	1626	A	C5-C6-N1	7.21	121.30	117.70
54	BA	1732	C	N1-C2-O2	7.21	123.22	118.90
21	AA	1289	A	C5-C6-N1	7.21	121.30	117.70
21	AA	640	A	C4-C5-C6	-7.20	113.40	117.00
45	BW	76	ARG	NE-CZ-NH2	-7.20	116.70	120.30
54	BA	661	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2103	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	2544	G	C8-N9-C4	-7.20	103.52	106.40
55	BB	66	A	C4-C5-C6	-7.20	113.40	117.00
54	BA	161	A	C4-C5-C6	-7.20	113.40	117.00
2	AC	71	ARG	NE-CZ-NH1	7.20	123.90	120.30
21	AA	696	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2071	A	N1-C6-N6	-7.20	114.28	118.60
37	BO	7	ARG	NE-CZ-NH1	7.19	123.90	120.30
21	AA	913	A	C4-C5-C6	-7.19	113.40	117.00
54	BA	192	C	N3-C2-O2	-7.19	116.87	121.90
54	BA	1829	A	C5-C6-N1	7.19	121.30	117.70
9	AJ	31	ARG	NE-CZ-NH1	7.19	123.90	120.30
21	AA	1201	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	503	A	N1-C6-N6	-7.19	114.28	118.60
54	BA	1653	G	O4'-C1'-N9	7.19	113.95	108.20
54	BA	2134	A	C5-C6-N1	7.19	121.30	117.70
6	AG	78	ARG	NE-CZ-NH1	7.19	123.89	120.30
21	AA	1394	A	C5-C6-N1	7.19	121.29	117.70
21	AA	238	A	C5-C6-N1	7.19	121.29	117.70
21	AA	547	A	C5-C6-N1	7.19	121.29	117.70
54	BA	251	A	C5-C6-N1	7.19	121.29	117.70
54	BA	1096	A	N1-C6-N6	-7.19	114.29	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	422	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	633	A	C5-C6-N1	7.18	121.29	117.70
54	BA	782	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	933	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	2855	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	2510	C	C6-N1-C2	-7.18	117.43	120.30
54	BA	445	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	1933	G	O4'-C1'-N9	7.18	113.94	108.20
21	AA	84	U	N3-C2-O2	-7.18	117.18	122.20
24	A3	45	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	99	U	O4'-C1'-N1	7.18	113.94	108.20
54	BA	324	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	514	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	1829	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	1782	U	O4'-C1'-N1	7.17	113.94	108.20
21	AA	101	A	C5-C6-N1	7.17	121.29	117.70
21	AA	1306	A	C5-C6-N1	7.17	121.29	117.70
54	BA	244	A	C5-C6-N1	7.17	121.29	117.70
54	BA	603	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	1676	A	C5-C6-N1	7.17	121.29	117.70
5	AF	24	ARG	NE-CZ-NH2	-7.17	116.72	120.30
13	AN	69	ARG	NH1-CZ-NH2	-7.17	111.52	119.40
21	AA	642	A	C5-C6-N1	7.17	121.28	117.70
21	AA	1397	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	1392	A	C5-C6-N1	7.17	121.28	117.70
54	BA	164	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	612	C	N3-C2-O2	-7.17	116.88	121.90
39	BQ	57	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	504	A	C5-C6-N1	7.16	121.28	117.70
54	BA	677	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	403	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	104	A	C4-C5-C6	-7.16	113.42	117.00
54	BA	2145	C	N3-C2-O2	-7.16	116.89	121.90
21	AA	78	A	C5-C6-N1	7.16	121.28	117.70
21	AA	1430	A	C4-C5-C6	-7.16	113.42	117.00
29	BG	54	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	1266	G	O4'-C1'-N9	7.16	113.93	108.20
21	AA	34	C	N3-C2-O2	-7.16	116.89	121.90
21	AA	412	A	C5-C6-N1	7.16	121.28	117.70
21	AA	706	A	C4-C5-C6	-7.16	113.42	117.00
54	BA	1433	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2392	A	C5-C6-N1	7.16	121.28	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	969	A	N1-C6-N6	-7.16	114.31	118.60
21	AA	496	A	N1-C6-N6	-7.16	114.31	118.60
21	AA	937	A	C4-C5-C6	-7.16	113.42	117.00
24	A3	60	A	C4-C5-C6	-7.16	113.42	117.00
54	BA	404	A	N1-C6-N6	-7.16	114.31	118.60
54	BA	1558	C	N1-C2-O2	7.16	123.19	118.90
54	BA	2009	A	C5-C6-N1	7.16	121.28	117.70
21	AA	502	A	C5-C6-N1	7.15	121.28	117.70
21	AA	312	C	N3-C2-O2	-7.15	116.89	121.90
21	AA	393	A	N1-C6-N6	-7.15	114.31	118.60
21	AA	687	A	C5-C6-N1	7.15	121.28	117.70
21	AA	1139	G	N3-C2-N2	-7.15	114.89	119.90
34	BL	2	ARG	NE-CZ-NH2	-7.15	116.72	120.30
54	BA	1039	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1086	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	2033	A	N1-C6-N6	-7.15	114.31	118.60
13	AN	61	ARG	NE-CZ-NH1	7.15	123.88	120.30
21	AA	996	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	191	A	C4-C5-C6	-7.15	113.42	117.00
54	BA	371	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2579	C	C6-N1-C2	-7.15	117.44	120.30
54	BA	788	A	C5-C6-N1	7.15	121.28	117.70
21	AA	1179	A	C4-C5-C6	-7.15	113.43	117.00
39	BQ	29	ARG	NE-CZ-NH1	7.15	123.87	120.30
54	BA	2658	C	N3-C2-O2	-7.15	116.90	121.90
21	AA	176	C	N3-C4-C5	7.15	124.76	121.90
21	AA	635	A	C4-C5-C6	-7.15	113.43	117.00
54	BA	1043	C	N3-C2-O2	-7.15	116.90	121.90
12	AM	91	ARG	NE-CZ-NH1	7.14	123.87	120.30
54	BA	1354	A	N1-C6-N6	-7.14	114.31	118.60
21	AA	460	A	C4-C5-C6	-7.14	113.43	117.00
39	BQ	54	ARG	NE-CZ-NH1	7.14	123.87	120.30
21	AA	49	U	O4'-C1'-N1	7.14	113.91	108.20
54	BA	1689	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2716	C	N3-C2-O2	-7.14	116.90	121.90
21	AA	246	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	753	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2322	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2572	A	N1-C6-N6	-7.14	114.32	118.60
54	BA	1754	A	C4-C5-C6	-7.13	113.43	117.00
54	BA	1894	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	2430	A	C5-C6-N1	7.13	121.27	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BI	64	ARG	NE-CZ-NH1	7.13	123.87	120.30
54	BA	1276	A	C5-C6-N1	7.13	121.27	117.70
54	BA	2278	A	N1-C6-N6	-7.13	114.32	118.60
54	BA	223	A	C4-C5-C6	-7.13	113.43	117.00
54	BA	2124	G	N1-C6-O6	-7.13	115.62	119.90
54	BA	2875	C	O4'-C1'-N1	7.13	113.91	108.20
21	AA	1492	A	N1-C6-N6	-7.13	114.32	118.60
54	BA	2542	A	C5-C6-N1	7.13	121.27	117.70
21	AA	1408	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1705	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	2795	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	497	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	1382	G	O4'-C1'-N9	7.13	113.90	108.20
54	BA	2327	A	C4-C5-C6	-7.13	113.44	117.00
21	AA	1509	C	N1-C2-O2	7.12	123.17	118.90
38	BP	92	ARG	NE-CZ-NH2	-7.12	116.74	120.30
54	BA	229	C	N3-C2-O2	-7.12	116.91	121.90
21	AA	483	C	N1-C2-O2	7.12	123.17	118.90
21	AA	1044	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1195	C	N3-C2-O2	-7.12	116.91	121.90
24	A3	66	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	590	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	1644	C	O4'-C1'-N1	7.12	113.90	108.20
54	BA	2518	A	N1-C6-N6	-7.12	114.33	118.60
21	AA	336	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	1502	A	C5-C6-N1	7.12	121.26	117.70
54	BA	975	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	1240	U	O4'-C1'-N1	7.12	113.90	108.20
54	BA	1998	A	C5-C6-N1	7.12	121.26	117.70
21	AA	600	A	C4-C5-C6	-7.12	113.44	117.00
10	AK	97	ARG	NE-CZ-NH1	7.12	123.86	120.30
21	AA	132	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	309	A	C4-C5-C6	-7.12	113.44	117.00
33	BK	98	ARG	NE-CZ-NH1	7.12	123.86	120.30
54	BA	156	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1014	A	C5-C6-N1	7.12	121.26	117.70
24	A3	22	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2711	A	C5-C6-N1	7.12	121.26	117.70
21	AA	210	C	N1-C2-O2	7.11	123.17	118.90
54	BA	164	C	O4'-C1'-N1	7.11	113.89	108.20
54	BA	1290	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	1572	A	C4-C5-C6	-7.11	113.44	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	189	A	C5-C6-N1	7.11	121.26	117.70
54	BA	209	C	N3-C2-O2	-7.11	116.92	121.90
21	AA	85	U	N3-C2-O2	-7.11	117.22	122.20
54	BA	398	C	N3-C2-O2	-7.11	116.92	121.90
21	AA	335	C	N3-C2-O2	-7.11	116.92	121.90
21	AA	532	A	C1'-O4'-C4'	-7.11	104.22	109.90
21	AA	1479	C	N1-C2-O2	7.11	123.17	118.90
54	BA	699	A	C5-C6-N1	7.11	121.25	117.70
54	BA	1689	A	C4-C5-C6	-7.11	113.45	117.00
4	AE	92	ARG	NE-CZ-NH1	7.11	123.85	120.30
21	AA	521	G	N1-C6-O6	-7.11	115.64	119.90
54	BA	909	A	C5-C6-N1	7.11	121.25	117.70
54	BA	1853	A	C4-C5-C6	-7.11	113.45	117.00
54	BA	1918	A	O4'-C1'-N9	7.11	113.89	108.20
54	BA	2758	A	C4-C5-C6	-7.11	113.45	117.00
21	AA	946	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	1730	C	N3-C2-O2	-7.10	116.93	121.90
12	AM	112	ARG	NE-CZ-NH1	7.10	123.85	120.30
21	AA	16	A	N1-C6-N6	-7.10	114.34	118.60
21	AA	1101	A	P-O3'-C3'	7.10	128.22	119.70
54	BA	331	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	759	A	N1-C6-N6	-7.10	114.34	118.60
21	AA	694	A	C4-C5-C6	-7.10	113.45	117.00
37	BO	13	ARG	NE-CZ-NH1	7.10	123.85	120.30
54	BA	1618	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2743	U	O4'-C1'-N1	7.10	113.88	108.20
21	AA	1318	A	C4-C5-C6	-7.10	113.45	117.00
22	A1	19	G	O4'-C1'-N9	7.10	113.88	108.20
54	BA	1268	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	2870	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	718	A	C5-C6-N1	7.10	121.25	117.70
21	AA	270	A	N1-C6-N6	-7.09	114.34	118.60
21	AA	655	A	C5-C6-N1	7.09	121.25	117.70
21	AA	1054	C	N3-C2-O2	-7.09	116.93	121.90
24	A3	59	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	1226	A	N1-C6-N6	-7.09	114.34	118.60
54	BA	2321	U	O4'-C1'-N1	7.09	113.88	108.20
21	AA	81	A	N1-C6-N6	-7.09	114.34	118.60
21	AA	1000	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	2822	G	N1-C6-O6	-7.09	115.64	119.90
21	AA	579	A	C5-C6-N1	7.09	121.25	117.70
54	BA	905	A	C5-C6-N1	7.09	121.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1974	C	N3-C2-O2	-7.09	116.94	121.90
54	BA	522	A	C5-C6-N1	7.09	121.24	117.70
21	AA	175	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	702	A	C5-C6-N1	7.09	121.24	117.70
22	A1	38	A	C4-C5-C6	-7.09	113.46	117.00
54	BA	1304	A	C5-C6-N1	7.09	121.24	117.70
54	BA	1544	A	C5-C6-N1	7.09	121.24	117.70
54	BA	2708	G	N1-C6-O6	-7.09	115.65	119.90
21	AA	600	A	C5-C6-N1	7.08	121.24	117.70
21	AA	1288	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	1977	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2482	A	C5-C6-N1	7.08	121.24	117.70
21	AA	1281	C	N3-C4-N4	-7.08	113.04	118.00
21	AA	470	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	980	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	1378	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	1019	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	1762	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	411	A	C5-C6-N1	7.07	121.24	117.70
21	AA	621	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	1261	A	C5-C6-N1	7.07	121.24	117.70
54	BA	378	C	O4'-C1'-N1	7.07	113.86	108.20
54	BA	2150	C	O4'-C1'-N1	7.07	113.86	108.20
54	BA	2826	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	139	U	O4'-C1'-N1	7.07	113.86	108.20
54	BA	1955	U	O4'-C1'-N1	7.07	113.86	108.20
21	AA	831	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	1496	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	2427	C	N3-C2-O2	-7.07	116.95	121.90
10	AK	105	ARG	NE-CZ-NH1	7.07	123.83	120.30
54	BA	1243	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1585	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1665	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	66	A	C5-C6-N1	7.06	121.23	117.70
21	AA	575	G	N1-C6-O6	-7.06	115.66	119.90
54	BA	1702	G	N1-C6-O6	-7.06	115.66	119.90
54	BA	1348	C	O4'-C1'-N1	7.06	113.85	108.20
54	BA	28	A	C5-C6-N1	7.06	121.23	117.70
54	BA	892	A	N1-C6-N6	-7.06	114.37	118.60
54	BA	1549	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	1578	U	O4'-C1'-N1	7.06	113.85	108.20
54	BA	1916	A	C4-C5-C6	-7.06	113.47	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1691	C	O4'-C1'-N1	7.06	113.84	108.20
54	BA	2091	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	325	A	C4-C5-C6	-7.05	113.47	117.00
21	AA	1239	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	199	A	C5-C6-N1	7.05	121.23	117.70
54	BA	689	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	1553	A	C4-C5-C6	-7.05	113.47	117.00
21	AA	629	A	C5-C6-N1	7.05	121.22	117.70
21	AA	1248	A	C5-C6-N1	7.05	121.22	117.70
54	BA	274	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	2031	A	C5-C6-N1	7.05	121.22	117.70
54	BA	680	C	N3-C2-O2	-7.05	116.97	121.90
25	BC	269	ARG	NE-CZ-NH1	7.05	123.82	120.30
54	BA	1985	C	O4'-C1'-N1	7.05	113.84	108.20
55	BB	113	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	1509	A	C5-C6-N1	7.04	121.22	117.70
21	AA	7	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1373	A	N1-C6-N6	-7.04	114.37	118.60
54	BA	609	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1877	A	C5-C6-N1	7.04	121.22	117.70
21	AA	73	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	533	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2163	A	N1-C6-N6	-7.04	114.38	118.60
21	AA	275	G	C8-N9-C4	-7.04	103.58	106.40
54	BA	2676	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	1030	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	1815	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	2103	C	N3-C4-C5	7.04	124.71	121.90
21	AA	483	C	N3-C2-O2	-7.03	116.98	121.90
21	AA	1412	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	2169	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2332	C	N1-C2-O2	7.03	123.12	118.90
27	BE	40	ARG	NE-CZ-NH2	-7.03	116.78	120.30
54	BA	920	A	C5-C6-N1	7.03	121.22	117.70
12	AM	70	ARG	NE-CZ-NH1	7.03	123.81	120.30
21	AA	1209	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1895	C	N3-C2-O2	-7.03	116.98	121.90
21	AA	228	A	C4-C5-C6	-7.03	113.48	117.00
28	BF	124	ARG	NE-CZ-NH1	7.03	123.81	120.30
21	AA	630	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	270	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	2814	A	C4-C5-C6	-7.03	113.49	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	55	ARG	NE-CZ-NH1	7.03	123.81	120.30
54	BA	1027	A	C5-C6-N1	7.03	121.21	117.70
54	BA	734	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	2275	C	N3-C2-O2	-7.02	116.98	121.90
21	AA	264	C	N3-C2-O2	-7.02	116.98	121.90
54	BA	21	A	C5-C6-N1	7.02	121.21	117.70
54	BA	837	C	N3-C2-O2	-7.02	116.98	121.90
54	BA	2827	C	N3-C2-O2	-7.02	116.98	121.90
54	BA	2117	A	O4'-C1'-N9	7.02	113.82	108.20
54	BA	2097	A	C5-C6-N1	7.02	121.21	117.70
18	AS	35	ARG	NE-CZ-NH1	7.02	123.81	120.30
54	BA	1020	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	1194	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1254	A	N1-C6-N6	-7.02	114.39	118.60
21	AA	1246	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1205	A	N1-C6-N6	-7.02	114.39	118.60
21	AA	596	A	C5-C6-N1	7.01	121.21	117.70
21	AA	249	U	N3-C2-O2	-7.01	117.29	122.20
21	AA	176	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	723	U	N3-C2-O2	-7.01	117.29	122.20
21	AA	1489	G	N1-C6-O6	-7.01	115.69	119.90
54	BA	244	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	1755	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	2614	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2755	C	O4'-C1'-N1	7.01	113.81	108.20
21	AA	790	A	C4-C5-C6	-7.01	113.50	117.00
21	AA	807	A	C5-C6-N1	7.01	121.20	117.70
46	BX	17	ARG	NE-CZ-NH1	7.01	123.81	120.30
54	BA	840	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	2777	G	N9-C4-C5	7.01	108.20	105.40
21	AA	1035	A	C5-C6-N1	7.01	121.20	117.70
21	AA	1521	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	1109	C	C3'-C2'-C1'	7.01	107.11	101.50
54	BA	1964	G	C3'-C2'-C1'	7.01	107.11	101.50
21	AA	676	A	C4-C5-C6	-7.01	113.50	117.00
21	AA	814	A	N1-C6-N6	-7.01	114.40	118.60
21	AA	978	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2003	A	C4-C5-C6	-7.01	113.50	117.00
55	BB	99	A	N1-C6-N6	-7.01	114.40	118.60
54	BA	793	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	1179	A	N1-C6-N6	-7.00	114.40	118.60
21	AA	971	G	N1-C6-O6	-7.00	115.70	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1387	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	1603	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	19	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1854	A	C5-C6-N1	7.00	121.20	117.70
21	AA	559	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1032	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1794	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	702	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1953	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1537	G	O4'-C1'-N9	6.99	113.80	108.20
54	BA	2682	A	C5-C6-N1	6.99	121.20	117.70
21	AA	1055	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	95	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	613	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	705	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	1434	A	O4'-C1'-N9	6.99	113.79	108.20
28	BF	111	ARG	NE-CZ-NH1	6.99	123.79	120.30
54	BA	272	A	O4'-C1'-N9	6.99	113.79	108.20
54	BA	2158	A	C5-C6-N1	6.99	121.19	117.70
21	AA	325	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2761	A	O4'-C1'-N9	6.99	113.79	108.20
21	AA	768	A	C5-C6-N1	6.98	121.19	117.70
54	BA	788	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	1130	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	1551	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2385	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	2823	A	C3'-C2'-C1'	6.98	107.09	101.50
21	AA	824	G	N9-C4-C5	6.98	108.19	105.40
54	BA	1551	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	2620	C	N3-C4-C5	6.98	124.69	121.90
21	AA	364	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	31	C	N1-C2-O2	6.98	123.09	118.90
54	BA	1040	A	N1-C6-N6	-6.98	114.41	118.60
21	AA	116	A	N1-C6-N6	-6.98	114.41	118.60
21	AA	411	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	845	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	2572	A	C5-C6-N1	6.98	121.19	117.70
21	AA	1061	G	N3-C4-C5	-6.98	125.11	128.60
54	BA	2691	C	N3-C2-O2	-6.98	117.02	121.90
21	AA	553	A	C4-C5-C6	-6.97	113.51	117.00
54	BA	948	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	1885	A	C4-C5-C6	-6.97	113.51	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2753	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	1004	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1095	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1990	C	O4'-C1'-N1	6.97	113.78	108.20
54	BA	2612	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	499	A	C5-C6-N1	6.97	121.19	117.70
22	A1	21	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1753	G	N3-C4-C5	-6.97	125.11	128.60
54	BA	2461	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	2705	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	263	A	C5-C6-N1	6.97	121.18	117.70
21	AA	1179	A	C5-C6-N1	6.97	121.19	117.70
21	AA	1217	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	1314	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	251	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	547	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2090	A	C6-C5-N7	6.97	137.18	132.30
54	BA	2723	C	N1-C2-O2	6.97	123.08	118.90
21	AA	1147	C	N3-C2-O2	-6.97	117.02	121.90
22	A1	58	A	C5-C6-N1	6.97	121.18	117.70
54	BA	61	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	332	A	C5-C6-N1	6.96	121.18	117.70
54	BA	641	U	O4'-C1'-N1	6.96	113.77	108.20
54	BA	1039	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1800	C	N1-C2-O2	6.96	123.08	118.90
21	AA	460	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1045	C	N3-C2-O2	-6.96	117.03	121.90
8	AI	94	ARG	NE-CZ-NH1	6.96	123.78	120.30
21	AA	1204	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1621	U	O4'-C1'-N1	6.96	113.77	108.20
21	AA	811	C	O4'-C1'-N1	6.96	113.77	108.20
21	AA	825	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1151	A	C5-C6-N1	6.96	121.18	117.70
54	BA	829	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1050	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1310	G	O4'-C1'-N9	6.96	113.77	108.20
54	BA	2207	C	N3-C2-O2	-6.96	117.03	121.90
21	AA	119	A	N1-C6-N6	-6.95	114.43	118.60
21	AA	706	A	N1-C6-N6	-6.95	114.43	118.60
21	AA	998	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	1475	G	C5-C6-N1	6.95	114.98	111.50
55	BB	34	A	C5-C6-N1	6.95	121.18	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	337	C	O4'-C1'-N1	6.95	113.76	108.20
54	BA	1558	C	N3-C2-O2	-6.95	117.03	121.90
21	AA	819	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	623	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	717	C	N1-C2-O2	6.95	123.07	118.90
54	BA	2019	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2471	A	C5-C6-N1	6.95	121.17	117.70
21	AA	564	C	N3-C2-O2	-6.95	117.04	121.90
29	BG	2	ARG	NE-CZ-NH1	6.95	123.77	120.30
54	BA	1146	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	1328	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	1598	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	2681	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	1401	G	C5-C6-N1	6.94	114.97	111.50
54	BA	587	C	N1-C2-O2	6.94	123.07	118.90
54	BA	1135	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	2841	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	346	G	C5-C6-N1	6.94	114.97	111.50
24	A3	11	A	N1-C6-N6	-6.94	114.44	118.60
31	BI	102	ARG	NE-CZ-NH1	6.94	123.77	120.30
54	BA	2198	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	2217	G	C5-C6-N1	6.94	114.97	111.50
32	BJ	69	ARG	NE-CZ-NH1	6.94	123.77	120.30
21	AA	397	A	C5-C6-N1	6.94	121.17	117.70
21	AA	1157	A	N1-C6-N6	-6.94	114.44	118.60
54	BA	1323	C	N3-C2-O2	-6.94	117.04	121.90
39	BQ	32	ARG	NE-CZ-NH2	6.94	123.77	120.30
54	BA	1596	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	2515	C	N3-C2-O2	-6.94	117.05	121.90
21	AA	712	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	1476	U	O4'-C1'-N1	6.93	113.75	108.20
54	BA	2516	A	C4-C5-C6	-6.93	113.53	117.00
5	AF	45	ARG	NE-CZ-NH1	6.93	123.77	120.30
21	AA	71	A	C5-C6-N1	6.93	121.17	117.70
21	AA	1365	G	N3-C2-N2	-6.93	115.05	119.90
54	BA	2114	A	C4-C5-C6	-6.93	113.53	117.00
21	AA	1329	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	21	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	2068	U	C1'-O4'-C4'	-6.93	104.36	109.90
54	BA	634	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	1652	A	C5-C6-N1	6.93	121.16	117.70
54	BA	2683	C	N3-C2-O2	-6.93	117.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AE	44	ARG	NE-CZ-NH1	6.93	123.76	120.30
21	AA	383	A	C4-C5-C6	-6.93	113.54	117.00
21	AA	806	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	2029	G	C5-C6-N1	6.93	114.96	111.50
54	BA	2045	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	2758	A	C5-C6-N1	6.93	121.16	117.70
54	BA	1669	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	1821	A	C5-C6-N1	6.93	121.16	117.70
54	BA	2104	C	N3-C4-C5	6.93	124.67	121.90
55	BB	53	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	233	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1021	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1367	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	2403	C	N3-C2-O2	-6.92	117.05	121.90
21	AA	267	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	1484	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	854	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	1042	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2297	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2819	G	C5-C6-N1	6.92	114.96	111.50
55	BB	52	A	C5-C6-N1	6.92	121.16	117.70
54	BA	781	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	1933	G	C8-N9-C4	-6.92	103.63	106.40
54	BA	2808	G	N1-C6-O6	-6.92	115.75	119.90
54	BA	2858	C	O4'-C1'-N1	6.92	113.73	108.20
54	BA	1386	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	95	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1954	G	N3-C4-C5	-6.91	125.14	128.60
54	BA	1029	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	1208	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	2469	A	C5-C6-N1	6.91	121.16	117.70
21	AA	797	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	599	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	2043	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	2483	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	932	C	O4'-C1'-N1	6.91	113.72	108.20
55	BB	99	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	1057	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	2183	A	N1-C6-N6	-6.90	114.46	118.60
7	AH	14	ARG	NE-CZ-NH1	6.90	123.75	120.30
21	AA	382	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	158	U	O4'-C1'-N1	6.90	113.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2338	C	N3-C4-C5	6.90	124.66	121.90
21	AA	972	C	N1-C2-O2	6.90	123.04	118.90
21	AA	1340	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1717	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2333	A	N1-C6-N6	-6.90	114.46	118.60
54	BA	2512	C	O4'-C1'-N1	6.90	113.72	108.20
21	AA	1231	G	N9-C4-C5	6.90	108.16	105.40
54	BA	1040	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1654	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	358	U	O4'-C1'-N1	6.89	113.72	108.20
11	AL	93	ARG	NE-CZ-NH1	6.89	123.75	120.30
54	BA	1204	A	O4'-C1'-N9	6.89	113.71	108.20
21	AA	545	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	212	G	O4'-C1'-N9	6.89	113.71	108.20
21	AA	756	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	2675	A	C5-C6-N1	6.89	121.14	117.70
21	AA	1269	A	C5-C6-N1	6.89	121.14	117.70
22	A1	61	C	N3-C2-O2	-6.89	117.08	121.90
24	A3	11	A	C5-C6-N1	6.89	121.14	117.70
54	BA	226	A	C5-C6-N1	6.89	121.14	117.70
54	BA	1053	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1382	G	C8-N9-C4	-6.89	103.64	106.40
21	AA	866	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	2378	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2887	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	1214	A	N1-C6-N6	-6.88	114.47	118.60
54	BA	1233	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	1558	C	N3-C4-C5	6.88	124.65	121.90
54	BA	2042	A	N1-C6-N6	-6.88	114.47	118.60
54	BA	2091	C	N1-C2-O2	6.88	123.03	118.90
54	BA	1096	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1293	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	2288	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	482	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1140	C	N3-C2-O2	-6.88	117.09	121.90
21	AA	1286	U	N3-C2-O2	-6.88	117.39	122.20
54	BA	128	C	N3-C2-O2	-6.88	117.09	121.90
54	BA	1213	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	1953	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2793	C	N3-C2-O2	-6.88	117.09	121.90
21	AA	1130	A	C5-C6-N1	6.88	121.14	117.70
21	AA	1092	A	C4-C5-C6	-6.87	113.56	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1145	A	C5-C6-N1	6.87	121.14	117.70
54	BA	2005	A	N1-C6-N6	-6.87	114.48	118.60
44	BV	21	ARG	NE-CZ-NH1	6.87	123.74	120.30
54	BA	1207	C	C6-N1-C2	-6.87	117.55	120.30
54	BA	2070	A	C5-C6-N1	6.87	121.14	117.70
54	BA	2398	U	O4'-C1'-N1	6.87	113.70	108.20
21	AA	695	A	C5-C6-N1	6.87	121.14	117.70
36	BN	69	ARG	NE-CZ-NH1	6.87	123.73	120.30
54	BA	1685	C	N3-C2-O2	-6.87	117.09	121.90
35	BM	114	ARG	NE-CZ-NH1	6.87	123.73	120.30
54	BA	666	A	N1-C6-N6	-6.87	114.48	118.60
54	BA	1247	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1477	A	N1-C6-N6	-6.87	114.48	118.60
54	BA	1525	A	N1-C6-N6	-6.87	114.48	118.60
55	BB	108	A	C5-C6-N1	6.87	121.13	117.70
21	AA	247	G	N9-C4-C5	6.87	108.15	105.40
21	AA	1101	A	N1-C6-N6	-6.87	114.48	118.60
54	BA	14	A	C5-C6-N1	6.87	121.13	117.70
54	BA	139	U	N3-C2-O2	-6.87	117.39	122.20
54	BA	1073	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	1114	C	N3-C2-O2	-6.87	117.09	121.90
55	BB	116	G	C8-N9-C4	-6.87	103.65	106.40
21	AA	55	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	2020	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2727	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	1126	U	N3-C2-O2	-6.86	117.40	122.20
21	AA	716	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	820	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1392	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	2644	G	N1-C6-O6	-6.86	115.78	119.90
54	BA	2883	A	C5-C6-N1	6.86	121.13	117.70
21	AA	25	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	826	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	1508	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	426	C	O4'-C1'-N1	6.86	113.69	108.20
54	BA	937	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2469	A	O4'-C1'-N9	6.86	113.69	108.20
21	AA	1111	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1912	A	N1-C6-N6	-6.86	114.49	118.60
54	BA	698	C	N3-C2-O2	-6.85	117.10	121.90
54	BA	2795	C	N1-C2-O2	6.85	123.01	118.90
55	BB	73	A	C4-C5-C6	-6.85	113.57	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	413	G	C5'-C4'-C3'	-6.85	105.04	116.00
54	BA	1437	C	N3-C2-O2	-6.85	117.11	121.90
21	AA	445	G	C5-C6-N1	6.85	114.92	111.50
54	BA	1288	G	N1-C6-O6	-6.85	115.79	119.90
21	AA	919	A	C4-C5-C6	-6.85	113.58	117.00
6	AG	3	ARG	NE-CZ-NH1	6.85	123.72	120.30
21	AA	114	U	O4'-C1'-N1	6.84	113.67	108.20
22	A1	72	C	N1-C2-O2	6.84	123.01	118.90
54	BA	2778	A	C4-C5-C6	-6.84	113.58	117.00
21	AA	679	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	878	A	N1-C6-N6	-6.84	114.49	118.60
21	AA	1196	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1338	G	C1'-O4'-C4'	-6.84	104.43	109.90
54	BA	1122	G	N3-C2-N2	-6.84	115.11	119.90
54	BA	1595	C	N1-C2-O2	6.84	123.01	118.90
54	BA	631	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1610	A	C5-C6-N1	6.84	121.12	117.70
21	AA	766	A	C4-C5-C6	-6.84	113.58	117.00
21	AA	1103	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1801	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	2530	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	800	A	N1-C6-N6	-6.84	114.50	118.60
54	BA	985	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1495	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1188	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2771	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	643	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	177	G	C5-C6-N1	6.83	114.92	111.50
44	BV	79	ARG	NE-CZ-NH1	6.83	123.72	120.30
54	BA	2466	C	O4'-C1'-N1	6.83	113.66	108.20
27	BE	67	ARG	NE-CZ-NH1	6.83	123.72	120.30
21	AA	893	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	2785	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1429	A	O4'-C1'-N9	6.83	113.66	108.20
34	BL	2	ARG	NE-CZ-NH1	6.83	123.71	120.30
54	BA	975	A	C6-C5-N7	6.83	137.08	132.30
54	BA	1625	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	341	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1251	A	C5-C6-N1	6.83	121.11	117.70
54	BA	68	G	C5-C6-N1	6.83	114.91	111.50
21	AA	906	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1172	C	N3-C2-O2	-6.82	117.12	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1463	C	O4'-C1'-N1	6.82	113.66	108.20
54	BA	1495	A	N1-C6-N6	-6.82	114.51	118.60
21	AA	195	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1101	U	O4'-C1'-N1	6.82	113.66	108.20
54	BA	2335	A	N1-C6-N6	-6.82	114.51	118.60
21	AA	765	G	O4'-C1'-N9	6.82	113.65	108.20
54	BA	203	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	2338	C	N1-C2-O2	6.82	122.99	118.90
54	BA	2527	C	N3-C2-O2	-6.82	117.13	121.90
55	BB	58	A	C5-C6-N1	6.82	121.11	117.70
21	AA	1523	G	C5-C6-N1	6.81	114.91	111.50
54	BA	1287	A	C5-C6-N1	6.81	121.11	117.70
55	BB	110	C	N3-C2-O2	-6.81	117.13	121.90
3	AD	183	ARG	NE-CZ-NH1	6.81	123.71	120.30
54	BA	142	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	2174	C	N1-C2-O2	6.81	122.99	118.90
54	BA	2717	C	N1-C2-O2	6.81	122.99	118.90
54	BA	254	G	C5'-C4'-O4'	6.81	117.27	109.10
54	BA	1348	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	938	A	O4'-C1'-N9	6.81	113.65	108.20
21	AA	1183	U	O4'-C1'-N1	6.81	113.65	108.20
22	A1	72	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	67	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	561	U	C3'-C2'-C1'	6.81	106.95	101.50
54	BA	2354	C	O4'-C1'-N1	6.81	113.65	108.20
54	BA	219	A	C4-C5-C6	-6.81	113.60	117.00
54	BA	2767	C	N3-C2-O2	-6.81	117.14	121.90
54	BA	995	C	N3-C2-O2	-6.80	117.14	121.90
55	BB	99	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1037	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	1229	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	1336	C	N1-C2-O2	6.80	122.98	118.90
21	AA	1366	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	1410	A	C5-C6-N1	6.80	121.10	117.70
54	BA	979	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	372	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	415	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	658	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	715	A	C5-C6-N1	6.80	121.10	117.70
21	AA	770	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	2079	U	O4'-C1'-N1	6.80	113.64	108.20
21	AA	608	A	C5-C6-N1	6.80	121.10	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	111	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	2790	U	O4'-C1'-N1	6.80	113.64	108.20
21	AA	1265	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	507	A	C5-C6-N1	6.79	121.10	117.70
54	BA	886	A	N1-C6-N6	-6.79	114.52	118.60
31	BI	133	ARG	NE-CZ-NH1	6.79	123.70	120.30
54	BA	125	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	131	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	1595	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	1668	A	N1-C6-N6	-6.79	114.52	118.60
54	BA	2879	A	C5-C6-N1	6.79	121.10	117.70
54	BA	311	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	2559	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	2707	U	O4'-C1'-N1	6.79	113.63	108.20
54	BA	1858	A	C5-C6-N1	6.79	121.09	117.70
27	BE	88	ARG	NE-CZ-NH2	-6.79	116.91	120.30
54	BA	2463	C	O4'-C1'-N1	6.79	113.63	108.20
54	BA	2901	C	N3-C4-C5	6.79	124.61	121.90
21	AA	703	G	N3-C4-C5	-6.79	125.21	128.60
54	BA	264	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	299	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	374	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	1044	C	N1-C2-O2	6.79	122.97	118.90
54	BA	1349	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	1414	C	O4'-C1'-N1	6.79	113.63	108.20
54	BA	1658	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	2295	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	1362	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1246	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1317	G	O4'-C1'-N9	6.78	113.63	108.20
54	BA	2171	A	N1-C6-N6	-6.78	114.53	118.60
54	BA	2215	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	2009	A	C4-C5-C6	-6.78	113.61	117.00
33	BK	17	ARG	NE-CZ-NH1	6.78	123.69	120.30
54	BA	483	A	C5-C6-N1	6.78	121.09	117.70
54	BA	538	A	C5-C6-N1	6.78	121.09	117.70
21	AA	215	C	N3-C2-O2	-6.78	117.16	121.90
54	BA	1638	C	N3-C2-O2	-6.78	117.16	121.90
54	BA	2099	U	O4'-C1'-N1	6.78	113.62	108.20
54	BA	2171	A	C4-C5-C6	-6.78	113.61	117.00
55	BB	54	G	N1-C6-O6	-6.78	115.83	119.90
21	AA	1405	G	N9-C4-C5	6.78	108.11	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	345	A	N1-C6-N6	-6.78	114.53	118.60
55	BB	12	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	706	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2253	G	C8-N9-C4	-6.78	103.69	106.40
54	BA	589	U	O4'-C1'-N1	6.77	113.62	108.20
54	BA	1241	A	C4-C5-C6	-6.77	113.61	117.00
22	A1	35	A	N1-C6-N6	-6.77	114.54	118.60
54	BA	1362	C	O4'-C1'-N1	6.77	113.62	108.20
54	BA	1398	C	N1-C2-O2	6.77	122.96	118.90
54	BA	163	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	354	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	1322	A	C4-C5-C6	-6.77	113.61	117.00
21	AA	1360	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	330	A	C5-C6-N1	6.77	121.08	117.70
54	BA	522	A	N1-C6-N6	-6.77	114.54	118.60
54	BA	575	A	C4-C5-C6	-6.77	113.62	117.00
54	BA	1853	A	C5-C6-N1	6.77	121.08	117.70
21	AA	1250	A	C4-C5-C6	-6.77	113.62	117.00
54	BA	2196	C	O4'-C1'-N1	6.77	113.61	108.20
21	AA	320	A	C5-C6-N1	6.77	121.08	117.70
21	AA	1044	A	C4-C5-C6	-6.77	113.62	117.00
21	AA	1129	C	N1-C2-O2	6.77	122.96	118.90
21	AA	996	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1427	C	N3-C2-O2	-6.76	117.16	121.90
25	BC	101	ARG	NE-CZ-NH1	6.76	123.68	120.30
54	BA	2883	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	147	G	N1-C6-O6	-6.76	115.84	119.90
21	AA	523	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1109	C	O4'-C1'-N1	6.76	113.61	108.20
21	AA	782	A	C4-C5-C6	-6.76	113.62	117.00
22	A1	72	C	N3-C4-C5	6.76	124.60	121.90
25	BC	155	ARG	NE-CZ-NH1	6.76	123.68	120.30
54	BA	1802	A	N1-C6-N6	-6.76	114.55	118.60
54	BA	2821	A	N1-C6-N6	-6.76	114.55	118.60
55	BB	46	A	C5-C6-N1	6.76	121.08	117.70
54	BA	509	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	172	A	C6-C5-N7	6.76	137.03	132.30
54	BA	115	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1614	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1676	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	275	C	N1-C2-O2	6.75	122.95	118.90
21	AA	767	A	C4-C5-C6	-6.75	113.62	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1479	C	N3-C4-C5	6.75	124.60	121.90
54	BA	873	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	925	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	1367	A	C5-C6-N1	6.75	121.08	117.70
21	AA	80	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1342	C	N1-C2-O2	6.75	122.95	118.90
54	BA	980	A	N1-C6-N6	-6.75	114.55	118.60
54	BA	344	A	N1-C6-N6	-6.75	114.55	118.60
54	BA	2270	A	C5-C6-N1	6.75	121.07	117.70
54	BA	2634	A	C5-C6-N1	6.75	121.07	117.70
54	BA	1289	C	O4'-C1'-N1	6.75	113.60	108.20
54	BA	1902	C	N3-C2-O2	-6.75	117.18	121.90
55	BB	18	G	N1-C6-O6	-6.75	115.85	119.90
54	BA	2273	A	C5-C6-N1	6.75	121.07	117.70
21	AA	1167	A	C4-C5-C6	-6.74	113.63	117.00
24	A3	14	A	C5-C6-N1	6.74	121.07	117.70
54	BA	599	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1932	A	N1-C6-N6	-6.74	114.55	118.60
55	BB	108	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	899	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	366	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1236	A	N1-C6-N6	-6.74	114.56	118.60
54	BA	462	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	1145	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	2725	A	N1-C6-N6	-6.74	114.56	118.60
22	A1	76	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	126	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2870	C	N1-C2-O2	6.74	122.94	118.90
21	AA	1116	U	C5-C6-N1	-6.74	119.33	122.70
21	AA	1410	A	O4'-C1'-N9	6.74	113.59	108.20
21	AA	1534	A	C5-C6-N1	6.74	121.07	117.70
54	BA	256	A	N1-C6-N6	-6.74	114.56	118.60
54	BA	613	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1594	U	C5-C6-N1	-6.74	119.33	122.70
21	AA	680	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	694	A	C5-C6-N1	6.73	121.07	117.70
21	AA	750	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	751	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	2620	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	270	A	C4-C5-C6	-6.73	113.64	117.00
21	AA	483	C	C3'-C2'-C1'	6.73	106.89	101.50
21	AA	1236	A	C5-C6-N1	6.73	121.07	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1832	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	1337	G	N3-C4-N9	6.73	130.04	126.00
22	A1	2	G	N3-C4-C5	-6.73	125.24	128.60
54	BA	1056	G	O4'-C1'-N9	6.73	113.58	108.20
54	BA	1446	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2008	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2135	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	863	A	N1-C6-N6	-6.73	114.56	118.60
21	AA	840	C	N1-C2-O2	6.73	122.94	118.90
54	BA	1579	A	C5-C6-N1	6.73	121.06	117.70
21	AA	285	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	2204	G	C5-C6-N1	6.72	114.86	111.50
21	AA	414	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	196	A	C5-C6-N1	6.72	121.06	117.70
54	BA	900	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1504	A	C5-C6-N1	6.72	121.06	117.70
21	AA	1136	C	N1-C2-O2	6.72	122.93	118.90
54	BA	96	C	N3-C2-O2	-6.72	117.19	121.90
21	AA	408	A	C5-C6-N1	6.72	121.06	117.70
21	AA	833	G	N1-C6-O6	-6.72	115.87	119.90
54	BA	471	A	N1-C6-N6	-6.72	114.57	118.60
54	BA	1114	C	N1-C2-O2	6.72	122.93	118.90
55	BB	3	C	O4'-C1'-N1	6.72	113.57	108.20
54	BA	1278	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	1829	A	N1-C6-N6	-6.72	114.57	118.60
54	BA	2104	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	2575	C	N1-C2-O2	6.72	122.93	118.90
54	BA	2620	C	N1-C2-O2	6.72	122.93	118.90
21	AA	758	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	201	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	398	C	N1-C2-O2	6.71	122.93	118.90
54	BA	505	A	N1-C6-N6	-6.71	114.57	118.60
21	AA	968	A	C5-C6-N1	6.71	121.06	117.70
21	AA	1431	A	C3'-C2'-C1'	6.71	106.87	101.50
54	BA	1672	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	2636	C	N1-C2-O2	6.71	122.93	118.90
54	BA	1640	A	C5-C6-N1	6.71	121.05	117.70
54	BA	2275	C	C3'-C2'-C1'	6.71	106.87	101.50
21	AA	129	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	519	C	C1'-O4'-C4'	-6.71	104.53	109.90
21	AA	1452	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	505	A	C5-C6-N1	6.71	121.05	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1724	G	N3-C4-C5	-6.71	125.25	128.60
25	BC	174	ARG	NE-CZ-NH1	6.71	123.65	120.30
54	BA	336	C	O4'-C1'-N1	6.71	113.56	108.20
54	BA	453	A	C5-C6-N1	6.71	121.05	117.70
54	BA	849	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	859	G	O4'-C1'-N9	6.71	113.56	108.20
54	BA	2739	U	C5-C6-N1	-6.71	119.35	122.70
21	AA	83	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	706	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1253	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1626	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2471	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2739	U	N3-C2-O2	-6.70	117.51	122.20
54	BA	957	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	364	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	743	A	C4-C5-C6	-6.70	113.65	117.00
24	A3	39	A	N1-C6-N6	-6.70	114.58	118.60
54	BA	1133	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1871	A	C4-C5-C6	-6.70	113.65	117.00
24	A3	11	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	899	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2534	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	145	G	N3-C2-N2	-6.69	115.21	119.90
54	BA	1695	G	C8-N9-C4	-6.69	103.72	106.40
54	BA	1776	G	N3-C4-C5	-6.69	125.25	128.60
21	AA	575	G	C5-C6-N1	6.69	114.85	111.50
54	BA	1155	A	N1-C6-N6	-6.69	114.58	118.60
54	BA	1906	G	N1-C6-O6	-6.69	115.89	119.90
54	BA	515	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	918	A	N1-C6-N6	-6.69	114.59	118.60
54	BA	1805	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	2282	G	N1-C6-O6	-6.69	115.89	119.90
54	BA	2418	A	C5-C6-N1	6.69	121.05	117.70
21	AA	1035	A	N1-C6-N6	-6.69	114.59	118.60
21	AA	270	A	C5-C6-N1	6.69	121.04	117.70
21	AA	463	U	C5-C6-N1	-6.69	119.36	122.70
21	AA	1345	U	C1'-O4'-C4'	-6.69	104.55	109.90
54	BA	239	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	1889	A	C5-C6-N1	6.69	121.04	117.70
54	BA	2782	G	C8-N9-C4	-6.69	103.72	106.40
21	AA	204	G	C5-C6-N1	6.69	114.84	111.50
54	BA	886	A	C5-C6-N1	6.69	121.04	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	349	A	C4-C5-C6	-6.68	113.66	117.00
33	BK	71	ARG	NE-CZ-NH1	6.68	123.64	120.30
54	BA	228	C	N3-C2-O2	-6.68	117.22	121.90
7	AH	116	ARG	NE-CZ-NH1	6.68	123.64	120.30
21	AA	754	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	404	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1275	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	1689	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	1794	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	2150	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	2433	A	C4-C5-C6	-6.68	113.66	117.00
55	BB	51	G	O4'-C1'-N9	6.68	113.54	108.20
21	AA	462	G	N1-C6-O6	-6.68	115.89	119.90
54	BA	118	A	C5-C6-N1	6.68	121.04	117.70
54	BA	281	C	O4'-C1'-N1	6.68	113.54	108.20
54	BA	2234	G	C8-N9-C4	-6.68	103.73	106.40
54	BA	345	A	C5-C6-N1	6.68	121.04	117.70
54	BA	508	A	C5-C6-N1	6.68	121.04	117.70
21	AA	413	G	O4'-C1'-N9	6.67	113.54	108.20
21	AA	1021	A	C5-C6-N1	6.67	121.04	117.70
24	A3	13	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	83	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	2092	U	N3-C2-O2	-6.67	117.53	122.20
54	BA	2632	A	N1-C6-N6	-6.67	114.60	118.60
21	AA	1016	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	1369	G	C5-C6-N1	6.67	114.84	111.50
54	BA	2305	U	O4'-C1'-N1	6.67	113.54	108.20
21	AA	1197	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	1959	G	N1-C6-O6	-6.67	115.90	119.90
21	AA	716	A	C5-C6-N1	6.67	121.03	117.70
21	AA	1152	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	1503	A	C1'-O4'-C4'	-6.67	104.57	109.90
54	BA	453	A	O4'-C1'-N9	6.67	113.53	108.20
54	BA	819	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	1384	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	1439	A	O4'-C1'-N9	6.67	113.53	108.20
54	BA	2411	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	32	C	N1-C2-O2	6.67	122.90	118.90
54	BA	1678	A	C5-C6-N1	6.67	121.03	117.70
54	BA	1803	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2756	U	N3-C2-O2	-6.67	117.53	122.20
21	AA	752	G	O4'-C1'-N9	6.66	113.53	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	17	C	N1-C2-O2	6.66	122.90	118.90
54	BA	758	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1204	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1327	A	C5-C6-N1	6.66	121.03	117.70
21	AA	790	A	C5-C6-N1	6.66	121.03	117.70
54	BA	472	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	981	A	N1-C6-N6	-6.66	114.60	118.60
21	AA	60	A	C4-C5-C6	-6.66	113.67	117.00
24	A3	58	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2039	U	O4'-C1'-N1	6.66	113.53	108.20
54	BA	2810	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	800	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2019	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2655	G	C8-N9-C4	-6.66	103.74	106.40
54	BA	2752	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	2129	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	2385	C	N1-C2-O2	6.66	122.89	118.90
54	BA	2863	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	529	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	635	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	901	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	2862	G	N1-C6-O6	-6.65	115.91	119.90
21	AA	879	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	1005	A	N1-C6-N6	-6.65	114.61	118.60
22	A1	6	A	C5-C6-N1	6.65	121.03	117.70
39	BQ	63	ARG	NE-CZ-NH1	6.65	123.62	120.30
54	BA	1189	A	C5-C6-N1	6.65	121.03	117.70
54	BA	2013	A	N1-C6-N6	-6.65	114.61	118.60
21	AA	222	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	2158	A	C4-C5-C6	-6.65	113.68	117.00
52	B3	12	ARG	NE-CZ-NH1	6.65	123.62	120.30
54	BA	316	C	N1-C2-O2	6.65	122.89	118.90
54	BA	1285	A	N1-C6-N6	-6.65	114.61	118.60
54	BA	1294	U	O4'-C1'-N1	6.65	113.52	108.20
54	BA	1786	A	C4-C5-C6	-6.65	113.68	117.00
21	AA	1437	A	N1-C6-N6	-6.65	114.61	118.60
22	A1	68	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1919	A	C5-C6-N1	6.65	121.02	117.70
21	AA	177	G	C2-N3-C4	6.64	115.22	111.90
21	AA	338	A	N1-C6-N6	-6.64	114.61	118.60
21	AA	1325	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1031	G	N1-C6-O6	-6.64	115.92	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1920	C	N3-C2-O2	-6.64	117.25	121.90
26	BD	184	ARG	NE-CZ-NH1	6.64	123.62	120.30
54	BA	651	G	C5'-C4'-O4'	6.64	117.07	109.10
54	BA	1978	A	C4-C5-C6	-6.64	113.68	117.00
10	AK	55	ARG	NE-CZ-NH1	6.64	123.62	120.30
35	BM	44	ARG	NE-CZ-NH1	6.64	123.62	120.30
54	BA	1794	A	C5-C6-N1	6.64	121.02	117.70
21	AA	210	C	N3-C4-C5	6.64	124.56	121.90
21	AA	431	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	346	A	C2-N3-C4	6.64	113.92	110.60
54	BA	513	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	998	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	494	G	C8-N9-C4	-6.63	103.75	106.40
21	AA	1022	A	C5-C6-N1	6.63	121.02	117.70
21	AA	1428	A	C4-C5-C6	-6.63	113.69	117.00
21	AA	1399	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	181	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	182	A	C5-C6-N1	6.63	121.02	117.70
54	BA	1307	A	C5-C6-N1	6.63	121.02	117.70
54	BA	1977	A	N1-C6-N6	-6.63	114.62	118.60
21	AA	188	C	N1-C2-O2	6.63	122.88	118.90
21	AA	338	A	C4-C5-C6	-6.63	113.69	117.00
21	AA	602	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	1565	C	O4'-C1'-N1	6.63	113.50	108.20
54	BA	2051	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	2251	G	C5-C6-N1	6.63	114.81	111.50
54	BA	2393	U	O4'-C1'-N1	6.63	113.50	108.20
21	AA	1395	C	N3-C2-O2	-6.62	117.26	121.90
21	AA	1418	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	2013	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	2503	A	C5-C6-N1	6.62	121.01	117.70
54	BA	1663	G	C5-C6-N1	6.62	114.81	111.50
54	BA	2055	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	432	A	C5-C6-N1	6.62	121.01	117.70
21	AA	489	C	O4'-C1'-N1	6.62	113.50	108.20
21	AA	526	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	1189	U	C5-C6-N1	-6.62	119.39	122.70
54	BA	1595	C	N3-C4-C5	6.62	124.55	121.90
55	BB	30	C	O4'-C1'-N1	6.62	113.49	108.20
46	BX	26	ARG	NE-CZ-NH1	6.62	123.61	120.30
54	BA	341	C	O4'-C1'-N1	6.62	113.49	108.20
54	BA	832	U	O4'-C1'-N1	6.62	113.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1863	G	N1-C6-O6	-6.62	115.93	119.90
2	AC	142	ARG	NE-CZ-NH2	-6.62	116.99	120.30
21	AA	6	G	C8-N9-C4	-6.62	103.75	106.40
54	BA	838	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1634	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1771	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	2265	U	O4'-C1'-N1	6.62	113.49	108.20
54	BA	2300	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	981	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	1368	G	N3-C4-C5	-6.61	125.29	128.60
54	BA	462	C	O4'-C1'-N1	6.61	113.49	108.20
21	AA	315	A	C5-C6-N1	6.61	121.00	117.70
54	BA	758	C	N1-C2-O2	6.61	122.86	118.90
54	BA	1848	A	C5-C6-N1	6.61	121.00	117.70
54	BA	2162	G	C8-N9-C4	-6.61	103.76	106.40
54	BA	2420	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	278	A	N1-C6-N6	-6.61	114.64	118.60
54	BA	988	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	1248	G	N3-C4-C5	-6.61	125.30	128.60
54	BA	2874	C	N3-C2-O2	-6.61	117.28	121.90
24	A3	68	C	N3-C2-O2	-6.60	117.28	121.90
12	AM	2	ARG	NE-CZ-NH2	6.60	123.60	120.30
54	BA	560	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	1049	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	715	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	2000	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	577	G	N1-C6-O6	-6.60	115.94	119.90
54	BA	699	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	912	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	1937	A	C5-C6-N1	6.60	121.00	117.70
54	BA	2037	A	N1-C6-N6	-6.60	114.64	118.60
55	BB	15	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	1352	U	C5-C6-N1	-6.60	119.40	122.70
21	AA	630	A	C5-C6-N1	6.59	121.00	117.70
21	AA	1341	U	O4'-C1'-N1	6.59	113.48	108.20
54	BA	1169	A	C5-C6-N1	6.59	121.00	117.70
21	AA	1487	G	C8-N9-C4	-6.59	103.76	106.40
21	AA	277	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	1381	U	N3-C2-O2	-6.59	117.59	122.20
54	BA	378	C	N3-C4-C5	6.59	124.54	121.90
54	BA	617	G	C5-C6-N1	6.59	114.80	111.50
54	BA	2723	C	N3-C4-C5	6.59	124.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2860	A	C5-C6-N1	6.59	121.00	117.70
54	BA	609	A	N1-C6-N6	-6.59	114.65	118.60
54	BA	2030	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	2875	C	N3-C2-O2	-6.59	117.29	121.90
15	AP	56	ARG	NE-CZ-NH1	6.59	123.59	120.30
21	AA	101	A	C4-C5-C6	-6.59	113.71	117.00
54	BA	1451	C	N1-C2-O2	6.59	122.85	118.90
21	AA	207	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	560	A	C4-C5-C6	-6.59	113.71	117.00
54	BA	219	A	C5-C6-N1	6.59	120.99	117.70
54	BA	1870	C	N1-C2-O2	6.59	122.85	118.90
54	BA	2312	U	O4'-C1'-N1	6.59	113.47	108.20
54	BA	2432	A	C5-C6-N1	6.59	120.99	117.70
21	AA	327	A	N1-C6-N6	-6.58	114.65	118.60
21	AA	1172	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	1201	A	C5-C6-N1	6.58	120.99	117.70
50	B1	43	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	1774	C	N1-C2-O2	6.58	122.85	118.90
54	BA	2175	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	2340	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	255	A	C5-C6-N1	6.58	120.99	117.70
54	BA	941	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2169	A	O4'-C1'-N9	6.58	113.47	108.20
54	BA	183	C	O4'-C1'-N1	6.58	113.47	108.20
54	BA	1352	U	N1-C2-N3	6.58	118.85	114.90
54	BA	1991	U	C5-C6-N1	-6.58	119.41	122.70
54	BA	1713	A	C5-C6-N1	6.58	120.99	117.70
24	A3	63	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	1301	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	1978	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	2374	C	N1-C2-O2	6.58	122.85	118.90
24	A3	38	A	C5-C6-N1	6.58	120.99	117.70
54	BA	687	C	O4'-C1'-N1	6.58	113.46	108.20
54	BA	1691	C	N3-C2-O2	-6.58	117.30	121.90
3	AD	103	ARG	NE-CZ-NH1	6.58	123.59	120.30
21	AA	300	A	C5-C6-N1	6.58	120.99	117.70
21	AA	308	C	N1-C2-O2	6.58	122.84	118.90
21	AA	566	G	N3-C4-C5	-6.58	125.31	128.60
21	AA	1128	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	2494	G	N1-C6-O6	-6.58	115.95	119.90
21	AA	36	C	C5'-C4'-C3'	-6.57	105.48	116.00
54	BA	420	C	N3-C2-O2	-6.57	117.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1453	A	C4-C5-C6	-6.57	113.71	117.00
54	BA	2835	A	C5-C6-N1	6.57	120.99	117.70
21	AA	165	G	N1-C6-O6	-6.57	115.96	119.90
21	AA	274	A	C5-C6-N1	6.57	120.99	117.70
54	BA	421	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	2478	A	C5-C6-N1	6.57	120.99	117.70
21	AA	321	A	C4-C5-C6	-6.57	113.71	117.00
21	AA	1029	U	N3-C2-O2	-6.57	117.60	122.20
54	BA	1971	U	O4'-C1'-N1	6.57	113.46	108.20
21	AA	1408	A	N1-C6-N6	-6.57	114.66	118.60
21	AA	511	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	595	A	N1-C6-N6	-6.57	114.66	118.60
22	A1	60	C	N1-C2-O2	6.57	122.84	118.90
42	BT	73	ARG	NE-CZ-NH1	6.57	123.58	120.30
54	BA	820	A	N1-C6-N6	-6.57	114.66	118.60
54	BA	2338	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	2354	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	610	U	C1'-O4'-C4'	-6.57	104.65	109.90
54	BA	255	A	N1-C6-N6	-6.57	114.66	118.60
54	BA	269	C	O4'-C1'-N1	6.57	113.45	108.20
54	BA	1028	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	2096	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	251	G	C8-N9-C4	-6.56	103.77	106.40
54	BA	415	A	C5-C6-N1	6.56	120.98	117.70
54	BA	1562	U	C5-C6-N1	-6.56	119.42	122.70
21	AA	381	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	580	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1788	C	N1-C2-O2	6.56	122.84	118.90
17	AR	72	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	474	G	O4'-C1'-N9	6.56	113.45	108.20
54	BA	2060	A	C6-C5-N7	6.56	136.89	132.30
54	BA	2539	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	379	C	N1-C2-O2	6.56	122.83	118.90
36	BN	22	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	501	A	N1-C6-N6	-6.56	114.67	118.60
54	BA	575	A	C1'-O4'-C4'	-6.56	104.65	109.90
54	BA	586	A	N1-C6-N6	-6.56	114.67	118.60
54	BA	2873	A	C5-C6-N1	6.56	120.98	117.70
54	BA	1173	U	O4'-C1'-N1	6.55	113.44	108.20
54	BA	2053	G	N3-C2-N2	-6.55	115.31	119.90
54	BA	2343	U	O4'-C1'-N1	6.55	113.44	108.20
54	BA	2173	A	C5-C6-N1	6.55	120.98	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	111	G	C5-C6-N1	6.55	114.78	111.50
21	AA	1093	A	N1-C6-N6	-6.55	114.67	118.60
29	BG	151	ARG	NE-CZ-NH1	6.55	123.58	120.30
54	BA	2327	A	C5-C6-N1	6.55	120.98	117.70
54	BA	2345	G	C5-C6-N1	6.55	114.78	111.50
54	BA	2820	A	C4-C5-C6	-6.55	113.72	117.00
21	AA	5	U	O4'-C1'-N1	6.55	113.44	108.20
21	AA	969	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	197	A	C5-C6-N1	6.55	120.97	117.70
54	BA	670	A	P-O3'-C3'	6.55	127.56	119.70
54	BA	996	A	C5-C6-N1	6.55	120.97	117.70
54	BA	1309	G	O4'-C1'-N9	6.55	113.44	108.20
54	BA	1872	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	2789	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	1004	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	554	U	O4'-C1'-N1	6.55	113.44	108.20
21	AA	445	G	N1-C6-O6	-6.55	115.97	119.90
54	BA	221	A	C5-C6-N1	6.55	120.97	117.70
54	BA	532	A	C2-N3-C4	6.55	113.87	110.60
54	BA	1639	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	2820	A	C5-C6-N1	6.55	120.97	117.70
54	BA	660	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	2076	U	N3-C2-O2	-6.54	117.62	122.20
21	AA	1121	U	O4'-C1'-N1	6.54	113.44	108.20
54	BA	1230	A	C5-C6-N1	6.54	120.97	117.70
54	BA	2078	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	1259	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	364	C	O4'-C1'-N1	6.54	113.43	108.20
54	BA	727	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	2258	C	N3-C2-O2	-6.54	117.32	121.90
17	AR	47	ARG	NE-CZ-NH1	6.54	123.57	120.30
51	B2	41	ARG	NE-CZ-NH1	6.54	123.57	120.30
54	BA	1996	C	O4'-C1'-N1	6.54	113.43	108.20
54	BA	2147	A	C5-C6-N1	6.54	120.97	117.70
54	BA	2225	A	N1-C6-N6	-6.54	114.68	118.60
54	BA	2646	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	608	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	2278	A	C5-C6-N1	6.54	120.97	117.70
24	A3	24	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1402	U	C5-C6-N1	-6.53	119.43	122.70
21	AA	816	A	C5-C6-N1	6.53	120.97	117.70
21	AA	81	A	C5-C6-N1	6.53	120.96	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	430	A	C5-C6-N1	6.53	120.96	117.70
54	BA	1936	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	2117	A	C5-C6-N1	6.53	120.96	117.70
54	BA	2458	G	N3-C4-C5	-6.53	125.34	128.60
22	A1	73	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1304	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1502	A	C5-C6-N1	6.53	120.96	117.70
54	BA	2032	G	N7-C8-N9	6.53	116.36	113.10
21	AA	453	G	C8-N9-C4	-6.52	103.79	106.40
54	BA	423	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	215	C	O4'-C1'-N1	6.52	113.42	108.20
21	AA	373	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	1279	G	N1-C6-O6	-6.52	115.99	119.90
54	BA	791	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	1480	C	O4'-C1'-N1	6.52	113.42	108.20
54	BA	1505	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	2644	G	N3-C2-N2	-6.52	115.33	119.90
21	AA	115	G	C5-C6-N1	6.52	114.76	111.50
21	AA	996	A	C4-C5-C6	-6.52	113.74	117.00
22	A1	43	G	N1-C6-O6	-6.52	115.99	119.90
54	BA	1793	C	N3-C4-C5	6.52	124.51	121.90
21	AA	609	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	310	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1103	A	N1-C6-N6	-6.52	114.69	118.60
54	BA	1344	U	O4'-C1'-N1	6.52	113.41	108.20
21	AA	52	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	502	A	N1-C6-N6	-6.51	114.69	118.60
54	BA	1502	A	N1-C6-N6	-6.51	114.69	118.60
54	BA	2764	A	C5-C6-N1	6.51	120.96	117.70
12	AM	92	ARG	NE-CZ-NH1	6.51	123.56	120.30
21	AA	810	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	812	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	934	U	O4'-C1'-N1	6.51	113.41	108.20
54	BA	1300	G	P-O3'-C3'	6.51	127.51	119.70
23	A2	82	A	C4-C5-C6	-6.51	113.75	117.00
21	AA	703	G	N1-C6-O6	-6.51	116.00	119.90
21	AA	1507	A	C5-C6-N1	6.51	120.95	117.70
25	BC	166	ARG	NE-CZ-NH1	6.51	123.55	120.30
21	AA	274	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1304	A	N1-C6-N6	-6.51	114.70	118.60
54	BA	1833	C	N3-C2-O2	-6.51	117.35	121.90
54	BA	154	U	C5-C6-N1	-6.50	119.45	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1650	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	620	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	787	A	N1-C6-N6	-6.50	114.70	118.60
21	AA	1493	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	256	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1398	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1938	A	O4'-C1'-N9	6.50	113.40	108.20
21	AA	874	G	N1-C6-O6	-6.50	116.00	119.90
54	BA	180	G	O4'-C1'-N9	6.50	113.40	108.20
54	BA	1126	A	C5-C6-N1	6.50	120.95	117.70
54	BA	811	U	O4'-C1'-N1	6.50	113.40	108.20
21	AA	484	G	C8-N9-C4	-6.50	103.80	106.40
21	AA	530	G	N3-C4-C5	-6.50	125.35	128.60
54	BA	730	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1436	G	C8-N9-C4	-6.50	103.80	106.40
21	AA	481	G	N1-C6-O6	-6.50	116.00	119.90
21	AA	1238	A	C4-C5-C6	-6.50	113.75	117.00
20	AU	32	ARG	NE-CZ-NH1	6.49	123.55	120.30
54	BA	2573	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	32	A	C5-C6-N1	6.49	120.94	117.70
21	AA	578	C	N3-C2-O2	-6.49	117.36	121.90
29	BG	162	ARG	NE-CZ-NH1	6.49	123.55	120.30
54	BA	1286	A	C5-C6-N1	6.49	120.94	117.70
54	BA	1662	U	O4'-C1'-N1	6.49	113.39	108.20
21	AA	374	A	C5-C6-N1	6.49	120.94	117.70
38	BP	102	ARG	NE-CZ-NH1	6.49	123.54	120.30
54	BA	1417	C	O4'-C1'-N1	6.49	113.39	108.20
54	BA	2031	A	C3'-C2'-C1'	6.49	106.69	101.50
54	BA	1930	G	C3'-C2'-C1'	-6.49	96.31	101.50
21	AA	181	A	C4-C5-C6	-6.49	113.76	117.00
21	AA	401	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	1251	A	C4-C5-C6	-6.49	113.76	117.00
35	BM	18	ARG	NE-CZ-NH1	6.49	123.54	120.30
54	BA	2166	U	C5-C6-N1	-6.49	119.46	122.70
54	BA	2340	A	C4-C5-C6	-6.49	113.76	117.00
21	AA	5	U	N3-C2-O2	-6.48	117.66	122.20
21	AA	320	A	N1-C6-N6	-6.48	114.71	118.60
44	BV	19	ARG	NE-CZ-NH1	6.48	123.54	120.30
21	AA	330	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	138	U	N3-C2-O2	-6.48	117.67	122.20
54	BA	2693	G	C5-C6-N1	6.48	114.74	111.50
21	AA	462	G	N9-C4-C5	6.48	107.99	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	487	A	C5-C6-N1	6.48	120.94	117.70
54	BA	2097	A	O4'-C1'-N9	6.48	113.38	108.20
54	BA	2590	A	O4'-C1'-N9	6.48	113.38	108.20
54	BA	2837	A	C5-C6-N1	6.48	120.94	117.70
55	BB	80	U	O4'-C1'-N1	6.48	113.38	108.20
21	AA	330	C	N3-C4-C5	6.47	124.49	121.90
21	AA	458	U	C5-C6-N1	-6.47	119.46	122.70
21	AA	1117	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	1364	U	N3-C2-O2	-6.47	117.67	122.20
37	BO	10	ARG	NE-CZ-NH1	6.47	123.54	120.30
54	BA	1472	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	182	A	C5-C6-N1	6.47	120.94	117.70
21	AA	282	A	C5-C6-N1	6.47	120.94	117.70
54	BA	816	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1155	A	C5-C6-N1	6.47	120.94	117.70
54	BA	1606	C	O4'-C1'-N1	6.47	113.38	108.20
54	BA	1476	U	C5-C6-N1	-6.47	119.47	122.70
54	BA	2020	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	1218	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	639	U	O4'-C1'-N1	6.47	113.38	108.20
54	BA	719	C	O4'-C1'-N1	6.47	113.38	108.20
21	AA	696	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	719	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1158	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1293	C	O4'-C1'-N1	6.47	113.37	108.20
54	BA	1745	A	C5-C6-N1	6.47	120.93	117.70
54	BA	2861	U	O4'-C1'-N1	6.47	113.37	108.20
21	AA	80	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	607	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	641	U	C3'-C2'-C1'	6.46	106.67	101.50
21	AA	1141	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	685	A	N1-C6-N6	-6.46	114.72	118.60
54	BA	2649	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2717	C	O4'-C1'-N1	6.46	113.37	108.20
54	BA	1869	G	N1-C6-O6	-6.46	116.02	119.90
3	AD	46	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	1110	A	C5-C6-N1	6.46	120.93	117.70
56	B5	7	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	177	G	N3-C4-C5	-6.46	125.37	128.60
21	AA	271	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1912	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	156	C	N3-C4-N4	-6.46	113.48	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	174	A	C5-C6-N1	6.46	120.93	117.70
21	AA	549	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	1252	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1303	C	N3-C2-O2	-6.46	117.38	121.90
41	BS	25	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	314	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	590	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	55	A	C5-C6-N1	6.46	120.93	117.70
54	BA	180	G	N1-C6-O6	-6.46	116.03	119.90
54	BA	632	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1545	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	2094	A	N1-C6-N6	-6.46	114.73	118.60
54	BA	1761	C	N1-C2-O2	6.46	122.77	118.90
24	A3	49	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	678	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	1032	A	N1-C6-N6	-6.45	114.73	118.60
54	BA	2712	C	N3-C2-O2	-6.45	117.38	121.90
21	AA	379	C	N3-C4-C5	6.45	124.48	121.90
54	BA	1439	A	C5-C6-N1	6.45	120.93	117.70
54	BA	1974	C	O4'-C1'-N1	6.45	113.36	108.20
21	AA	1478	U	N3-C2-O2	-6.45	117.69	122.20
54	BA	565	C	N1-C2-O2	6.45	122.77	118.90
54	BA	1098	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	2355	G	N1-C6-O6	-6.45	116.03	119.90
21	AA	432	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	452	A	N1-C6-N6	-6.45	114.73	118.60
28	BF	94	ARG	NE-CZ-NH1	6.45	123.53	120.30
54	BA	1113	U	C5-C6-N1	-6.45	119.47	122.70
54	BA	2381	A	C6-C5-N7	6.45	136.81	132.30
54	BA	692	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1938	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	8	A	C5-C6-N1	6.45	120.92	117.70
24	A3	44	A	C5-C6-N1	6.45	120.92	117.70
54	BA	1735	A	C5-C6-N1	6.45	120.92	117.70
54	BA	1741	C	N1-C2-O2	6.45	122.77	118.90
54	BA	1985	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	2110	G	C3'-C2'-C1'	-6.45	96.34	101.50
55	BB	78	A	C5-C6-N1	6.45	120.92	117.70
54	BA	28	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2358	A	C4-C5-C6	-6.44	113.78	117.00
55	BB	46	A	C4-C5-C6	-6.44	113.78	117.00
23	A2	79	A	C4-C5-C6	-6.44	113.78	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BH	116	ARG	NE-CZ-NH2	-6.44	117.08	120.30
54	BA	299	A	N1-C6-N6	-6.44	114.73	118.60
54	BA	890	C	N3-C2-O2	-6.44	117.39	121.90
24	A3	26	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	16	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	70	G	O4'-C1'-N9	6.44	113.35	108.20
54	BA	582	A	C6-C5-N7	6.44	136.81	132.30
54	BA	970	U	O4'-C1'-N1	6.44	113.35	108.20
54	BA	1028	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1210	G	O4'-C1'-N9	6.44	113.35	108.20
54	BA	1580	A	C5-C6-N1	6.44	120.92	117.70
21	AA	896	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	188	G	N1-C6-O6	-6.44	116.04	119.90
54	BA	2236	U	O4'-C1'-N1	6.44	113.35	108.20
23	A2	80	C	N1-C2-O2	6.44	122.76	118.90
54	BA	2191	A	C5-C6-N1	6.44	120.92	117.70
54	BA	2486	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	1175	A	C5-C6-N1	6.43	120.92	117.70
55	BB	22	U	O4'-C1'-N1	6.43	113.35	108.20
54	BA	411	G	N3-C2-N2	-6.43	115.40	119.90
54	BA	1889	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	2858	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1335	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1868	C	N3-C2-O2	-6.43	117.40	121.90
24	A3	62	C	N1-C2-O2	6.43	122.76	118.90
21	AA	418	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	610	U	O4'-C1'-N1	6.43	113.34	108.20
21	AA	1022	A	C4-C5-C6	-6.43	113.79	117.00
22	A1	26	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	1583	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	2024	G	N1-C6-O6	-6.43	116.04	119.90
54	BA	297	G	N1-C6-O6	-6.42	116.05	119.90
21	AA	726	C	N3-C2-O2	-6.42	117.40	121.90
21	AA	853	C	O4'-C1'-N1	6.42	113.34	108.20
54	BA	1553	A	N1-C6-N6	-6.42	114.75	118.60
54	BA	2901	C	N3-C2-O2	-6.42	117.40	121.90
21	AA	1363	A	C5-C6-N1	6.42	120.91	117.70
3	AD	127	ARG	NE-CZ-NH1	6.42	123.51	120.30
21	AA	231	U	O4'-C1'-N1	6.42	113.34	108.20
21	AA	459	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	779	C	O4'-C1'-N1	6.42	113.33	108.20
54	BA	13	A	C5-C6-N1	6.42	120.91	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	227	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	564	C	N1-C2-O2	6.42	122.75	118.90
54	BA	1189	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1590	A	N1-C6-N6	-6.42	114.75	118.60
54	BA	2790	U	N3-C2-O2	-6.42	117.71	122.20
21	AA	536	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	654	A	O4'-C1'-N9	6.42	113.33	108.20
54	BA	2205	A	N1-C6-N6	-6.42	114.75	118.60
21	AA	167	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1370	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1586	A	N1-C6-N6	-6.41	114.75	118.60
21	AA	344	A	C4-C5-C6	-6.41	113.79	117.00
21	AA	926	G	N1-C6-O6	-6.41	116.05	119.90
21	AA	990	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	1280	A	C5-C6-N1	6.41	120.91	117.70
54	BA	52	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	241	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	1056	G	N3-C4-C5	-6.41	125.39	128.60
54	BA	1934	C	O4'-C1'-N1	6.41	113.33	108.20
55	BB	118	C	N1-C2-O2	6.41	122.75	118.90
21	AA	251	G	N7-C8-N9	6.41	116.30	113.10
21	AA	304	U	O4'-C1'-N1	6.41	113.33	108.20
21	AA	736	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	999	C	N3-C4-C5	6.41	124.46	121.90
54	BA	1143	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	1679	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	1744	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	1927	A	C5-C6-N1	6.41	120.91	117.70
54	BA	2578	G	C1'-O4'-C4'	-6.41	104.77	109.90
54	BA	757	G	C5-C6-N1	6.41	114.70	111.50
54	BA	1151	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	1324	A	C5-C6-N1	6.40	120.90	117.70
21	AA	664	G	N3-C4-C5	-6.40	125.40	128.60
54	BA	581	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2359	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	53	A	C5-C6-N1	6.40	120.90	117.70
21	AA	739	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	1130	A	N1-C6-N6	-6.40	114.76	118.60
32	BJ	37	ARG	NE-CZ-NH2	-6.40	117.10	120.30
21	AA	1134	G	N1-C6-O6	-6.40	116.06	119.90
54	BA	450	G	N3-C4-C5	-6.40	125.40	128.60
54	BA	572	A	N1-C6-N6	-6.40	114.76	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	661	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	921	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2752	C	N3-C4-C5	6.40	124.46	121.90
21	AA	1299	A	C4-C5-C6	-6.40	113.80	117.00
38	BP	100	ARG	NE-CZ-NH2	-6.40	117.10	120.30
54	BA	540	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	908	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1383	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1609	A	C5-C6-N1	6.40	120.90	117.70
54	BA	2001	C	O4'-C1'-N1	6.39	113.32	108.20
54	BA	1823	G	C5-C6-N1	6.39	114.70	111.50
54	BA	2442	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	2757	A	N1-C6-N6	-6.39	114.77	118.60
21	AA	569	C	N3-C2-O2	-6.39	117.43	121.90
21	AA	709	U	O4'-C1'-N1	6.39	113.31	108.20
21	AA	941	G	N1-C6-O6	-6.39	116.06	119.90
21	AA	1494	G	C8-N9-C4	-6.39	103.84	106.40
54	BA	195	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	1498	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2765	A	N1-C6-N6	-6.39	114.77	118.60
21	AA	509	A	C4-C5-C6	-6.39	113.81	117.00
21	AA	1108	G	N9-C4-C5	6.39	107.95	105.40
54	BA	32	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2755	C	C3'-C2'-C1'	6.39	106.61	101.50
7	AH	83	ARG	NE-CZ-NH1	6.39	123.49	120.30
21	AA	1070	U	O4'-C1'-N1	6.39	113.31	108.20
54	BA	473	G	C8-N9-C4	-6.39	103.85	106.40
54	BA	1045	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2758	A	N1-C6-N6	-6.39	114.77	118.60
21	AA	288	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	1496	C	N3-C4-C5	6.38	124.45	121.90
54	BA	732	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	753	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	1807	G	O4'-C1'-N9	6.38	113.31	108.20
54	BA	2336	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	2619	C	O4'-C1'-N1	6.38	113.31	108.20
21	AA	127	G	C8-N9-C4	-6.38	103.85	106.40
21	AA	353	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	374	A	N1-C6-N6	-6.38	114.77	118.60
21	AA	897	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	1830	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2788	C	N3-C2-O2	-6.38	117.43	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AN	9	ARG	NE-CZ-NH1	6.38	123.49	120.30
54	BA	4	U	C5-C6-N1	-6.38	119.51	122.70
54	BA	320	A	C5-C6-N1	6.38	120.89	117.70
54	BA	1368	G	C5-C6-N1	6.38	114.69	111.50
21	AA	34	C	N1-C2-O2	6.38	122.73	118.90
21	AA	189	A	N1-C6-N6	-6.38	114.77	118.60
21	AA	1000	A	C5-C6-N1	6.38	120.89	117.70
21	AA	1287	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	95	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2639	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2668	G	N9-C4-C5	6.38	107.95	105.40
21	AA	807	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	815	A	C5-C6-N1	6.38	120.89	117.70
21	AA	930	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	416	U	O4'-C1'-N1	6.38	113.30	108.20
54	BA	1535	A	C4-C5-C6	-6.38	113.81	117.00
9	AJ	89	ARG	NE-CZ-NH1	6.37	123.49	120.30
11	AL	35	ARG	NE-CZ-NH1	6.37	123.49	120.30
21	AA	1413	A	N1-C6-N6	-6.37	114.78	118.60
21	AA	1504	G	C5-C6-N1	6.37	114.69	111.50
22	A1	32	C	N3-C2-O2	-6.37	117.44	121.90
22	A1	52	G	C8-N9-C4	-6.37	103.85	106.40
54	BA	641	U	C5-C6-N1	-6.37	119.51	122.70
54	BA	1844	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2362	C	N3-C4-C5	6.37	124.45	121.90
55	BB	29	A	C5-C6-N1	6.37	120.89	117.70
54	BA	181	A	N1-C6-N6	-6.37	114.78	118.60
54	BA	1330	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1205	A	C5-C6-N1	6.37	120.88	117.70
21	AA	389	A	C5-C6-N1	6.37	120.88	117.70
54	BA	79	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1477	A	C4-C5-C6	-6.37	113.82	117.00
21	AA	759	A	C5-C6-N1	6.37	120.88	117.70
21	AA	984	C	N3-C2-O2	-6.37	117.44	121.90
40	BR	80	ARG	NE-CZ-NH2	6.37	123.48	120.30
54	BA	896	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	930	G	N1-C6-O6	-6.37	116.08	119.90
54	BA	2813	A	C5-C6-N1	6.37	120.88	117.70
21	AA	120	A	N1-C6-N6	-6.36	114.78	118.60
21	AA	651	C	N3-C2-O2	-6.36	117.44	121.90
21	AA	1201	A	P-O3'-C3'	6.36	127.34	119.70
21	AA	1363	A	N1-C6-N6	-6.36	114.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BE	40	ARG	NE-CZ-NH1	6.36	123.48	120.30
54	BA	292	U	C5-C6-N1	-6.36	119.52	122.70
54	BA	438	G	O4'-C1'-N9	6.36	113.29	108.20
21	AA	1469	C	C3'-C2'-C1'	6.36	106.59	101.50
54	BA	1345	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1636	U	O4'-C1'-N1	6.36	113.29	108.20
54	BA	2079	U	C5-C6-N1	-6.36	119.52	122.70
54	BA	2183	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2646	C	N1-C2-O2	6.36	122.72	118.90
54	BA	140	C	C2-N3-C4	-6.36	116.72	119.90
54	BA	314	C	O4'-C1'-N1	6.36	113.28	108.20
54	BA	2146	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2587	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	609	A	C5-C6-N1	6.36	120.88	117.70
54	BA	171	U	O4'-C1'-N1	6.36	113.28	108.20
54	BA	1151	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1975	G	C5-C6-N1	6.36	114.68	111.50
21	AA	1234	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	1272	A	N1-C6-N6	-6.35	114.79	118.60
21	AA	303	A	C5-C6-N1	6.35	120.88	117.70
21	AA	1036	A	C5-C6-N1	6.35	120.88	117.70
21	AA	1429	A	C6-C5-N7	6.35	136.75	132.30
54	BA	767	U	O4'-C1'-N1	6.35	113.28	108.20
54	BA	1426	G	C8-N9-C4	-6.35	103.86	106.40
54	BA	1603	A	C5-C6-N1	6.35	120.88	117.70
54	BA	1686	C	O4'-C1'-N1	6.35	113.28	108.20
22	A1	28	C	N3-C2-O2	-6.35	117.45	121.90
41	BS	92	ARG	NE-CZ-NH1	6.35	123.47	120.30
54	BA	402	A	C5-C6-N1	6.35	120.88	117.70
54	BA	1053	C	O4'-C1'-N1	6.35	113.28	108.20
54	BA	1070	A	C5-C6-N1	6.35	120.88	117.70
54	BA	2355	G	N3-C4-C5	-6.35	125.43	128.60
55	BB	37	C	N3-C4-C5	6.35	124.44	121.90
21	AA	16	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	136	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	743	A	C5-C6-N1	6.35	120.87	117.70
54	BA	1204	A	C2-N3-C4	6.35	113.77	110.60
54	BA	1325	U	C4-C5-C6	6.35	123.51	119.70
54	BA	1594	U	O4'-C1'-N1	6.35	113.28	108.20
54	BA	2837	A	N1-C6-N6	-6.35	114.79	118.60
21	AA	1412	C	N3-C4-C5	6.35	124.44	121.90
54	BA	1637	A	C4-C5-C6	-6.35	113.83	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2547	A	C5-C6-N1	6.35	120.87	117.70
21	AA	465	A	C5-C6-N1	6.34	120.87	117.70
22	A1	27	C	N1-C2-O2	6.34	122.71	118.90
54	BA	275	C	N3-C4-C5	6.34	124.44	121.90
54	BA	607	U	O4'-C1'-N1	6.34	113.28	108.20
54	BA	2201	G	N1-C6-O6	-6.34	116.09	119.90
54	BA	2212	A	N1-C6-N6	-6.34	114.79	118.60
21	AA	1469	C	N1-C2-O2	6.34	122.71	118.90
54	BA	461	C	N3-C2-O2	-6.34	117.46	121.90
3	AD	2	ARG	NE-CZ-NH1	6.34	123.47	120.30
21	AA	359	G	N9-C4-C5	6.34	107.94	105.40
21	AA	912	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	1328	C	N3-C2-O2	-6.34	117.46	121.90
25	BC	268	ARG	NE-CZ-NH1	6.34	123.47	120.30
54	BA	817	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1402	U	O4'-C1'-N1	6.34	113.27	108.20
54	BA	1704	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1997	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2144	G	N1-C6-O6	-6.34	116.10	119.90
21	AA	1311	A	C5-C6-N1	6.34	120.87	117.70
22	A1	62	C	N3-C4-C5	6.34	124.43	121.90
54	BA	1990	C	N3-C2-O2	-6.34	117.47	121.90
54	BA	2541	A	C4-C5-C6	-6.34	113.83	117.00
55	BB	90	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	1267	C	N1-C2-O2	6.33	122.70	118.90
24	A3	3	C	N3-C4-C5	6.33	124.43	121.90
54	BA	992	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1385	A	C4-C5-C6	-6.33	113.83	117.00
21	AA	120	A	C5-C6-N1	6.33	120.87	117.70
21	AA	226	G	N3-C2-N2	-6.33	115.47	119.90
21	AA	510	A	C6-C5-N7	6.33	136.73	132.30
54	BA	740	C	O4'-C1'-N1	6.33	113.27	108.20
54	BA	2668	G	C8-N9-C4	-6.33	103.87	106.40
55	BB	97	C	N3-C2-O2	-6.33	117.47	121.90
41	BS	8	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	1214	A	C5-C6-N1	6.33	120.86	117.70
54	BA	1965	C	N3-C4-C5	6.33	124.43	121.90
55	BB	105	G	O4'-C1'-N9	6.33	113.27	108.20
21	AA	148	G	N3-C4-C5	-6.33	125.44	128.60
21	AA	699	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1133	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	2062	A	O4'-C1'-N9	6.33	113.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	23	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	508	A	N1-C6-N6	-6.33	114.80	118.60
54	BA	1000	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	718	A	N1-C6-N6	-6.32	114.81	118.60
21	AA	728	A	C2-N3-C4	6.32	113.76	110.60
21	AA	1036	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	447	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1570	A	O4'-C1'-N9	6.32	113.26	108.20
54	BA	2564	A	C5-C6-N1	6.32	120.86	117.70
21	AA	1011	C	N3-C2-O2	-6.32	117.47	121.90
51	B2	35	ARG	NE-CZ-NH1	6.32	123.46	120.30
54	BA	246	C	N3-C2-O2	-6.32	117.47	121.90
8	AI	10	ARG	NE-CZ-NH1	6.32	123.46	120.30
24	A3	72	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	89	A	N1-C6-N6	-6.32	114.81	118.60
54	BA	948	C	O4'-C1'-N1	6.32	113.26	108.20
54	BA	1114	C	N3-C4-C5	6.32	124.43	121.90
54	BA	1286	A	N1-C6-N6	-6.32	114.81	118.60
21	AA	195	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	1005	A	C5-C6-N1	6.32	120.86	117.70
14	AO	87	ARG	NE-CZ-NH1	6.32	123.46	120.30
18	AS	2	ARG	NE-CZ-NH1	6.32	123.46	120.30
21	AA	217	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	572	A	C1'-O4'-C4'	-6.32	104.85	109.90
21	AA	1085	U	C5-C6-N1	-6.32	119.54	122.70
24	A3	22	A	C4-C5-C6	-6.32	113.84	117.00
45	BW	24	ARG	NE-CZ-NH1	6.32	123.46	120.30
54	BA	1140	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	1755	A	C4-C5-C6	-6.32	113.84	117.00
19	AT	73	ARG	NH1-CZ-NH2	-6.32	112.45	119.40
21	AA	534	U	N3-C2-O2	-6.32	117.78	122.20
21	AA	740	U	O4'-C1'-N1	6.32	113.25	108.20
24	A3	14	A	N1-C6-N6	-6.32	114.81	118.60
29	BG	152	ARG	NE-CZ-NH1	6.32	123.46	120.30
54	BA	501	A	C5-C6-N1	6.32	120.86	117.70
54	BA	729	G	C8-N9-C4	-6.32	103.87	106.40
54	BA	2640	G	C5-C6-N1	6.32	114.66	111.50
55	BB	43	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	514	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	190	A	C5-C6-N1	6.31	120.86	117.70
21	AA	1239	A	C5-C6-N1	6.31	120.86	117.70
55	BB	16	G	C8-N9-C4	-6.31	103.88	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	308	C	N3-C4-N4	-6.31	113.58	118.00
21	AA	379	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	2068	U	C5-C6-N1	-6.31	119.55	122.70
21	AA	689	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	166	U	O4'-C1'-N1	6.31	113.25	108.20
54	BA	965	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	640	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1318	U	N3-C2-O2	-6.31	117.79	122.20
54	BA	435	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	486	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1257	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1755	A	C5-C6-N1	6.30	120.85	117.70
54	BA	257	C	N3-C2-O2	-6.30	117.49	121.90
22	A1	65	C	N3-C2-O2	-6.30	117.49	121.90
24	A3	16	C	N1-C2-O2	6.30	122.68	118.90
54	BA	516	C	N1-C2-O2	6.30	122.68	118.90
54	BA	814	C	O4'-C1'-N1	6.30	113.24	108.20
54	BA	2815	C	N3-C2-O2	-6.30	117.49	121.90
55	BB	113	C	N1-C2-O2	6.30	122.68	118.90
17	AR	72	ARG	NE-CZ-NH2	-6.30	117.15	120.30
54	BA	1014	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2521	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2530	A	C5-C6-N1	6.30	120.85	117.70
54	BA	2232	C	N3-C2-O2	-6.30	117.49	121.90
55	BB	14	U	O4'-C1'-N1	6.30	113.24	108.20
10	AK	68	ARG	NE-CZ-NH1	6.30	123.45	120.30
21	AA	15	G	C5-C6-N1	6.30	114.65	111.50
21	AA	1320	C	N1-C2-O2	6.30	122.68	118.90
54	BA	765	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	972	A	C5-C6-N1	6.30	120.85	117.70
54	BA	1442	U	C5-C6-N1	-6.30	119.55	122.70
54	BA	2305	U	C5-C6-N1	-6.30	119.55	122.70
54	BA	2636	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	931	C	N1-C2-O2	6.29	122.68	118.90
22	A1	26	A	N1-C6-N6	-6.29	114.82	118.60
54	BA	2863	C	N3-C4-C5	6.29	124.42	121.90
41	BS	110	ARG	NE-CZ-NH1	6.29	123.45	120.30
54	BA	1042	G	N1-C6-O6	-6.29	116.12	119.90
54	BA	1527	G	N1-C6-O6	-6.29	116.12	119.90
21	AA	743	A	C4-C5-C6	-6.29	113.86	117.00
51	B2	34	ARG	NE-CZ-NH1	6.29	123.45	120.30
54	BA	334	C	N3-C2-O2	-6.29	117.50	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AI	108	ARG	NE-CZ-NH1	6.29	123.44	120.30
21	AA	304	U	N1-C2-N3	6.29	118.67	114.90
21	AA	352	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	645	C	N1-C2-O2	6.29	122.67	118.90
54	BA	2546	U	C5-C6-N1	-6.29	119.56	122.70
54	BA	2800	A	C5-C6-N1	6.29	120.84	117.70
24	A3	27	G	N3-C2-N2	-6.29	115.50	119.90
55	BB	65	U	C5-C6-N1	-6.29	119.56	122.70
21	AA	311	C	C6-N1-C2	-6.29	117.79	120.30
21	AA	872	A	C2-N3-C4	6.29	113.74	110.60
21	AA	1456	A	N1-C6-N6	-6.29	114.83	118.60
54	BA	1705	A	N1-C6-N6	-6.29	114.83	118.60
54	BA	191	A	N1-C6-N6	-6.28	114.83	118.60
54	BA	2468	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	223	A	C5-C6-N1	6.28	120.84	117.70
21	AA	833	G	O4'-C1'-N9	6.28	113.23	108.20
54	BA	1558	C	O4'-C1'-N1	6.28	113.22	108.20
21	AA	519	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	1100	C	N1-C2-O2	6.28	122.67	118.90
54	BA	1512	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2135	A	C5-C6-N1	6.28	120.84	117.70
54	BA	2386	A	C6-C5-N7	6.28	136.70	132.30
21	AA	469	C	N3-C2-O2	-6.28	117.51	121.90
21	AA	595	A	C5-C6-N1	6.28	120.84	117.70
54	BA	796	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1836	C	O4'-C1'-N1	6.28	113.22	108.20
20	AU	46	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	1539	U	N3-C2-O2	-6.28	117.81	122.20
54	BA	2388	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	2458	G	O4'-C1'-N9	6.28	113.22	108.20
54	BA	2741	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	2886	A	C5-C6-N1	6.28	120.84	117.70
21	AA	1109	C	N1-C2-O2	6.27	122.66	118.90
21	AA	1256	A	N1-C6-N6	-6.27	114.84	118.60
21	AA	1404	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1833	C	N1-C2-O2	6.27	122.66	118.90
54	BA	2051	A	C5-C6-N1	6.27	120.84	117.70
21	AA	142	G	C5-C6-N1	6.27	114.64	111.50
21	AA	926	G	C8-N9-C4	-6.27	103.89	106.40
54	BA	950	G	N3-C2-N2	-6.27	115.51	119.90
54	BA	2224	G	C8-N9-C4	-6.27	103.89	106.40
54	BA	2531	A	C5-C6-N1	6.27	120.84	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AL	13	ARG	NE-CZ-NH1	6.27	123.44	120.30
54	BA	1759	A	C5-C6-N1	6.27	120.83	117.70
54	BA	1806	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2456	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	182	A	O4'-C1'-N9	6.27	113.21	108.20
21	AA	494	G	O4'-C1'-N9	6.27	113.22	108.20
21	AA	793	U	C1'-O4'-C4'	-6.27	104.89	109.90
54	BA	6	A	C5-C6-N1	6.27	120.83	117.70
54	BA	1690	A	N1-C6-N6	-6.27	114.84	118.60
54	BA	2247	A	C5-C6-N1	6.27	120.83	117.70
55	BB	12	C	O4'-C1'-N1	6.27	113.21	108.20
21	AA	526	C	N1-C2-O2	6.27	122.66	118.90
21	AA	872	A	C4-C5-C6	-6.27	113.87	117.00
21	AA	919	A	C6-C5-N7	6.27	136.69	132.30
54	BA	1701	A	C4-C5-C6	-6.27	113.87	117.00
54	BA	1515	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1722	A	C5-C6-N1	6.26	120.83	117.70
54	BA	2040	G	C5-C6-N1	6.26	114.63	111.50
54	BA	2498	C	N3-C2-O2	-6.26	117.52	121.90
55	BB	113	C	N3-C4-C5	6.26	124.41	121.90
24	A3	58	A	N1-C6-N6	-6.26	114.84	118.60
21	AA	1139	G	N9-C4-C5	6.26	107.91	105.40
54	BA	990	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2788	C	O4'-C1'-N1	6.26	113.21	108.20
14	AO	52	ARG	NE-CZ-NH1	6.26	123.43	120.30
21	AA	164	G	C8-N9-C4	-6.26	103.90	106.40
54	BA	430	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	195	A	N1-C6-N6	-6.26	114.84	118.60
54	BA	2439	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	970	C	N1-C2-O2	6.26	122.65	118.90
21	AA	1430	A	N1-C6-N6	-6.26	114.85	118.60
54	BA	385	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2045	C	N1-C2-O2	6.26	122.65	118.90
54	BA	2336	A	C5-C6-N1	6.26	120.83	117.70
55	BB	80	U	N1-C2-N3	6.26	118.65	114.90
54	BA	592	A	C4-C5-C6	-6.25	113.87	117.00
21	AA	1108	G	N3-C2-N2	-6.25	115.52	119.90
21	AA	1449	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	2028	U	O4'-C1'-N1	6.25	113.20	108.20
21	AA	493	A	C2-N3-C4	6.25	113.73	110.60
54	BA	130	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	1587	G	N3-C4-C5	-6.25	125.47	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AU	44	ARG	NE-CZ-NH1	6.25	123.42	120.30
21	AA	970	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	1263	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	2108	A	C5-C6-N1	6.25	120.83	117.70
54	BA	2443	C	N3-C4-C5	6.25	124.40	121.90
54	BA	2469	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	19	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	269	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	2052	A	N1-C6-N6	-6.25	114.85	118.60
54	BA	2693	G	N1-C6-O6	-6.25	116.15	119.90
54	BA	2715	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	2808	G	C5-C6-N1	6.25	114.62	111.50
21	AA	67	C	O4'-C1'-N1	6.25	113.20	108.20
54	BA	1759	A	C8-N9-C4	-6.25	103.30	105.80
54	BA	1890	A	C5-C6-N1	6.25	120.82	117.70
54	BA	746	U	C5-C6-N1	-6.25	119.58	122.70
54	BA	1980	G	C5-C6-N1	6.25	114.62	111.50
54	BA	2269	G	N9-C4-C5	6.25	107.90	105.40
21	AA	614	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	1526	G	C8-N9-C4	-6.24	103.90	106.40
22	A1	47	U	N3-C2-O2	-6.24	117.83	122.20
54	BA	1100	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1340	U	P-O3'-C3'	6.24	127.19	119.70
21	AA	176	C	N1-C2-O2	6.24	122.64	118.90
21	AA	892	A	C5-N7-C8	-6.24	100.78	103.90
54	BA	311	A	C5-C6-N1	6.24	120.82	117.70
54	BA	749	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1095	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1357	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	13	U	O4'-C1'-N1	6.24	113.19	108.20
21	AA	110	C	O4'-C1'-N1	6.24	113.19	108.20
21	AA	1157	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	36	G	C5-C6-N1	6.24	114.62	111.50
54	BA	1315	C	C6-N1-C2	-6.24	117.81	120.30
54	BA	1641	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	2160	C	N1-C2-O2	6.24	122.64	118.90
21	AA	110	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1030	C	O4'-C1'-N1	6.24	113.19	108.20
54	BA	2095	A	N1-C6-N6	-6.24	114.86	118.60
24	A3	36	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	2704	C	O4'-C1'-N1	6.24	113.19	108.20
55	BB	19	C	N3-C2-O2	-6.24	117.53	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	17	U	N3-C2-O2	-6.23	117.84	122.20
54	BA	1928	A	C5-C6-N1	6.23	120.82	117.70
54	BA	2230	G	O4'-C1'-N9	6.23	113.19	108.20
21	AA	427	U	N3-C2-O2	-6.23	117.84	122.20
21	AA	1324	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	1478	U	C5-C6-N1	-6.23	119.58	122.70
54	BA	177	G	N3-C2-N2	-6.23	115.54	119.90
54	BA	1798	U	C5-C6-N1	-6.23	119.58	122.70
54	BA	1393	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	1443	U	C5-C6-N1	-6.23	119.58	122.70
54	BA	2902	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	648	A	C5-C6-N1	6.23	120.81	117.70
21	AA	1522	U	N3-C2-O2	-6.23	117.84	122.20
22	A1	62	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	565	C	N3-C4-C5	6.23	124.39	121.90
54	BA	1924	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1274	A	C5-C6-N1	6.23	120.81	117.70
54	BA	643	A	C5-C6-N1	6.23	120.81	117.70
54	BA	897	C	C6-N1-C2	-6.23	117.81	120.30
54	BA	1535	A	O4'-C1'-N9	6.23	113.18	108.20
21	AA	1256	A	O4'-C1'-N9	6.22	113.18	108.20
54	BA	1117	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	1543	G	C5-C6-N1	6.22	114.61	111.50
54	BA	1847	A	C1'-O4'-C4'	-6.22	104.92	109.90
21	AA	369	G	N9-C4-C5	6.22	107.89	105.40
54	BA	532	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	814	A	C5-C6-N1	6.22	120.81	117.70
54	BA	2555	U	O4'-C1'-N1	6.22	113.18	108.20
21	AA	459	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	1161	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1384	A	C5-C6-N1	6.22	120.81	117.70
54	BA	1550	C	N3-C4-C5	6.22	124.39	121.90
54	BA	2825	G	C5-C6-N1	6.22	114.61	111.50
13	AN	24	ARG	NE-CZ-NH2	-6.22	117.19	120.30
21	AA	36	C	C5'-C4'-O4'	6.22	116.56	109.10
21	AA	233	C	N1-C2-O2	6.22	122.63	118.90
54	BA	927	A	C5-C6-N1	6.22	120.81	117.70
54	BA	1266	G	C5-C6-N1	6.22	114.61	111.50
54	BA	198	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1495	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1516	G	O4'-C1'-N9	6.21	113.17	108.20
54	BA	310	A	N1-C6-N6	-6.21	114.87	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2088	A	C5-C6-N1	6.21	120.81	117.70
54	BA	2144	G	O4'-C1'-N9	6.21	113.17	108.20
21	AA	95	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	1509	C	N3-C4-C5	6.21	124.38	121.90
54	BA	269	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2624	G	N3-C4-C5	-6.21	125.49	128.60
54	BA	1428	C	N3-C2-O2	-6.21	117.55	121.90
55	BB	81	G	N3-C4-C5	-6.21	125.50	128.60
21	AA	363	A	C5-C6-N1	6.21	120.80	117.70
54	BA	34	U	O4'-C1'-N1	6.21	113.17	108.20
54	BA	1601	G	N9-C4-C5	6.21	107.88	105.40
54	BA	1604	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1692	U	C5-C6-N1	-6.21	119.60	122.70
21	AA	402	G	N1-C6-O6	-6.21	116.18	119.90
21	AA	1275	A	C5-C6-N1	6.21	120.80	117.70
21	AA	1468	A	C4-C5-C6	-6.21	113.90	117.00
26	BD	58	ASN	C-N-CA	6.21	137.21	121.70
54	BA	439	A	C6-C5-N7	6.21	136.65	132.30
54	BA	889	C	N1-C2-O2	6.21	122.62	118.90
54	BA	1052	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	1325	U	N1-C2-N3	6.21	118.62	114.90
54	BA	2795	C	N3-C4-C5	6.21	124.38	121.90
54	BA	1357	C	O4'-C1'-N1	6.21	113.16	108.20
54	BA	474	G	N1-C6-O6	-6.20	116.18	119.90
54	BA	2274	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	2142	A	C5-C6-N1	6.20	120.80	117.70
21	AA	1141	C	N1-C2-O2	6.20	122.62	118.90
21	AA	1360	A	C5-C6-N1	6.20	120.80	117.70
21	AA	1443	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	485	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1577	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2807	U	O4'-C1'-N1	6.20	113.16	108.20
54	BA	1437	C	O4'-C1'-N1	6.20	113.16	108.20
55	BB	13	G	O4'-C1'-N9	6.20	113.16	108.20
55	BB	42	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1438	G	O4'-C1'-N9	6.20	113.16	108.20
54	BA	1422	G	N1-C6-O6	-6.20	116.18	119.90
21	AA	1067	A	C5-C6-N1	6.20	120.80	117.70
54	BA	353	C	O4'-C1'-N1	6.20	113.16	108.20
54	BA	368	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1298	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1817	G	C5-C6-N1	6.20	114.60	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2123	G	N1-C6-O6	-6.20	116.18	119.90
54	BA	2799	A	C5-C6-N1	6.20	120.80	117.70
54	BA	2197	U	C5-C6-N1	-6.19	119.60	122.70
54	BA	2021	C	N1-C2-O2	6.19	122.62	118.90
24	A3	63	C	N1-C2-O2	6.19	122.61	118.90
54	BA	578	G	N1-C6-O6	-6.19	116.19	119.90
54	BA	2072	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	2638	G	C8-N9-C4	-6.19	103.92	106.40
55	BB	39	A	C5-C6-N1	6.19	120.80	117.70
21	AA	188	C	N3-C4-C5	6.19	124.38	121.90
54	BA	585	G	C8-N9-C4	-6.19	103.92	106.40
21	AA	1226	C	N1-C2-O2	6.19	122.61	118.90
21	AA	1405	G	N1-C6-O6	-6.19	116.19	119.90
54	BA	909	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	2222	C	N1-C2-O2	6.18	122.61	118.90
21	AA	72	A	C5-C6-N1	6.18	120.79	117.70
21	AA	1322	C	N1-C2-O2	6.18	122.61	118.90
54	BA	1978	A	C5-C6-N1	6.18	120.79	117.70
54	BA	428	A	C5-C6-N1	6.18	120.79	117.70
54	BA	605	G	N1-C6-O6	-6.18	116.19	119.90
54	BA	692	C	O4'-C1'-N1	6.18	113.14	108.20
54	BA	782	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	898	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1936	A	P-O3'-C3'	6.18	127.12	119.70
54	BA	1955	U	C1'-O4'-C4'	-6.18	104.96	109.90
54	BA	1970	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2173	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2476	A	C5-C6-N1	6.18	120.79	117.70
21	AA	1237	C	N1-C2-O2	6.18	122.61	118.90
54	BA	878	A	C5-C6-N1	6.18	120.79	117.70
54	BA	1251	C	N3-C2-O2	-6.18	117.58	121.90
21	AA	340	U	N1-C2-N3	6.18	118.61	114.90
54	BA	344	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1967	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	2052	A	C5-C6-N1	6.18	120.79	117.70
54	BA	2404	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	2517	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	2855	C	O4'-C1'-N1	6.18	113.14	108.20
12	AM	97	ARG	NE-CZ-NH1	6.17	123.39	120.30
21	AA	36	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1113	U	O4'-C1'-N1	6.17	113.14	108.20
21	AA	449	G	C8-N9-C4	-6.17	103.93	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	890	G	O4'-C1'-N9	6.17	113.14	108.20
54	BA	9	G	C5-C6-N1	6.17	114.59	111.50
54	BA	734	A	C5-C6-N1	6.17	120.79	117.70
54	BA	66	C	O4'-C1'-N1	6.17	113.14	108.20
54	BA	460	A	C5-C6-N1	6.17	120.79	117.70
54	BA	1010	A	C4-C5-C6	-6.17	113.91	117.00
3	AD	62	ARG	NH1-CZ-NH2	-6.17	112.61	119.40
21	AA	845	A	C2-N3-C4	6.17	113.69	110.60
21	AA	1112	C	N1-C2-O2	6.17	122.60	118.90
54	BA	1285	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	99	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	193	C	N3-C4-C5	6.17	124.37	121.90
21	AA	712	A	C5-C6-N1	6.17	120.78	117.70
54	BA	1320	C	N1-C2-O2	6.17	122.60	118.90
21	AA	1173	U	C5-C6-N1	-6.17	119.62	122.70
54	BA	1209	U	C5-C6-N1	-6.17	119.62	122.70
54	BA	2333	A	C5-C6-N1	6.17	120.78	117.70
54	BA	84	A	C5-C6-N1	6.17	120.78	117.70
54	BA	2465	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	732	C	N3-C2-O2	-6.16	117.58	121.90
54	BA	515	A	O4'-C1'-N9	6.16	113.13	108.20
54	BA	928	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	2876	G	C5-C6-N1	6.16	114.58	111.50
21	AA	777	A	C5-C6-N1	6.16	120.78	117.70
21	AA	995	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	493	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	663	A	C5-C6-N1	6.16	120.78	117.70
54	BA	1674	G	C5-C6-N1	6.16	114.58	111.50
54	BA	2636	C	N3-C4-C5	6.16	124.36	121.90
21	AA	81	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	226	G	C8-N9-C4	-6.16	103.94	106.40
21	AA	1275	A	C4-C5-C6	-6.16	113.92	117.00
24	A3	36	A	C5-C6-N1	6.16	120.78	117.70
54	BA	677	A	N1-C6-N6	-6.16	114.91	118.60
54	BA	947	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1914	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	971	G	O4'-C1'-N9	6.16	113.12	108.20
21	AA	1174	G	C5-C6-N1	6.16	114.58	111.50
32	BJ	27	ARG	NE-CZ-NH2	-6.16	117.22	120.30
54	BA	1112	G	N1-C6-O6	-6.16	116.21	119.90
54	BA	2074	U	C5-C6-N1	-6.16	119.62	122.70
21	AA	535	A	C5-C6-N1	6.15	120.78	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BH	116	ARG	NE-CZ-NH1	6.15	123.38	120.30
21	AA	31	G	O4'-C1'-N9	6.15	113.12	108.20
21	AA	286	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2545	G	N1-C6-O6	-6.15	116.21	119.90
21	AA	26	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	112	U	O4'-C1'-N1	6.15	113.12	108.20
54	BA	645	C	N3-C4-C5	6.15	124.36	121.90
54	BA	671	C	N3-C4-C5	6.15	124.36	121.90
21	AA	753	A	N1-C6-N6	-6.15	114.91	118.60
21	AA	1394	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	1553	A	C5-C6-N1	6.15	120.78	117.70
54	BA	2352	A	C5-C6-N1	6.15	120.77	117.70
21	AA	135	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	722	A	N1-C6-N6	-6.15	114.91	118.60
54	BA	2691	C	O4'-C1'-N1	6.15	113.12	108.20
54	BA	32	C	N3-C4-C5	6.15	124.36	121.90
54	BA	347	A	C5-C6-N1	6.15	120.77	117.70
54	BA	1438	U	C5-C6-N1	-6.15	119.63	122.70
54	BA	2142	A	C4-C5-C6	-6.15	113.93	117.00
16	AQ	10	ARG	NE-CZ-NH1	6.14	123.37	120.30
21	AA	346	G	N3-C4-C5	-6.14	125.53	128.60
21	AA	1377	A	C5-C6-N1	6.14	120.77	117.70
54	BA	2280	G	C4'-C3'-C2'	-6.14	96.45	102.60
54	BA	2540	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2632	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	663	G	O4'-C1'-N9	6.14	113.11	108.20
55	BB	2	G	N1-C6-O6	-6.14	116.22	119.90
21	AA	474	G	N1-C6-O6	-6.14	116.22	119.90
24	A3	20	G	C5-C6-N1	6.14	114.57	111.50
54	BA	1282	U	O4'-C1'-N1	6.14	113.11	108.20
54	BA	2655	G	N7-C8-N9	6.14	116.17	113.10
54	BA	600	G	C5-C6-N1	6.14	114.57	111.50
54	BA	1468	U	O4'-C1'-N1	6.14	113.11	108.20
21	AA	908	A	C5-C6-N1	6.14	120.77	117.70
21	AA	1190	G	P-O3'-C3'	6.14	127.06	119.70
21	AA	1400	C	N3-C2-O2	-6.14	117.61	121.90
54	BA	2016	U	N3-C2-O2	-6.14	117.90	122.20
54	BA	2309	A	C5-C6-N1	6.14	120.77	117.70
21	AA	20	U	N1-C2-N3	6.13	118.58	114.90
21	AA	1488	G	N9-C4-C5	6.13	107.85	105.40
22	A1	14	A	C5-C6-N1	6.13	120.77	117.70
54	BA	301	G	N3-C4-C5	-6.13	125.53	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	693	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	995	C	N1-C2-O2	6.13	122.58	118.90
54	BA	1722	A	C4-C5-C6	-6.13	113.93	117.00
55	BB	24	G	N1-C6-O6	-6.13	116.22	119.90
54	BA	352	A	C5-C6-N1	6.13	120.77	117.70
21	AA	1099	G	N1-C6-O6	-6.13	116.22	119.90
51	B2	21	ARG	NE-CZ-NH1	6.13	123.37	120.30
54	BA	717	C	N3-C4-C5	6.13	124.35	121.90
54	BA	2240	U	O4'-C1'-N1	6.13	113.11	108.20
54	BA	1222	U	C5-C6-N1	-6.13	119.64	122.70
21	AA	339	C	O4'-C1'-N1	6.13	113.10	108.20
32	BJ	35	ARG	NE-CZ-NH1	6.13	123.36	120.30
54	BA	2496	C	C3'-C2'-C1'	6.13	106.40	101.50
1	AB	207	ARG	NE-CZ-NH1	6.13	123.36	120.30
21	AA	619	U	N3-C2-O2	-6.13	117.91	122.20
21	AA	946	A	N1-C6-N6	-6.13	114.92	118.60
21	AA	1406	U	N1-C2-N3	6.13	118.58	114.90
21	AA	1516	G	C8-N9-C4	-6.13	103.95	106.40
22	A1	76	A	O4'-C1'-N9	6.13	113.10	108.20
24	A3	39	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	482	A	C3'-C2'-C1'	6.13	106.40	101.50
54	BA	2066	C	O4'-C1'-N1	6.13	113.10	108.20
54	BA	2449	U	C5-C6-N1	-6.13	119.64	122.70
21	AA	1012	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	1120	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	38	A	C5-C6-N1	6.12	120.76	117.70
54	BA	1124	G	N1-C6-O6	-6.12	116.22	119.90
54	BA	1937	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2799	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	339	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	457	G	N1-C6-O6	-6.12	116.23	119.90
21	AA	1249	C	N3-C2-O2	-6.12	117.61	121.90
55	BB	65	U	N3-C2-O2	-6.12	117.91	122.20
21	AA	637	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	249	C	P-O3'-C3'	6.12	127.05	119.70
54	BA	2514	U	C5-C6-N1	-6.12	119.64	122.70
54	BA	1908	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2082	A	C5-C6-N1	6.12	120.76	117.70
21	AA	605	U	C5-C6-N1	-6.12	119.64	122.70
54	BA	165	A	C5-C6-N1	6.12	120.76	117.70
54	BA	415	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1308	A	C5-C6-N1	6.12	120.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1712	U	C5-C6-N1	-6.12	119.64	122.70
54	BA	1866	A	C5-C6-N1	6.12	120.76	117.70
54	BA	2132	U	C5-C6-N1	-6.12	119.64	122.70
54	BA	670	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	55	G	N1-C6-O6	-6.12	116.23	119.90
54	BA	1233	C	O4'-C1'-N1	6.12	113.09	108.20
54	BA	1393	A	C5-C6-N1	6.12	120.76	117.70
54	BA	1592	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2350	C	N1-C2-O2	6.12	122.57	118.90
55	BB	71	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	373	U	N3-C2-O2	-6.11	117.92	122.20
54	BA	1965	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2068	U	N3-C2-O2	-6.11	117.92	122.20
2	AC	10	ARG	NE-CZ-NH2	-6.11	117.25	120.30
21	AA	615	G	C5-C6-N1	6.11	114.56	111.50
21	AA	697	U	O4'-C1'-N1	6.11	113.09	108.20
21	AA	869	G	N3-C2-N2	-6.11	115.62	119.90
21	AA	119	A	O4'-C1'-N9	6.11	113.09	108.20
21	AA	355	C	N3-C4-N4	-6.11	113.72	118.00
21	AA	411	A	N1-C6-N6	-6.11	114.93	118.60
54	BA	340	A	C5-C6-N1	6.11	120.75	117.70
54	BA	839	U	O4'-C1'-N1	6.11	113.09	108.20
54	BA	2754	U	O4'-C1'-N1	6.11	113.09	108.20
24	A3	74	A	C4-C5-C6	-6.11	113.95	117.00
36	BN	64	ARG	NE-CZ-NH2	-6.11	117.25	120.30
54	BA	523	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	533	G	C5-C6-N1	6.11	114.55	111.50
54	BA	1455	G	C5-C6-N1	6.11	114.55	111.50
54	BA	2576	G	N3-C4-C5	-6.11	125.55	128.60
21	AA	452	A	C5-C6-N1	6.11	120.75	117.70
21	AA	1409	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	782	A	C5-C6-N1	6.11	120.75	117.70
54	BA	1646	C	N3-C4-C5	6.11	124.34	121.90
54	BA	2427	C	N3-C4-C5	6.11	124.34	121.90
21	AA	1332	A	N1-C6-N6	-6.10	114.94	118.60
54	BA	1194	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2788	C	C5'-C4'-O4'	6.10	116.42	109.10
54	BA	311	A	N1-C6-N6	-6.10	114.94	118.60
54	BA	1033	U	C5-C6-N1	-6.10	119.65	122.70
54	BA	2467	C	N3-C2-O2	-6.10	117.63	121.90
55	BB	106	G	C5-C6-N1	6.10	114.55	111.50
21	AA	619	U	C5-C6-N1	-6.10	119.65	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	873	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2336	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	496	A	C5-C6-N1	6.10	120.75	117.70
21	AA	658	C	N1-C2-O2	6.10	122.56	118.90
54	BA	91	A	C5-C6-N1	6.10	120.75	117.70
54	BA	679	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	2430	A	N1-C6-N6	-6.10	114.94	118.60
21	AA	354	G	C8-N9-C4	-6.10	103.96	106.40
21	AA	535	A	C3'-C2'-C1'	6.10	106.38	101.50
54	BA	917	A	C5-C6-N1	6.10	120.75	117.70
54	BA	1380	G	C5-C6-N1	6.10	114.55	111.50
54	BA	1442	U	N3-C2-O2	-6.10	117.93	122.20
54	BA	2441	U	O4'-C1'-N1	6.10	113.08	108.20
21	AA	1230	C	O4'-C1'-N1	6.10	113.08	108.20
21	AA	1256	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	490	C	O4'-C1'-N1	6.10	113.08	108.20
54	BA	1938	A	N1-C6-N6	-6.10	114.94	118.60
21	AA	901	A	C5-C6-N1	6.09	120.75	117.70
21	AA	1063	C	N3-C2-O2	-6.09	117.63	121.90
21	AA	1510	C	N3-C2-O2	-6.09	117.63	121.90
54	BA	487	C	N1-C2-O2	6.09	122.56	118.90
54	BA	1862	G	N1-C6-O6	-6.09	116.24	119.90
21	AA	151	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	974	A	C5-C6-N1	6.09	120.75	117.70
54	BA	91	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	944	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2126	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	1513	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	807	U	N3-C2-O2	-6.09	117.94	122.20
54	BA	2496	C	N1-C2-O2	6.09	122.55	118.90
54	BA	2628	C	O4'-C1'-N1	6.09	113.07	108.20
21	AA	28	A	C5-C6-N1	6.09	120.74	117.70
21	AA	49	U	C5-C6-N1	-6.09	119.66	122.70
54	BA	2513	A	C5-C6-N1	6.09	120.74	117.70
21	AA	27	G	C5-C6-N1	6.09	114.54	111.50
21	AA	532	A	C4-C5-C6	-6.09	113.96	117.00
21	AA	948	C	N3-C2-O2	-6.09	117.64	121.90
23	A2	89	U	O4'-C1'-N1	6.08	113.07	108.20
39	BQ	52	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	413	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	761	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	974	G	O4'-C1'-N9	6.08	113.07	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	527	G	N1-C6-O6	-6.08	116.25	119.90
21	AA	1248	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	565	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	892	A	C5-C6-N1	6.08	120.74	117.70
54	BA	1123	C	O4'-C1'-N1	6.08	113.07	108.20
54	BA	1999	C	N1-C2-O2	6.08	122.55	118.90
55	BB	71	C	N3-C4-C5	6.08	124.33	121.90
21	AA	63	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	313	A	C6-C5-N7	6.08	136.56	132.30
21	AA	455	G	N7-C8-N9	6.08	116.14	113.10
21	AA	1430	A	C5-C6-N1	6.08	120.74	117.70
54	BA	546	U	N3-C2-O2	-6.08	117.94	122.20
54	BA	809	G	C8-N9-C4	-6.08	103.97	106.40
54	BA	866	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1499	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	1826	G	C4'-C3'-C2'	-6.08	96.52	102.60
21	AA	480	U	C5-C6-N1	-6.08	119.66	122.70
54	BA	38	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	401	A	C5-C6-N1	6.08	120.74	117.70
54	BA	1102	C	N3-C4-C5	6.08	124.33	121.90
54	BA	2166	U	O4'-C1'-N1	6.08	113.06	108.20
54	BA	2521	C	N1-C2-O2	6.08	122.55	118.90
54	BA	527	C	N3-C4-C5	6.08	124.33	121.90
54	BA	1206	G	N7-C8-N9	6.08	116.14	113.10
54	BA	2317	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2416	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	69	C	N1-C2-O2	6.08	122.55	118.90
54	BA	1819	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2216	G	C5-C6-N1	6.08	114.54	111.50
54	BA	2333	A	C4-C5-C6	-6.08	113.96	117.00
55	BB	4	C	N3-C2-O2	-6.08	117.65	121.90
21	AA	57	G	N1-C6-O6	-6.07	116.26	119.90
54	BA	233	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	716	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	1753	G	C8-N9-C4	-6.07	103.97	106.40
54	BA	2080	A	C6-C5-N7	6.07	136.55	132.30
21	AA	507	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	222	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	1406	U	O4'-C1'-N1	6.07	113.06	108.20
54	BA	1742	U	O4'-C1'-N1	6.07	113.06	108.20
21	AA	56	U	O4'-C1'-N1	6.07	113.06	108.20
21	AA	171	A	C4-C5-C6	-6.07	113.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	433	C	N3-C4-C5	6.07	124.33	121.90
54	BA	676	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	873	C	N1-C2-O2	6.07	122.54	118.90
54	BA	1175	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	1576	U	C5-C6-N1	-6.07	119.67	122.70
54	BA	1634	A	C5-C6-N1	6.07	120.73	117.70
54	BA	2094	A	C5-C6-N1	6.07	120.73	117.70
54	BA	2216	G	N3-C4-C5	-6.07	125.56	128.60
54	BA	2449	U	N3-C2-O2	-6.07	117.95	122.20
21	AA	451	A	O4'-C1'-N9	6.07	113.05	108.20
54	BA	484	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2312	U	C5-C6-N1	-6.07	119.67	122.70
21	AA	553	A	N1-C6-N6	-6.07	114.96	118.60
21	AA	1097	C	N3-C2-O2	-6.07	117.66	121.90
21	AA	1505	G	O4'-C1'-N9	6.07	113.05	108.20
54	BA	168	G	C5-C6-N1	6.07	114.53	111.50
54	BA	2778	A	N1-C6-N6	-6.07	114.96	118.60
21	AA	929	G	C8-N9-C4	-6.06	103.97	106.40
54	BA	1611	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1772	A	C6-C5-N7	6.06	136.54	132.30
21	AA	347	G	C8-N9-C4	-6.06	103.97	106.40
21	AA	789	U	N3-C2-O2	-6.06	117.96	122.20
54	BA	754	U	O4'-C1'-N1	6.06	113.05	108.20
54	BA	951	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1104	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1752	C	O4'-C1'-N1	6.06	113.05	108.20
54	BA	2044	C	N1-C2-O2	6.06	122.54	118.90
54	BA	2356	U	C5-C6-N1	-6.06	119.67	122.70
54	BA	2417	C	N3-C2-O2	-6.06	117.66	121.90
22	A1	74	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	466	A	C5-C6-N1	6.06	120.73	117.70
54	BA	541	A	C5-C6-N1	6.06	120.73	117.70
28	BF	6	TYR	CB-CG-CD2	-6.06	117.36	121.00
54	BA	1640	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	1533	C	N1-C2-O2	6.06	122.53	118.90
54	BA	142	A	C5-C6-N1	6.06	120.73	117.70
54	BA	1698	A	N1-C6-N6	-6.06	114.97	118.60
21	AA	160	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	41	G	C5-C6-N1	6.05	114.53	111.50
22	A1	20	G	O4'-C1'-N9	6.05	113.04	108.20
54	BA	159	G	C5-C6-N1	6.05	114.53	111.50
55	BB	14	U	C5-C6-N1	-6.05	119.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BE	88	ARG	NE-CZ-NH1	6.05	123.33	120.30
54	BA	181	A	C5-C6-N1	6.05	120.73	117.70
55	BB	91	C	N3-C2-O2	-6.05	117.66	121.90
55	BB	112	G	C5-C6-N1	6.05	114.53	111.50
21	AA	378	G	C5-C6-N1	6.05	114.53	111.50
21	AA	1341	U	C5-C6-N1	-6.05	119.67	122.70
21	AA	1510	C	N1-C2-O2	6.05	122.53	118.90
54	BA	20	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	309	A	C5-C6-N1	6.05	120.73	117.70
54	BA	1918	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	2113	U	C5-C6-N1	-6.05	119.67	122.70
54	BA	2377	A	N1-C6-N6	-6.05	114.97	118.60
54	BA	522	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	1625	C	O4'-C1'-N1	6.05	113.04	108.20
54	BA	2050	C	N1-C2-O2	6.05	122.53	118.90
54	BA	2281	A	C5-C6-N1	6.05	120.72	117.70
54	BA	2710	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1119	U	O4'-C1'-N1	6.05	113.04	108.20
54	BA	1130	U	O4'-C1'-N1	6.05	113.04	108.20
54	BA	1503	A	C5-C6-N1	6.05	120.72	117.70
54	BA	1617	C	N1-C2-O2	6.05	122.53	118.90
54	BA	1828	G	C3'-C2'-C1'	-6.05	96.66	101.50
21	AA	352	C	C6-N1-C2	-6.05	117.88	120.30
21	AA	525	C	N3-C2-O2	-6.05	117.67	121.90
23	A2	92	U	N3-C2-O2	-6.05	117.97	122.20
54	BA	246	C	O4'-C1'-N1	6.05	113.04	108.20
54	BA	405	U	O4'-C1'-N1	6.05	113.04	108.20
54	BA	444	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	681	G	C5-C6-N1	6.05	114.52	111.50
54	BA	2289	G	C8-N9-C4	-6.05	103.98	106.40
21	AA	108	G	N3-C4-C5	-6.04	125.58	128.60
21	AA	468	A	C2-N3-C4	6.04	113.62	110.60
21	AA	1401	G	N3-C4-C5	-6.04	125.58	128.60
54	BA	1379	U	O4'-C1'-N1	6.04	113.04	108.20
54	BA	1395	A	C5-C6-N1	6.04	120.72	117.70
54	BA	1667	G	C8-N9-C4	-6.04	103.98	106.40
54	BA	2024	G	N3-C4-C5	-6.04	125.58	128.60
54	BA	2183	A	C5-C6-N1	6.04	120.72	117.70
54	BA	2246	G	N3-C4-C5	-6.04	125.58	128.60
6	AG	108	ARG	NE-CZ-NH1	6.04	123.32	120.30
21	AA	193	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	272	C	N3-C2-O2	-6.04	117.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	744	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	1091	U	N1-C2-N3	6.04	118.53	114.90
21	AA	1369	C	N3-C2-O2	-6.04	117.67	121.90
28	BF	147	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	42	A	C6-C5-N7	6.04	136.53	132.30
54	BA	60	G	O4'-C1'-N9	6.04	113.03	108.20
54	BA	474	G	N9-C4-C5	6.04	107.82	105.40
54	BA	633	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2331	G	N3-C4-C5	-6.04	125.58	128.60
21	AA	900	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	517	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	960	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2340	A	C5-C6-N1	6.04	120.72	117.70
54	BA	2390	U	O4'-C1'-N1	6.04	113.03	108.20
54	BA	2394	C	O4'-C1'-N1	6.04	113.03	108.20
21	AA	1093	A	C5-C6-N1	6.04	120.72	117.70
54	BA	715	A	C3'-C2'-C1'	6.04	106.33	101.50
54	BA	1918	A	C5-C6-N1	6.04	120.72	117.70
54	BA	2712	C	N3-C4-C5	6.04	124.32	121.90
21	AA	360	G	C5-C6-N1	6.04	114.52	111.50
54	BA	184	C	N1-C2-O2	6.04	122.52	118.90
54	BA	1317	G	N1-C6-O6	-6.04	116.28	119.90
54	BA	272	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	685	A	C5-C6-N1	6.04	120.72	117.70
54	BA	2276	G	C5-C6-N1	6.04	114.52	111.50
54	BA	2349	G	N1-C6-O6	-6.04	116.28	119.90
21	AA	342	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	611	C	N1-C2-O2	6.03	122.52	118.90
21	AA	1423	G	C5-C6-N1	6.03	114.52	111.50
54	BA	1768	C	N1-C2-O2	6.03	122.52	118.90
54	BA	2805	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	1076	U	C5-C6-N1	-6.03	119.68	122.70
54	BA	548	G	C3'-C2'-C1'	6.03	106.33	101.50
54	BA	1321	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	1000	A	N1-C6-N6	-6.03	114.98	118.60
54	BA	39	G	N3-C2-N2	-6.03	115.68	119.90
54	BA	411	G	N9-C4-C5	6.03	107.81	105.40
54	BA	478	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	2311	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	2371	G	C4'-C3'-C2'	-6.03	96.57	102.60
21	AA	1447	A	C5-C6-N1	6.03	120.71	117.70
54	BA	1082	U	C5-C6-N1	-6.03	119.69	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1668	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	1946	U	O4'-C1'-N1	6.03	113.02	108.20
21	AA	1117	A	C6-C5-N7	6.03	136.52	132.30
54	BA	544	C	N1-C2-O2	6.03	122.52	118.90
54	BA	1049	C	O4'-C1'-N1	6.03	113.02	108.20
54	BA	1670	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1764	C	O4'-C1'-N1	6.03	113.02	108.20
54	BA	2591	C	O4'-C1'-N1	6.03	113.02	108.20
54	BA	622	G	C5-C6-N1	6.02	114.51	111.50
54	BA	1040	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2049	G	N3-C4-C5	-6.02	125.59	128.60
54	BA	1867	G	O4'-C1'-N9	6.02	113.02	108.20
54	BA	2228	G	C8-N9-C4	-6.02	103.99	106.40
54	BA	2478	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2506	U	O4'-C1'-N1	6.02	113.02	108.20
54	BA	2580	U	N3-C2-O2	-6.02	117.98	122.20
21	AA	1499	A	N1-C6-N6	-6.02	114.99	118.60
54	BA	382	A	C5-C6-N1	6.02	120.71	117.70
54	BA	502	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	712	G	C5-C6-N1	6.02	114.51	111.50
54	BA	2085	U	O4'-C1'-N1	6.02	113.02	108.20
54	BA	2743	U	C5-C6-N1	-6.02	119.69	122.70
55	BB	19	C	N1-C2-O2	6.02	122.51	118.90
21	AA	1522	U	N1-C2-N3	6.02	118.51	114.90
54	BA	1096	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2170	A	C4-C5-C6	-6.02	113.99	117.00
22	A1	69	A	C3'-C2'-C1'	6.02	106.31	101.50
21	AA	459	A	C5-C6-N1	6.01	120.71	117.70
54	BA	972	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	2130	U	N1-C2-N3	6.01	118.51	114.90
54	BA	2345	G	N1-C6-O6	-6.01	116.29	119.90
21	AA	551	U	C5-C6-N1	-6.01	119.69	122.70
54	BA	378	C	N1-C2-O2	6.01	122.51	118.90
54	BA	2045	C	N3-C4-C5	6.01	124.31	121.90
55	BB	27	C	N1-C2-O2	6.01	122.51	118.90
21	AA	975	A	C5-C6-N1	6.01	120.70	117.70
21	AA	1115	U	C5-C6-N1	-6.01	119.69	122.70
21	AA	1237	C	O4'-C1'-N1	6.01	113.01	108.20
54	BA	610	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1031	G	C5-C6-N1	6.01	114.51	111.50
54	BA	1874	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	2443	C	N1-C2-O2	6.01	122.51	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	935	A	C5-C6-N1	6.01	120.70	117.70
21	AA	1239	A	C4-C5-C6	-6.01	114.00	117.00
21	AA	1282	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1260	A	C6-C5-N7	6.01	136.51	132.30
54	BA	1870	C	N3-C4-C5	6.01	124.30	121.90
54	BA	2110	G	C1'-O4'-C4'	-6.01	105.09	109.90
54	BA	2321	U	N3-C2-O2	-6.01	117.99	122.20
54	BA	2608	G	N3-C4-C5	-6.01	125.59	128.60
21	AA	789	U	C5-C6-N1	-6.01	119.70	122.70
21	AA	832	G	N1-C6-O6	-6.01	116.30	119.90
54	BA	1044	C	N3-C4-C5	6.01	124.30	121.90
21	AA	841	C	N3-C4-C5	6.01	124.30	121.90
21	AA	1227	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	1327	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2379	G	N1-C6-O6	-6.01	116.30	119.90
54	BA	2557	G	O4'-C1'-N9	6.01	113.00	108.20
54	BA	981	A	C5-C6-N1	6.00	120.70	117.70
54	BA	2395	C	O4'-C1'-N1	6.00	113.00	108.20
21	AA	319	G	C5-C6-N1	6.00	114.50	111.50
21	AA	782	A	C5-C6-N1	6.00	120.70	117.70
21	AA	926	G	N9-C4-C5	6.00	107.80	105.40
21	AA	1146	A	N1-C6-N6	-6.00	115.00	118.60
21	AA	1434	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	673	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	1505	A	C5-C6-N1	6.00	120.70	117.70
21	AA	417	G	N1-C6-O6	-6.00	116.30	119.90
21	AA	920	U	N3-C2-O2	-6.00	118.00	122.20
21	AA	940	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1148	U	C5-C6-N1	-6.00	119.70	122.70
21	AA	1522	U	C5-C6-N1	-6.00	119.70	122.70
54	BA	952	G	N1-C6-O6	-6.00	116.30	119.90
54	BA	2437	G	C5-C6-N1	6.00	114.50	111.50
21	AA	1019	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1768	C	N3-C4-C5	6.00	124.30	121.90
54	BA	2606	C	N3-C4-C5	6.00	124.30	121.90
54	BA	1766	G	C5-C6-N1	6.00	114.50	111.50
55	BB	86	G	N1-C6-O6	-6.00	116.30	119.90
21	AA	532	A	N1-C6-N6	-6.00	115.00	118.60
21	AA	277	C	N3-C4-C5	6.00	124.30	121.90
54	BA	602	A	N1-C6-N6	-5.99	115.00	118.60
54	BA	1251	C	C3'-C2'-C1'	5.99	106.30	101.50
54	BA	1316	U	O4'-C1'-N1	5.99	113.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1417	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	1793	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	2347	C	C3'-C2'-C1'	5.99	106.30	101.50
54	BA	2873	A	O4'-C1'-N9	5.99	112.99	108.20
55	BB	80	U	C5-C6-N1	-5.99	119.70	122.70
21	AA	631	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	905	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	2765	A	O4'-C1'-N9	5.99	112.99	108.20
21	AA	1297	G	N3-C2-N2	-5.99	115.71	119.90
54	BA	1154	G	O4'-C1'-N9	5.99	112.99	108.20
54	BA	2497	A	C5-C6-N1	5.99	120.69	117.70
21	AA	197	A	C5-C6-N1	5.99	120.69	117.70
21	AA	328	C	C1'-O4'-C4'	-5.99	105.11	109.90
54	BA	938	G	N1-C6-O6	-5.99	116.31	119.90
54	BA	1106	G	N1-C6-O6	-5.99	116.31	119.90
54	BA	1187	G	N1-C6-O6	-5.99	116.31	119.90
54	BA	1420	A	C6-C5-N7	5.99	136.49	132.30
54	BA	2883	A	N1-C6-N6	-5.99	115.01	118.60
21	AA	613	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	542	C	O4'-C1'-N1	5.99	112.99	108.20
21	AA	214	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	385	C	N3-C2-O2	-5.99	117.71	121.90
22	A1	73	A	C5-C6-N1	5.99	120.69	117.70
54	BA	2113	U	N3-C2-O2	-5.99	118.01	122.20
54	BA	2196	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	111	G	N1-C6-O6	-5.98	116.31	119.90
21	AA	1281	C	N1-C2-O2	5.98	122.49	118.90
54	BA	118	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	757	G	N1-C6-O6	-5.98	116.31	119.90
54	BA	1502	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1704	C	N1-C2-O2	5.98	122.49	118.90
54	BA	2568	U	O4'-C1'-N1	5.98	112.99	108.20
21	AA	422	C	N1-C2-O2	5.98	122.49	118.90
21	AA	533	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1072	G	C5-C6-N1	5.98	114.49	111.50
21	AA	1332	A	C5-C6-N1	5.98	120.69	117.70
21	AA	1477	U	N1-C2-N3	5.98	118.49	114.90
47	BY	29	ARG	NE-CZ-NH1	5.98	123.29	120.30
54	BA	1359	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1392	A	N1-C6-N6	-5.98	115.01	118.60
54	BA	1515	A	C5-C6-N1	5.98	120.69	117.70
54	BA	1602	U	O4'-C1'-N1	5.98	112.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	527	G	O4'-C1'-N9	5.98	112.98	108.20
54	BA	3	U	C5-C6-N1	-5.98	119.71	122.70
55	BB	25	U	C5-C6-N1	-5.98	119.71	122.70
21	AA	171	A	C6-C5-N7	5.98	136.48	132.30
21	AA	423	G	O4'-C1'-N9	5.98	112.98	108.20
21	AA	1151	A	P-O3'-C3'	5.98	126.87	119.70
24	A3	3	C	N3-C2-O2	-5.98	117.72	121.90
24	A3	63	C	N3-C4-C5	5.98	124.29	121.90
54	BA	1924	C	O4'-C1'-N1	5.98	112.98	108.20
54	BA	2044	C	N3-C4-C5	5.98	124.29	121.90
54	BA	2624	G	C5-C6-N1	5.98	114.49	111.50
21	AA	186	C	N1-C2-O2	5.98	122.48	118.90
54	BA	678	C	C6-N1-C2	-5.98	117.91	120.30
54	BA	2683	C	N3-C4-C5	5.98	124.29	121.90
21	AA	635	A	C5-C6-N1	5.97	120.69	117.70
54	BA	1601	G	C8-N9-C4	-5.97	104.01	106.40
54	BA	1752	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	1037	C	N1-C2-O2	5.97	122.48	118.90
21	AA	1056	U	C5-C6-N1	-5.97	119.71	122.70
54	BA	143	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	844	A	N1-C6-N6	-5.97	115.02	118.60
54	BA	1496	A	C5-C6-N1	5.97	120.69	117.70
54	BA	2135	A	O4'-C1'-N9	5.97	112.98	108.20
21	AA	311	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	674	G	C8-N9-C4	-5.97	104.01	106.40
21	AA	1182	G	N1-C6-O6	-5.97	116.32	119.90
24	A3	68	C	N1-C2-O2	5.97	122.48	118.90
54	BA	2512	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	183	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	297	G	C5-C6-N1	5.97	114.48	111.50
54	BA	411	G	C8-N9-C4	-5.97	104.01	106.40
54	BA	1165	A	C5-C6-N1	5.97	120.68	117.70
54	BA	1705	A	C5-C6-N1	5.97	120.68	117.70
54	BA	2847	U	O4'-C1'-N1	5.97	112.97	108.20
54	BA	712	G	N1-C6-O6	-5.97	116.32	119.90
54	BA	1013	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1332	G	C5-C6-N1	5.97	114.48	111.50
54	BA	2033	A	C5-C6-N1	5.97	120.68	117.70
54	BA	2175	C	N3-C4-C5	5.97	124.29	121.90
21	AA	356	A	C6-C5-N7	5.96	136.47	132.30
21	AA	409	U	C5-C6-N1	-5.96	119.72	122.70
21	AA	768	A	C4-C5-C6	-5.96	114.02	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1087	G	C5-C6-N1	5.96	114.48	111.50
54	BA	907	G	O4'-C1'-N9	5.96	112.97	108.20
54	BA	1241	A	O4'-C1'-N9	5.96	112.97	108.20
54	BA	1514	G	C8-N9-C4	-5.96	104.01	106.40
54	BA	1873	G	O4'-C1'-N9	5.96	112.97	108.20
21	AA	931	C	O4'-C1'-N1	5.96	112.97	108.20
54	BA	2290	G	C5-C6-N1	5.96	114.48	111.50
54	BA	2426	A	O4'-C1'-N9	5.96	112.97	108.20
21	AA	749	A	C5-C6-N1	5.96	120.68	117.70
21	AA	803	G	N1-C6-O6	-5.96	116.32	119.90
21	AA	877	G	N7-C8-N9	5.96	116.08	113.10
21	AA	934	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	1054	C	N1-C2-O2	5.96	122.48	118.90
27	BE	102	ARG	NE-CZ-NH1	5.96	123.28	120.30
54	BA	301	G	O4'-C1'-N9	5.96	112.97	108.20
54	BA	1229	C	N1-C2-O2	5.96	122.48	118.90
55	BB	95	U	N3-C2-O2	-5.96	118.03	122.20
54	BA	1730	C	N1-C2-O2	5.96	122.48	118.90
54	BA	1814	G	C5-C6-N1	5.96	114.48	111.50
21	AA	817	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	881	G	C5-C6-N1	5.96	114.48	111.50
54	BA	69	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	121	G	O4'-C1'-N9	5.96	112.97	108.20
54	BA	265	A	O4'-C1'-N9	5.96	112.97	108.20
54	BA	579	G	C5'-C4'-O4'	5.96	116.25	109.10
54	BA	1140	C	O4'-C1'-N1	5.96	112.97	108.20
54	BA	1156	A	C5-C6-N1	5.96	120.68	117.70
54	BA	1973	G	C8-N9-C4	-5.96	104.02	106.40
54	BA	2775	G	C5-C6-N1	5.96	114.48	111.50
21	AA	1021	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	736	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	922	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2174	C	N3-C4-N4	-5.96	113.83	118.00
22	A1	76	A	N1-C6-N6	-5.96	115.03	118.60
54	BA	4	U	O4'-C1'-N1	5.96	112.96	108.20
54	BA	2579	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	35	G	N1-C6-O6	-5.95	116.33	119.90
54	BA	624	C	N1-C2-O2	5.95	122.47	118.90
54	BA	1170	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	196	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	816	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	995	C	N3-C4-C5	5.95	124.28	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1284	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	35	G	C1'-O4'-C4'	-5.95	105.14	109.90
21	AA	718	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	793	U	C5-C6-N1	-5.95	119.72	122.70
46	BX	10	ARG	NE-CZ-NH1	5.95	123.28	120.30
54	BA	471	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	804	A	C5-C6-N1	5.95	120.68	117.70
54	BA	1727	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	2165	C	N1-C2-O2	5.95	122.47	118.90
54	BA	2326	C	N1-C2-O2	5.95	122.47	118.90
21	AA	1494	G	N9-C4-C5	5.95	107.78	105.40
54	BA	100	U	N1-C2-N3	5.95	118.47	114.90
54	BA	109	C	N1-C2-O2	5.95	122.47	118.90
54	BA	1363	C	N1-C2-O2	5.95	122.47	118.90
54	BA	1652	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	1696	G	C5-C6-N1	5.95	114.47	111.50
54	BA	1768	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	1892	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	2326	C	N3-C4-C5	5.95	124.28	121.90
54	BA	680	C	O4'-C1'-N1	5.95	112.96	108.20
54	BA	883	G	N1-C6-O6	-5.95	116.33	119.90
21	AA	194	C	N1-C2-O2	5.95	122.47	118.90
21	AA	779	C	N3-C4-N4	-5.95	113.84	118.00
21	AA	1496	C	N1-C2-O2	5.95	122.47	118.90
54	BA	759	G	N7-C8-N9	5.95	116.07	113.10
54	BA	828	U	N3-C2-O2	-5.95	118.04	122.20
54	BA	1223	G	C5-C6-N1	5.95	114.47	111.50
54	BA	1816	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	2102	G	N3-C4-C5	-5.95	125.63	128.60
21	AA	612	C	N1-C2-O2	5.94	122.47	118.90
54	BA	750	A	P-O3'-C3'	5.94	126.83	119.70
54	BA	2331	G	C5-C6-N1	5.94	114.47	111.50
10	AK	127	ARG	NE-CZ-NH1	5.94	123.27	120.30
21	AA	443	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	1228	C	N1-C2-O2	5.94	122.47	118.90
54	BA	7	G	N3-C2-N2	-5.94	115.74	119.90
54	BA	503	A	O4'-C1'-N9	5.94	112.95	108.20
54	BA	516	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1967	C	O4'-C1'-N1	5.94	112.95	108.20
54	BA	2645	G	C5-C6-N1	5.94	114.47	111.50
8	AI	44	ARG	NE-CZ-NH1	5.94	123.27	120.30
54	BA	720	U	C5-C6-N1	-5.94	119.73	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1229	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1267	U	C5-C6-N1	-5.94	119.73	122.70
54	BA	2098	U	C5-C6-N1	-5.94	119.73	122.70
21	AA	1207	G	N3-C2-N2	-5.94	115.74	119.90
22	A1	23	A	N1-C6-N6	-5.94	115.04	118.60
25	BC	13	ARG	NE-CZ-NH1	5.94	123.27	120.30
54	BA	450	G	N1-C6-O6	-5.94	116.34	119.90
54	BA	1165	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	2258	C	O4'-C1'-N1	5.94	112.95	108.20
54	BA	2660	A	C5-C6-N1	5.94	120.67	117.70
21	AA	461	A	C5-C6-N1	5.94	120.67	117.70
54	BA	888	C	N3-C2-O2	-5.94	117.75	121.90
54	BA	2840	C	N3-C2-O2	-5.94	117.75	121.90
21	AA	1289	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	1320	C	N3-C4-C5	5.93	124.27	121.90
54	BA	1	G	C4'-C3'-C2'	-5.93	96.67	102.60
54	BA	1119	U	C5-C6-N1	-5.93	119.73	122.70
54	BA	1205	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1878	G	C8-N9-C4	-5.93	104.03	106.40
54	BA	2516	A	C5-C6-N1	5.93	120.67	117.70
13	AN	41	ARG	NE-CZ-NH1	5.93	123.27	120.30
21	AA	132	C	N1-C2-O2	5.93	122.46	118.90
21	AA	1065	U	C3'-C2'-C1'	5.93	106.25	101.50
54	BA	5	A	N1-C6-N6	-5.93	115.04	118.60
54	BA	77	G	N1-C6-O6	-5.93	116.34	119.90
54	BA	490	C	N1-C2-O2	5.93	122.46	118.90
54	BA	1827	U	N3-C2-O2	-5.93	118.05	122.20
54	BA	2577	A	N1-C6-N6	-5.93	115.04	118.60
21	AA	1014	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2186	G	N1-C6-O6	-5.93	116.34	119.90
21	AA	840	C	N3-C4-C5	5.93	124.27	121.90
21	AA	1296	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	1066	U	O4'-C1'-N1	5.93	112.94	108.20
54	BA	1472	C	N1-C2-O2	5.93	122.46	118.90
54	BA	1940	U	N3-C2-O2	-5.93	118.05	122.20
54	BA	1989	G	C8-N9-C4	-5.93	104.03	106.40
54	BA	2420	C	N1-C2-O2	5.93	122.46	118.90
55	BB	76	G	N3-C4-C5	-5.93	125.64	128.60
54	BA	2372	U	O4'-C1'-N1	5.93	112.94	108.20
54	BA	1485	U	O4'-C1'-N1	5.93	112.94	108.20
54	BA	2616	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	869	G	N9-C4-C5	5.92	107.77	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	964	A	C4-C5-C6	-5.92	114.04	117.00
29	BG	68	ARG	NE-CZ-NH1	5.92	123.26	120.30
54	BA	3	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	1126	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1289	C	C3'-C2'-C1'	5.92	106.24	101.50
54	BA	1331	G	N1-C6-O6	-5.92	116.35	119.90
54	BA	1635	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2110	G	C5-C6-N1	5.92	114.46	111.50
21	AA	882	C	N3-C2-O2	-5.92	117.75	121.90
21	AA	972	C	C3'-C2'-C1'	5.92	106.24	101.50
21	AA	1117	A	C2-N3-C4	5.92	113.56	110.60
21	AA	1472	U	C5-C6-N1	-5.92	119.74	122.70
54	BA	723	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	2349	G	N3-C4-C5	-5.92	125.64	128.60
54	BA	2600	A	C4-C5-C6	-5.92	114.04	117.00
56	B5	53	ARG	NE-CZ-NH1	5.92	123.26	120.30
21	AA	1123	U	C1'-O4'-C4'	-5.92	105.16	109.90
54	BA	2452	C	N3-C4-C5	5.92	124.27	121.90
54	BA	2611	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	468	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	926	G	N3-C4-C5	-5.92	125.64	128.60
24	A3	44	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1383	A	N1-C6-N6	-5.92	115.05	118.60
15	AP	51	ARG	NE-CZ-NH1	5.92	123.26	120.30
21	AA	1338	G	C5-C6-N1	5.92	114.46	111.50
55	BB	100	G	C8-N9-C4	-5.92	104.03	106.40
21	AA	87	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	2433	A	C6-C5-N7	5.92	136.44	132.30
21	AA	186	C	N3-C4-C5	5.91	124.27	121.90
22	A1	66	A	C6-C5-N7	5.91	136.44	132.30
54	BA	108	G	O4'-C1'-N9	5.91	112.93	108.20
54	BA	395	U	O4'-C1'-N1	5.91	112.93	108.20
54	BA	1379	U	N3-C2-O2	-5.91	118.06	122.20
54	BA	2023	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	1298	U	N3-C2-O2	-5.91	118.06	122.20
21	AA	1356	G	C5-C6-N1	5.91	114.46	111.50
54	BA	702	U	O4'-C1'-N1	5.91	112.93	108.20
54	BA	853	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	973	G	N1-C6-O6	-5.91	116.35	119.90
21	AA	1389	C	C1'-O4'-C4'	-5.91	105.17	109.90
22	A1	68	C	N1-C2-O2	5.91	122.45	118.90
54	BA	1308	A	C4-C5-C6	-5.91	114.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1830	C	C6-N1-C2	-5.91	117.94	120.30
54	BA	1923	U	O4'-C1'-N1	5.91	112.93	108.20
54	BA	2900	A	C6-C5-N7	5.91	136.44	132.30
21	AA	685	G	N9-C4-C5	5.91	107.76	105.40
51	B2	19	ARG	NE-CZ-NH1	5.91	123.25	120.30
54	BA	1386	C	N1-C2-O2	5.91	122.45	118.90
54	BA	2138	G	O4'-C1'-N9	5.91	112.93	108.20
21	AA	306	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	930	C	O4'-C1'-N1	5.91	112.92	108.20
21	AA	1514	G	C5-C6-N1	5.91	114.45	111.50
22	A1	59	U	O4'-C1'-N1	5.91	112.92	108.20
54	BA	61	C	N1-C2-O2	5.91	122.44	118.90
54	BA	363	G	C5-C6-N1	5.91	114.45	111.50
54	BA	587	C	N3-C4-C5	5.91	124.26	121.90
54	BA	1081	U	O4'-C1'-N1	5.91	112.92	108.20
21	AA	1490	U	C5-C6-N1	-5.90	119.75	122.70
36	BN	96	ARG	NE-CZ-NH1	5.90	123.25	120.30
37	BO	111	ARG	NE-CZ-NH1	5.90	123.25	120.30
54	BA	145	C	N3-C4-N4	-5.90	113.87	118.00
54	BA	641	U	N3-C2-O2	-5.90	118.07	122.20
54	BA	1675	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	1777	U	C5'-C4'-O4'	5.90	116.18	109.10
9	AJ	7	ARG	NE-CZ-NH1	5.90	123.25	120.30
21	AA	971	G	C5-C6-N1	5.90	114.45	111.50
21	AA	1527	U	N3-C2-O2	-5.90	118.07	122.20
24	A3	20	G	N1-C6-O6	-5.90	116.36	119.90
35	BM	51	ARG	NE-CZ-NH1	5.90	123.25	120.30
54	BA	21	A	N1-C6-N6	-5.90	115.06	118.60
54	BA	121	G	N9-C4-C5	5.90	107.76	105.40
54	BA	982	C	N1-C1'-C2'	5.90	121.67	114.00
54	BA	1089	A	C2-N3-C4	5.90	113.55	110.60
54	BA	1306	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	1586	A	C5-C6-N1	5.90	120.65	117.70
54	BA	1819	A	C2-N3-C4	5.90	113.55	110.60
54	BA	2359	C	N1-C2-O2	5.90	122.44	118.90
54	BA	2463	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	438	G	C5-C6-N1	5.90	114.45	111.50
54	BA	1398	C	N3-C4-C5	5.90	124.26	121.90
21	AA	498	A	C6-C5-N7	5.90	136.43	132.30
21	AA	570	G	C5-C6-N1	5.90	114.45	111.50
21	AA	1019	A	C5-C6-N1	5.90	120.65	117.70
54	BA	1378	A	C5-C6-N1	5.90	120.65	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1646	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	2005	A	C5-C6-N1	5.90	120.65	117.70
55	BB	85	G	C8-N9-C4	-5.90	104.04	106.40
21	AA	532	A	C5-C6-N1	5.90	120.65	117.70
54	BA	787	C	N1-C2-O2	5.90	122.44	118.90
54	BA	2466	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	2505	G	N1-C6-O6	-5.90	116.36	119.90
55	BB	104	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	506	G	N1-C6-O6	-5.89	116.36	119.90
54	BA	648	G	C5-C6-N1	5.89	114.45	111.50
54	BA	1025	G	N1-C6-O6	-5.89	116.36	119.90
54	BA	2497	A	P-O3'-C3'	5.89	126.77	119.70
21	AA	162	A	C6-C5-N7	5.89	136.42	132.30
21	AA	1350	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	1402	U	N3-C2-O2	-5.89	118.08	122.20
54	BA	2202	U	O4'-C1'-N1	5.89	112.92	108.20
54	BA	2551	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	2868	A	C5-C6-N1	5.89	120.65	117.70
6	AG	137	ARG	NE-CZ-NH1	5.89	123.25	120.30
21	AA	58	C	N1-C2-O2	5.89	122.44	118.90
21	AA	649	A	C5-C6-N1	5.89	120.64	117.70
21	AA	705	G	C5-C6-N1	5.89	114.45	111.50
21	AA	848	C	N3-C4-C5	5.89	124.26	121.90
54	BA	457	A	C6-C5-N7	5.89	136.42	132.30
54	BA	1686	C	N1-C2-O2	5.89	122.43	118.90
54	BA	1788	C	N3-C4-C5	5.89	124.26	121.90
54	BA	2316	G	N1-C6-O6	-5.89	116.37	119.90
54	BA	220	G	N3-C4-C5	-5.89	125.66	128.60
54	BA	396	G	N1-C6-O6	-5.89	116.37	119.90
54	BA	738	G	N9-C4-C5	5.89	107.75	105.40
54	BA	2114	A	N1-C6-N6	-5.89	115.07	118.60
21	AA	621	A	C5-C6-N1	5.88	120.64	117.70
21	AA	798	U	O4'-C1'-N1	5.88	112.91	108.20
54	BA	406	G	N1-C6-O6	-5.88	116.37	119.90
54	BA	1979	U	O4'-C1'-N1	5.88	112.91	108.20
23	A2	87	U	O4'-C1'-N1	5.88	112.91	108.20
54	BA	1415	U	O4'-C1'-N1	5.88	112.91	108.20
55	BB	118	C	N3-C4-C5	5.88	124.25	121.90
21	AA	1421	G	C8-N9-C4	-5.88	104.05	106.40
54	BA	1048	A	C5-C6-N1	5.88	120.64	117.70
21	AA	39	G	N1-C6-O6	-5.88	116.37	119.90
54	BA	48	G	C8-N9-C4	-5.88	104.05	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BC	261	ARG	NE-CZ-NH1	5.88	123.24	120.30
42	BT	12	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	1827	U	C5-C6-N1	-5.88	119.76	122.70
54	BA	2640	G	N1-C6-O6	-5.88	116.37	119.90
55	BB	94	A	C5-C6-N1	5.88	120.64	117.70
21	AA	1257	A	C4-C5-C6	-5.88	114.06	117.00
24	A3	54	G	N3-C4-C5	-5.88	125.66	128.60
54	BA	537	G	N1-C6-O6	-5.88	116.37	119.90
54	BA	784	G	C8-N9-C4	-5.88	104.05	106.40
54	BA	1071	G	C8-N9-C4	-5.88	104.05	106.40
54	BA	53	A	N1-C6-N6	-5.88	115.08	118.60
54	BA	2429	G	N1-C6-O6	-5.88	116.38	119.90
54	BA	2698	U	O4'-C1'-N1	5.88	112.90	108.20
21	AA	56	U	N1-C2-N3	5.87	118.42	114.90
21	AA	395	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	999	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	1035	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	1428	A	C2-N3-C4	5.87	113.54	110.60
22	A1	25	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	422	A	C5-C6-N1	5.87	120.64	117.70
54	BA	1296	G	N3-C2-N2	-5.87	115.79	119.90
54	BA	2784	U	C5-C6-N1	-5.87	119.76	122.70
21	AA	563	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	1129	C	N3-C4-C5	5.87	124.25	121.90
54	BA	156	A	N1-C6-N6	-5.87	115.08	118.60
54	BA	1147	A	C5-C6-N1	5.87	120.64	117.70
54	BA	1278	C	N1-C2-O2	5.87	122.42	118.90
54	BA	1567	G	C5-C6-N1	5.87	114.44	111.50
54	BA	1747	U	O4'-C1'-N1	5.87	112.90	108.20
54	BA	1987	A	C6-C5-N7	5.87	136.41	132.30
54	BA	2205	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2443	C	N3-C4-N4	-5.87	113.89	118.00
54	BA	2476	A	C4-C5-C6	-5.87	114.06	117.00
55	BB	37	C	N1-C2-O2	5.87	122.42	118.90
21	AA	1530	G	N3-C2-N2	-5.87	115.79	119.90
54	BA	2815	C	N1-C2-O2	5.87	122.42	118.90
54	BA	2901	C	N1-C2-O2	5.87	122.42	118.90
21	AA	308	C	N3-C4-C5	5.87	124.25	121.90
21	AA	324	G	C5-C6-N1	5.87	114.44	111.50
21	AA	1521	C	O4'-C1'-N1	5.87	112.89	108.20
21	AA	1254	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	1305	C	N3-C2-O2	-5.87	117.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	522	C	N3-C4-C5	5.87	124.25	121.90
21	AA	821	G	C5-C6-N1	5.87	114.43	111.50
21	AA	1365	G	C8-N9-C4	-5.87	104.05	106.40
54	BA	121	G	C3'-C2'-C1'	5.87	106.19	101.50
54	BA	205	G	N7-C8-N9	5.87	116.03	113.10
54	BA	860	U	O4'-C1'-N1	5.87	112.89	108.20
54	BA	2767	C	N3-C4-C5	5.87	124.25	121.90
21	AA	276	G	N1-C6-O6	-5.86	116.38	119.90
21	AA	306	A	C5-C6-N1	5.86	120.63	117.70
21	AA	402	G	C5-C6-N1	5.86	114.43	111.50
25	BC	270	ARG	NE-CZ-NH1	5.86	123.23	120.30
54	BA	210	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	467	G	N1-C6-O6	-5.86	116.38	119.90
54	BA	901	C	N1-C2-O2	5.86	122.42	118.90
54	BA	2535	G	C5-C6-N1	5.86	114.43	111.50
21	AA	109	A	C1'-O4'-C4'	-5.86	105.21	109.90
21	AA	783	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	1122	U	C5-C6-N1	-5.86	119.77	122.70
21	AA	1452	C	N1-C2-O2	5.86	122.42	118.90
21	AA	1477	U	C5-C6-N1	-5.86	119.77	122.70
54	BA	2073	C	O4'-C1'-N1	5.86	112.89	108.20
53	B4	12	ARG	NE-CZ-NH1	5.86	123.23	120.30
54	BA	208	C	O4'-C1'-N1	5.86	112.89	108.20
54	BA	1001	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1175	A	O4'-C1'-N9	5.86	112.89	108.20
54	BA	1537	G	N1-C6-O6	-5.86	116.38	119.90
54	BA	2269	G	N3-C2-N2	-5.86	115.80	119.90
54	BA	2602	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	648	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	293	U	C5-C6-N1	-5.86	119.77	122.70
54	BA	637	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	766	U	O4'-C1'-N1	5.86	112.89	108.20
11	AL	8	ARG	NE-CZ-NH1	5.86	123.23	120.30
54	BA	1436	G	N9-C4-C5	5.86	107.74	105.40
54	BA	2299	U	O4'-C1'-N1	5.86	112.89	108.20
55	BB	50	A	N1-C6-N6	-5.86	115.08	118.60
21	AA	105	G	C8-N9-C4	-5.86	104.06	106.40
21	AA	284	C	N1-C2-O2	5.86	122.41	118.90
21	AA	307	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	556	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	102	U	O4'-C1'-N1	5.86	112.88	108.20
54	BA	249	C	N3-C2-O2	-5.86	117.80	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	490	C	C6-N1-C2	-5.86	117.96	120.30
54	BA	2298	A	C5-C6-N1	5.86	120.63	117.70
54	BA	2324	U	O4'-C1'-N1	5.86	112.89	108.20
54	BA	2644	G	N9-C4-C5	5.86	107.74	105.40
54	BA	815	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	1077	A	C5-C6-N1	5.85	120.63	117.70
54	BA	2136	G	C8-N9-C4	-5.85	104.06	106.40
54	BA	2667	C	N3-C4-C5	5.85	124.24	121.90
21	AA	681	A	C6-C5-N7	5.85	136.40	132.30
21	AA	1219	A	C5-C6-N1	5.85	120.63	117.70
22	A1	21	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	1695	G	N3-C2-N2	-5.85	115.80	119.90
54	BA	2265	U	C5-C6-N1	-5.85	119.77	122.70
21	AA	173	U	N3-C2-O2	-5.85	118.10	122.20
54	BA	826	U	N3-C2-O2	-5.85	118.10	122.20
54	BA	1826	G	N9-C4-C5	5.85	107.74	105.40
55	BB	50	A	C4-C5-C6	-5.85	114.08	117.00
21	AA	276	G	C5-C6-N1	5.85	114.42	111.50
21	AA	925	G	C5-C6-N1	5.85	114.42	111.50
54	BA	612	G	C5-C6-N1	5.85	114.42	111.50
54	BA	1075	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	1217	U	O4'-C1'-N1	5.85	112.88	108.20
54	BA	1905	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	2039	U	C5-C6-N1	-5.85	119.78	122.70
54	BA	2531	A	C4-C5-C6	-5.85	114.08	117.00
55	BB	61	G	N1-C6-O6	-5.85	116.39	119.90
54	BA	272	A	C5-C6-N1	5.85	120.62	117.70
54	BA	2064	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	2202	U	C5-C6-N1	-5.85	119.78	122.70
21	AA	1137	C	N3-C4-C5	5.85	124.24	121.90
54	BA	472	A	C5-C6-N1	5.85	120.62	117.70
54	BA	2863	C	N1-C2-O2	5.85	122.41	118.90
21	AA	1416	G	N3-C4-C5	-5.84	125.68	128.60
54	BA	2343	U	N3-C2-O2	-5.84	118.11	122.20
54	BA	2731	G	N1-C6-O6	-5.84	116.39	119.90
54	BA	1093	G	O4'-C1'-N9	5.84	112.88	108.20
21	AA	1214	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	115	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	1142	A	C6-C5-N7	5.84	136.39	132.30
54	BA	1224	U	C5-C6-N1	-5.84	119.78	122.70
54	BA	1391	U	O4'-C1'-N1	5.84	112.87	108.20
54	BA	2143	C	N3-C2-O2	-5.84	117.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2822	G	N3-C4-C5	-5.84	125.68	128.60
55	BB	70	C	N1-C2-O2	5.84	122.41	118.90
21	AA	359	G	C8-N9-C4	-5.84	104.06	106.40
54	BA	624	C	N3-C4-C5	5.84	124.24	121.90
54	BA	1122	G	C8-N9-C4	-5.84	104.06	106.40
5	AF	86	ARG	NE-CZ-NH1	5.84	123.22	120.30
21	AA	315	A	N1-C6-N6	-5.84	115.10	118.60
21	AA	392	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	513	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1596	A	N1-C6-N6	-5.84	115.10	118.60
54	BA	2690	U	N3-C2-O2	-5.84	118.11	122.20
21	AA	479	U	N3-C2-O2	-5.84	118.11	122.20
21	AA	1336	C	C1'-O4'-C4'	-5.84	105.23	109.90
24	A3	75	C	N1-C2-O2	5.84	122.40	118.90
54	BA	1349	C	N3-C4-C5	5.84	124.23	121.90
54	BA	2067	G	C5-C6-N1	5.84	114.42	111.50
54	BA	2306	C	N1-C2-O2	5.84	122.40	118.90
21	AA	199	A	C5-C6-N1	5.83	120.62	117.70
54	BA	182	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	1391	U	C5-C6-N1	-5.83	119.78	122.70
54	BA	1427	A	P-O3'-C3'	5.83	126.70	119.70
16	AQ	61	ARG	NE-CZ-NH1	5.83	123.22	120.30
21	AA	238	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	421	U	C5-C6-N1	-5.83	119.78	122.70
54	BA	602	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	2020	A	N1-C6-N6	-5.83	115.10	118.60
54	BA	2418	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	14	U	N3-C2-O2	-5.83	118.12	122.20
21	AA	428	G	N1-C6-O6	-5.83	116.40	119.90
21	AA	1407	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	1456	A	C5-C6-N1	5.83	120.62	117.70
54	BA	776	G	N3-C2-N2	-5.83	115.82	119.90
54	BA	898	C	O4'-C1'-N1	5.83	112.87	108.20
54	BA	2033	A	O4'-C1'-N9	5.83	112.86	108.20
54	BA	2059	A	C4-C5-C6	-5.83	114.08	117.00
55	BB	26	C	N1-C2-O2	5.83	122.40	118.90
21	AA	153	C	N3-C4-C5	5.83	124.23	121.90
21	AA	262	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	292	U	O4'-C1'-N1	5.83	112.86	108.20
54	BA	1866	A	C4-C5-C6	-5.83	114.08	117.00
55	BB	58	A	N1-C6-N6	-5.83	115.10	118.60
21	AA	1396	A	C5-C6-N1	5.83	120.61	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1492	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	362	A	C5-C6-N1	5.83	120.61	117.70
54	BA	1187	G	N3-C4-C5	-5.83	125.69	128.60
54	BA	1961	C	N1-C2-O2	5.83	122.40	118.90
21	AA	243	A	P-O3'-C3'	5.83	126.69	119.70
21	AA	322	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	1343	G	C5-C6-N1	5.83	114.41	111.50
32	BJ	13	ARG	NE-CZ-NH2	-5.83	117.39	120.30
54	BA	1387	A	O4'-C1'-N9	5.83	112.86	108.20
21	AA	1084	G	N1-C6-O6	-5.82	116.41	119.90
22	A1	75	C	N3-C2-O2	-5.82	117.82	121.90
54	BA	547	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1906	G	C5-C6-N1	5.82	114.41	111.50
54	BA	2253	G	N9-C4-C5	5.82	107.73	105.40
54	BA	2298	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2368	C	N1-C2-O2	5.82	122.39	118.90
54	BA	2412	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2498	C	N1-C2-O2	5.82	122.39	118.90
21	AA	784	A	C4-C5-C6	-5.82	114.09	117.00
22	A1	67	U	C5-C6-N1	-5.82	119.79	122.70
54	BA	663	G	C5-C6-N1	5.82	114.41	111.50
54	BA	801	G	C5-C6-N1	5.82	114.41	111.50
54	BA	2461	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2741	A	C5-C6-N1	5.82	120.61	117.70
54	BA	2744	G	C5-C6-N1	5.82	114.41	111.50
54	BA	1129	A	C5-C6-N1	5.82	120.61	117.70
54	BA	1164	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1512	C	N1-C2-O2	5.82	122.39	118.90
54	BA	1909	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2234	G	N7-C8-N9	5.82	116.01	113.10
54	BA	2548	U	O4'-C1'-N1	5.82	112.86	108.20
54	BA	2744	G	O4'-C1'-N9	5.82	112.86	108.20
21	AA	634	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	866	A	C5-C6-N1	5.82	120.61	117.70
54	BA	1728	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1893	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	647	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	1074	G	N3-C2-N2	-5.82	115.83	119.90
21	AA	1352	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	971	G	N3-C4-C5	-5.82	125.69	128.60
54	BA	1270	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1507	C	N3-C2-O2	-5.82	117.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1613	G	N9-C4-C5	5.82	107.73	105.40
54	BA	2059	A	N1-C6-N6	-5.82	115.11	118.60
54	BA	2193	G	C5-C6-N1	5.82	114.41	111.50
54	BA	2519	U	O4'-C1'-N1	5.82	112.85	108.20
54	BA	2676	C	N1-C2-O2	5.82	122.39	118.90
54	BA	1703	G	C5-C6-N1	5.81	114.41	111.50
54	BA	2818	U	C5-C6-N1	-5.81	119.79	122.70
3	AD	25	ARG	NE-CZ-NH1	5.81	123.21	120.30
21	AA	192	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	1155	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	176	A	C5-C6-N1	5.81	120.61	117.70
54	BA	964	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	1541	C	C4'-C3'-C2'	-5.81	96.79	102.60
54	BA	1559	U	N3-C2-O2	-5.81	118.13	122.20
54	BA	1847	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	38	A	N1-C6-N6	-5.81	115.11	118.60
54	BA	681	G	N1-C6-O6	-5.81	116.41	119.90
54	BA	1323	C	C5'-C4'-O4'	5.81	116.07	109.10
54	BA	2214	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2497	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	170	U	C5-C6-N1	-5.81	119.80	122.70
21	AA	1228	C	N3-C4-C5	5.81	124.22	121.90
54	BA	2803	G	C5-C6-N1	5.81	114.40	111.50
54	BA	887	U	O4'-C1'-N1	5.81	112.85	108.20
54	BA	1359	A	C6-C5-N7	5.81	136.37	132.30
21	AA	732	C	N3-C4-C5	5.81	124.22	121.90
34	BL	123	ARG	NE-CZ-NH1	5.81	123.20	120.30
54	BA	8	C	N3-C2-O2	-5.81	117.84	121.90
54	BA	119	A	O4'-C1'-N9	5.81	112.84	108.20
54	BA	1646	C	C2-N3-C4	-5.81	117.00	119.90
21	AA	1347	G	C8-N9-C4	-5.80	104.08	106.40
54	BA	2429	G	N3-C4-C5	-5.80	125.70	128.60
54	BA	2533	U	O4'-C1'-N1	5.80	112.84	108.20
54	BA	234	U	C5-C6-N1	-5.80	119.80	122.70
54	BA	506	G	O4'-C1'-N9	5.80	112.84	108.20
54	BA	1272	A	C5-C6-N1	5.80	120.60	117.70
21	AA	303	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	505	G	N3-C2-N2	-5.80	115.84	119.90
54	BA	805	G	N1-C6-O6	-5.80	116.42	119.90
54	BA	2015	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	44	A	C5-C6-N1	5.80	120.60	117.70
21	AA	994	A	C4-C5-C6	-5.80	114.10	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	526	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	673	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	838	C	N1-C2-O2	5.80	122.38	118.90
54	BA	1075	C	N1-C2-O2	5.80	122.38	118.90
54	BA	1342	A	C5-C6-N1	5.80	120.60	117.70
54	BA	1409	U	N3-C2-O2	-5.80	118.14	122.20
54	BA	1796	U	N1-C2-N3	5.80	118.38	114.90
54	BA	1909	C	O4'-C1'-N1	5.80	112.84	108.20
54	BA	2378	A	C5-C6-N1	5.80	120.60	117.70
12	AM	86	ARG	NE-CZ-NH1	5.80	123.20	120.30
21	AA	518	C	C3'-C2'-C1'	5.80	106.14	101.50
21	AA	1271	A	C5-C6-N1	5.80	120.60	117.70
21	AA	45	G	O4'-C1'-N9	5.80	112.84	108.20
21	AA	1109	C	C2-N3-C4	-5.80	117.00	119.90
54	BA	1339	G	N3-C4-C5	-5.80	125.70	128.60
54	BA	2048	G	C8-N9-C4	-5.80	104.08	106.40
54	BA	2230	G	N1-C6-O6	-5.80	116.42	119.90
21	AA	1327	C	N3-C2-O2	-5.79	117.84	121.90
21	AA	1421	G	N9-C4-C5	5.79	107.72	105.40
54	BA	1767	G	C5-C6-N1	5.79	114.40	111.50
21	AA	283	U	C5-C6-N1	-5.79	119.80	122.70
21	AA	421	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	543	G	C5-C6-N1	5.79	114.40	111.50
54	BA	1986	C	O4'-C1'-N1	5.79	112.83	108.20
21	AA	331	G	O4'-C4'-C3'	5.79	110.73	106.10
21	AA	355	C	N1-C2-O2	5.79	122.38	118.90
21	AA	387	U	N3-C2-O2	-5.79	118.15	122.20
21	AA	488	C	N3-C2-O2	-5.79	117.85	121.90
21	AA	633	G	N1-C6-O6	-5.79	116.42	119.90
21	AA	1208	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1711	A	P-O3'-C3'	5.79	126.65	119.70
54	BA	2670	A	C4-C5-C6	-5.79	114.10	117.00
11	AL	113	ARG	NE-CZ-NH1	5.79	123.19	120.30
21	AA	250	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	422	C	N3-C4-C5	5.79	124.22	121.90
54	BA	716	A	C1'-O4'-C4'	-5.79	105.27	109.90
54	BA	1934	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1956	U	N3-C2-O2	-5.79	118.15	122.20
54	BA	2184	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2571	U	C5-C6-N1	-5.79	119.81	122.70
1	AB	224	ARG	NE-CZ-NH2	-5.79	117.41	120.30
54	BA	140	C	N3-C4-C5	5.79	124.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1787	A	C5-C6-N1	5.79	120.59	117.70
54	BA	2468	A	O4'-C1'-N9	5.79	112.83	108.20
21	AA	701	U	C5-C6-N1	-5.79	119.81	122.70
21	AA	1412	C	N1-C2-O2	5.79	122.37	118.90
21	AA	1529	G	O4'-C1'-N9	5.79	112.83	108.20
54	BA	561	G	N1-C6-O6	-5.79	116.43	119.90
54	BA	845	A	C5-C6-N1	5.79	120.59	117.70
54	BA	1029	A	C5-C6-N1	5.79	120.59	117.70
54	BA	1717	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2280	G	C8-N9-C4	-5.79	104.09	106.40
54	BA	2792	A	C5-C6-N1	5.79	120.59	117.70
21	AA	620	C	N1-C2-O2	5.78	122.37	118.90
21	AA	1489	G	C5-C6-N1	5.78	114.39	111.50
54	BA	41	C	N1-C2-O2	5.78	122.37	118.90
54	BA	656	G	C8-N9-C4	-5.78	104.09	106.40
54	BA	821	A	C6-C5-N7	5.78	136.35	132.30
54	BA	2350	C	N3-C4-C5	5.78	124.21	121.90
54	BA	2854	G	N9-C4-C5	5.78	107.71	105.40
54	BA	291	G	N3-C2-N2	-5.78	115.85	119.90
54	BA	1094	U	C5'-C4'-O4'	5.78	116.04	109.10
21	AA	49	U	N3-C2-O2	-5.78	118.15	122.20
21	AA	452	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	1069	C	N3-C2-O2	-5.78	117.85	121.90
22	A1	18	G	C5-C6-N1	5.78	114.39	111.50
54	BA	101	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	216	A	N1-C6-N6	-5.78	115.13	118.60
54	BA	524	G	N1-C6-O6	-5.78	116.43	119.90
54	BA	1319	C	N3-C2-O2	-5.78	117.85	121.90
21	AA	354	G	N3-C4-C5	-5.78	125.71	128.60
54	BA	1389	G	C8-N9-C4	-5.78	104.09	106.40
54	BA	1592	C	O4'-C1'-N1	5.78	112.82	108.20
54	BA	1677	A	N1-C6-N6	-5.78	115.13	118.60
20	AU	34	ARG	NE-CZ-NH1	5.78	123.19	120.30
22	A1	70	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	622	G	N1-C6-O6	-5.78	116.43	119.90
54	BA	1439	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1725	U	C5-C6-N1	-5.78	119.81	122.70
54	BA	2264	C	O4'-C1'-N1	5.78	112.82	108.20
54	BA	2363	G	C5-C6-N1	5.78	114.39	111.50
21	AA	799	G	C5-C6-N1	5.78	114.39	111.50
21	AA	839	C	O4'-C1'-N1	5.78	112.82	108.20
54	BA	225	C	N3-C2-O2	-5.78	117.86	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	982	C	C6-N1-C2	-5.78	117.99	120.30
54	BA	1200	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	1290	C	N1-C2-O2	5.78	122.36	118.90
54	BA	2498	C	O4'-C1'-N1	5.78	112.82	108.20
21	AA	394	G	N3-C2-N2	-5.77	115.86	119.90
21	AA	481	G	N3-C4-C5	-5.77	125.71	128.60
25	BC	213	ARG	NE-CZ-NH2	-5.77	117.41	120.30
54	BA	1374	G	N1-C6-O6	-5.77	116.44	119.90
54	BA	2422	C	N3-C2-O2	-5.77	117.86	121.90
2	AC	131	ARG	NE-CZ-NH1	5.77	123.19	120.30
21	AA	857	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	1438	G	N9-C4-C5	5.77	107.71	105.40
54	BA	1383	A	O4'-C1'-N9	5.77	112.82	108.20
54	BA	1545	A	C6-C5-N7	5.77	136.34	132.30
54	BA	1692	U	N3-C2-O2	-5.77	118.16	122.20
54	BA	2362	C	O4'-C1'-N1	5.77	112.82	108.20
21	AA	1508	A	C6-C5-N7	5.77	136.34	132.30
54	BA	936	A	C5-C6-N1	5.77	120.58	117.70
54	BA	2633	G	O4'-C1'-N9	5.77	112.82	108.20
55	BB	35	C	C2-N3-C4	-5.77	117.02	119.90
21	AA	414	A	C3'-C2'-C1'	5.77	106.12	101.50
21	AA	1188	A	C6-C5-N7	5.77	136.34	132.30
21	AA	1200	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	1238	A	C6-C5-N7	5.77	136.34	132.30
21	AA	1246	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	487	C	C5'-C4'-O4'	5.77	116.02	109.10
54	BA	1633	G	C5-C6-N1	5.77	114.39	111.50
54	BA	1947	C	O4'-C1'-N1	5.77	112.81	108.20
54	BA	2087	G	C8-N9-C4	-5.77	104.09	106.40
21	AA	21	G	N3-C4-C5	-5.77	125.72	128.60
21	AA	217	C	N1-C2-O2	5.77	122.36	118.90
21	AA	1063	C	N3-C4-C5	5.77	124.21	121.90
54	BA	2433	A	O4'-C1'-N9	5.77	112.81	108.20
21	AA	354	G	N9-C4-C5	5.77	107.71	105.40
21	AA	738	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	837	U	O4'-C1'-N1	5.77	112.81	108.20
21	AA	1121	U	C5-C6-N1	-5.77	119.82	122.70
21	AA	1499	A	C4-C5-C6	-5.77	114.12	117.00
24	A3	6	G	C8-N9-C4	-5.77	104.09	106.40
54	BA	466	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	1229	C	N3-C4-C5	5.77	124.21	121.90
54	BA	1475	G	N1-C6-O6	-5.77	116.44	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2163	A	C5-C6-N1	5.77	120.58	117.70
54	BA	2359	C	N3-C4-C5	5.77	124.21	121.90
54	BA	2604	U	C5-C6-N1	-5.77	119.82	122.70
21	AA	100	G	N1-C6-O6	-5.76	116.44	119.90
21	AA	357	G	N7-C8-N9	5.76	115.98	113.10
54	BA	223	A	C6-C5-N7	5.76	136.33	132.30
14	AO	71	ARG	NE-CZ-NH1	5.76	123.18	120.30
21	AA	463	U	O4'-C1'-N1	5.76	112.81	108.20
21	AA	723	U	N1-C2-N3	5.76	118.36	114.90
29	BG	162	ARG	NE-CZ-NH2	-5.76	117.42	120.30
54	BA	1105	U	O4'-C1'-N1	5.76	112.81	108.20
54	BA	1150	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2109	U	C5-C6-N1	-5.76	119.82	122.70
54	BA	2543	G	N3-C2-N2	-5.76	115.87	119.90
54	BA	2866	U	C5-C6-N1	-5.76	119.82	122.70
21	AA	1148	U	N3-C2-O2	-5.76	118.17	122.20
21	AA	1162	C	N3-C2-O2	-5.76	117.87	121.90
23	A2	87	U	C5-C6-N1	-5.76	119.82	122.70
54	BA	1281	G	N1-C6-O6	-5.76	116.44	119.90
54	BA	1423	G	O4'-C1'-N9	5.76	112.81	108.20
54	BA	1434	A	C2-N3-C4	5.76	113.48	110.60
54	BA	1635	A	C5-C6-N1	5.76	120.58	117.70
54	BA	2178	C	C6-N1-C2	-5.76	118.00	120.30
54	BA	2428	G	O4'-C1'-N9	5.76	112.81	108.20
54	BA	2762	C	O4'-C1'-N1	5.76	112.81	108.20
54	BA	2824	C	C2-N3-C4	-5.76	117.02	119.90
21	AA	475	C	N1-C2-O2	5.76	122.36	118.90
21	AA	1181	G	C8-N9-C4	-5.76	104.10	106.40
54	BA	738	G	N1-C6-O6	-5.76	116.44	119.90
55	BB	23	G	N3-C4-C5	-5.76	125.72	128.60
21	AA	211	G	O4'-C1'-N9	5.76	112.81	108.20
21	AA	1477	U	N3-C2-O2	-5.76	118.17	122.20
54	BA	525	U	O4'-C1'-N1	5.76	112.81	108.20
54	BA	1764	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2015	A	O4'-C1'-N9	5.76	112.81	108.20
54	BA	2289	G	N9-C4-C5	5.76	107.70	105.40
54	BA	2558	C	N3-C2-O2	-5.76	117.87	121.90
9	AJ	68	ARG	NE-CZ-NH1	5.75	123.18	120.30
21	AA	280	C	N1-C2-O2	5.75	122.35	118.90
54	BA	2022	U	O4'-C1'-N1	5.75	112.80	108.20
21	AA	142	G	N1-C6-O6	-5.75	116.45	119.90
21	AA	447	G	N7-C8-N9	5.75	115.98	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	708	C	N3-C2-O2	-5.75	117.87	121.90
21	AA	1096	C	C6-N1-C2	-5.75	118.00	120.30
21	AA	1472	U	N3-C2-O2	-5.75	118.17	122.20
54	BA	106	C	C6-N1-C2	-5.75	118.00	120.30
54	BA	143	C	O4'-C1'-N1	5.75	112.80	108.20
54	BA	432	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	564	C	N3-C4-C5	5.75	124.20	121.90
54	BA	1123	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	1453	A	N1-C6-N6	-5.75	115.15	118.60
21	AA	632	U	C5-C6-N1	-5.75	119.82	122.70
21	AA	695	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	1180	A	C5-C6-N1	5.75	120.58	117.70
54	BA	1511	G	C5-C6-N1	5.75	114.38	111.50
54	BA	2833	U	C5-C6-N1	-5.75	119.82	122.70
55	BB	30	C	N3-C4-N4	-5.75	113.97	118.00
21	AA	371	A	C6-C5-N7	5.75	136.32	132.30
24	A3	42	C	N3-C2-O2	-5.75	117.88	121.90
25	BC	202	ARG	NE-CZ-NH1	5.75	123.17	120.30
54	BA	986	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	2208	C	O4'-C1'-N1	5.75	112.80	108.20
21	AA	885	G	N3-C4-C5	-5.75	125.72	128.60
21	AA	1132	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	1137	C	C2-N3-C4	-5.75	117.03	119.90
21	AA	1267	C	O4'-C1'-N1	5.75	112.80	108.20
22	A1	11	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	97	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	854	C	O4'-C1'-N1	5.75	112.80	108.20
54	BA	1085	A	C1'-O4'-C4'	-5.75	105.30	109.90
54	BA	1167	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	1462	C	N1-C2-O2	5.75	122.35	118.90
54	BA	301	G	C8-N9-C4	-5.75	104.10	106.40
54	BA	1391	U	N1-C2-N3	5.75	118.35	114.90
54	BA	1538	G	N1-C6-O6	-5.75	116.45	119.90
54	BA	1749	A	C5-C6-N1	5.75	120.57	117.70
21	AA	90	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	159	G	C1'-O4'-C4'	-5.75	105.30	109.90
21	AA	232	G	N1-C6-O6	-5.75	116.45	119.90
21	AA	334	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	1041	G	O4'-C1'-N9	5.75	112.80	108.20
21	AA	1395	C	N1-C2-O2	5.75	122.35	118.90
54	BA	58	G	N3-C2-N2	-5.75	115.88	119.90
54	BA	512	G	O4'-C1'-N9	5.75	112.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1374	G	C5-C6-N1	5.75	114.37	111.50
21	AA	1472	U	O4'-C1'-N1	5.74	112.80	108.20
54	BA	194	G	N1-C6-O6	-5.74	116.45	119.90
54	BA	1152	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	2205	A	C5-C6-N1	5.74	120.57	117.70
54	BA	2364	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	520	G	N1-C6-O6	-5.74	116.45	119.90
54	BA	1690	A	C4-C5-C6	-5.74	114.13	117.00
18	AS	36	ARG	NE-CZ-NH2	-5.74	117.43	120.30
21	AA	522	C	N1-C2-O2	5.74	122.34	118.90
25	BC	62	ARG	NE-CZ-NH1	5.74	123.17	120.30
54	BA	73	A	N1-C6-N6	-5.74	115.16	118.60
54	BA	1222	U	N3-C2-O2	-5.74	118.18	122.20
54	BA	1702	G	N3-C4-C5	-5.74	125.73	128.60
55	BB	106	G	N1-C6-O6	-5.74	116.46	119.90
21	AA	963	G	C5-C6-N1	5.74	114.37	111.50
21	AA	1138	G	N3-C4-C5	-5.74	125.73	128.60
54	BA	220	G	C8-N9-C4	-5.74	104.10	106.40
54	BA	1145	C	O4'-C1'-N1	5.74	112.79	108.20
54	BA	1832	C	N3-C4-C5	5.74	124.20	121.90
54	BA	183	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	286	U	N1-C2-N3	5.74	118.34	114.90
54	BA	2792	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	403	C	N1-C2-O2	5.74	122.34	118.90
21	AA	583	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	1473	G	C5-C6-N1	5.74	114.37	111.50
54	BA	49	A	O4'-C1'-N9	5.74	112.79	108.20
54	BA	645	C	C2-N3-C4	-5.74	117.03	119.90
54	BA	784	G	N1-C6-O6	-5.74	116.46	119.90
54	BA	1356	G	O4'-C1'-N9	5.74	112.79	108.20
54	BA	1588	G	C5-C6-N1	5.74	114.37	111.50
54	BA	2667	C	N3-C2-O2	-5.74	117.89	121.90
54	BA	2891	U	C5-C6-N1	-5.74	119.83	122.70
21	AA	45	G	C5-C6-N1	5.73	114.37	111.50
32	BJ	95	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	469	G	N1-C6-O6	-5.73	116.46	119.90
54	BA	669	G	C3'-C2'-C1'	5.73	106.09	101.50
21	AA	722	G	C5-C6-N1	5.73	114.37	111.50
21	AA	966	G	N1-C6-O6	-5.73	116.46	119.90
54	BA	45	G	N1-C6-O6	-5.73	116.46	119.90
54	BA	802	A	N1-C6-N6	-5.73	115.16	118.60
54	BA	1386	C	N3-C4-C5	5.73	124.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1463	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2301	C	O4'-C1'-N1	5.73	112.79	108.20
54	BA	2321	U	N1-C2-N3	5.73	118.34	114.90
21	AA	221	C	C5'-C4'-O4'	5.73	115.98	109.10
21	AA	316	C	C3'-C2'-C1'	5.73	106.08	101.50
21	AA	501	C	N1-C2-O2	5.73	122.34	118.90
23	A2	89	U	C5-C6-N1	-5.73	119.83	122.70
54	BA	140	C	N1-C2-O2	5.73	122.34	118.90
54	BA	441	U	C4'-C3'-C2'	-5.73	96.87	102.60
54	BA	474	G	N3-C4-C5	-5.73	125.73	128.60
54	BA	1082	U	O4'-C1'-N1	5.73	112.78	108.20
54	BA	1460	U	O4'-C1'-N1	5.73	112.78	108.20
21	AA	1492	A	C5-C6-N1	5.73	120.56	117.70
54	BA	238	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2112	G	N7-C8-N9	5.73	115.97	113.10
54	BA	2765	A	C5-C6-N1	5.73	120.56	117.70
4	AE	156	ARG	NE-CZ-NH1	5.73	123.16	120.30
21	AA	838	G	N1-C6-O6	-5.73	116.46	119.90
21	AA	1285	A	C6-C5-N7	5.73	136.31	132.30
54	BA	316	C	N3-C4-C5	5.73	124.19	121.90
54	BA	624	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	735	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	1063	G	C1'-O4'-C4'	-5.73	105.32	109.90
21	AA	130	A	C6-C5-N7	5.73	136.31	132.30
21	AA	936	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	1150	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	2348	U	O4'-C1'-N1	5.73	112.78	108.20
21	AA	665	A	C6-C5-N7	5.72	136.31	132.30
21	AA	1369	C	N1-C2-O2	5.72	122.33	118.90
21	AA	1499	A	C5-C6-N1	5.72	120.56	117.70
54	BA	1583	A	C5-C6-N1	5.72	120.56	117.70
54	BA	1748	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	1964	G	O4'-C1'-N9	5.72	112.78	108.20
54	BA	2362	C	N3-C4-N4	-5.72	113.99	118.00
54	BA	2782	G	N7-C8-N9	5.72	115.96	113.10
2	AC	39	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	AC	64	ARG	NE-CZ-NH1	5.72	123.16	120.30
21	AA	263	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	495	A	C5'-C4'-C3'	-5.72	106.84	116.00
21	AA	582	C	N3-C4-C5	5.72	124.19	121.90
21	AA	808	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	865	C	N3-C2-O2	-5.72	117.89	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1089	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1102	C	N1-C2-O2	5.72	122.33	118.90
54	BA	1435	G	N7-C8-N9	5.72	115.96	113.10
54	BA	2018	G	N3-C4-C5	-5.72	125.74	128.60
54	BA	2082	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2854	G	N1-C6-O6	-5.72	116.47	119.90
12	AM	108	ARG	NE-CZ-NH1	5.72	123.16	120.30
21	AA	121	U	O4'-C1'-N1	5.72	112.78	108.20
24	A3	5	G	N7-C8-N9	5.72	115.96	113.10
54	BA	73	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	473	G	N7-C8-N9	5.72	115.96	113.10
21	AA	61	G	N3-C4-C5	-5.72	125.74	128.60
21	AA	72	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	128	G	O4'-C1'-N9	5.72	112.78	108.20
34	BL	41	ARG	NE-CZ-NH2	-5.72	117.44	120.30
54	BA	621	A	C5'-C4'-C3'	-5.72	106.85	116.00
54	BA	732	C	N1-C2-O2	5.72	122.33	118.90
54	BA	1544	A	C5'-C4'-O4'	5.72	115.96	109.10
54	BA	1901	A	C5-C6-N1	5.72	120.56	117.70
54	BA	2007	U	O4'-C1'-N1	5.72	112.78	108.20
54	BA	322	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1397	U	N1-C2-N3	5.72	118.33	114.90
21	AA	340	U	N3-C2-O2	-5.72	118.20	122.20
21	AA	350	G	C5-C6-N1	5.72	114.36	111.50
21	AA	814	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	744	U	O4'-C1'-N1	5.72	112.77	108.20
54	BA	1668	A	C5-C6-N1	5.72	120.56	117.70
54	BA	2375	G	C5-C6-N1	5.72	114.36	111.50
54	BA	2611	C	O4'-C1'-N1	5.72	112.77	108.20
14	AO	83	ARG	NE-CZ-NH1	5.71	123.16	120.30
21	AA	703	G	C5-C6-N1	5.71	114.36	111.50
21	AA	1080	A	C5-N7-C8	-5.71	101.04	103.90
21	AA	1109	C	N3-C4-C5	5.71	124.19	121.90
23	A2	87	U	N3-C2-O2	-5.71	118.20	122.20
54	BA	68	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	131	A	N1-C6-N6	-5.71	115.17	118.60
54	BA	959	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1527	G	N3-C4-C5	-5.71	125.74	128.60
26	BD	169	ARG	NE-CZ-NH1	5.71	123.16	120.30
21	AA	1101	A	O4'-C1'-N9	5.71	112.77	108.20
54	BA	472	A	N1-C6-N6	-5.71	115.17	118.60
54	BA	647	G	N3-C4-C5	-5.71	125.74	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1100	C	O4'-C1'-N1	5.71	112.77	108.20
21	AA	676	A	C6-C5-N7	5.71	136.30	132.30
21	AA	1344	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	651	G	C8-N9-C4	-5.71	104.12	106.40
54	BA	886	A	C4'-C3'-C2'	-5.71	96.89	102.60
54	BA	2880	C	N1-C2-O2	5.71	122.33	118.90
21	AA	842	U	O4'-C4'-C3'	5.71	110.67	106.10
22	A1	1	G	N3-C4-C5	-5.71	125.75	128.60
54	BA	457	A	C3'-C2'-C1'	-5.71	96.93	101.50
54	BA	479	A	C6-C5-N7	5.71	136.30	132.30
54	BA	1181	U	O4'-C1'-N1	5.71	112.77	108.20
54	BA	1851	U	O4'-C1'-N1	5.71	112.77	108.20
54	BA	2180	U	O4'-C1'-N1	5.71	112.77	108.20
54	BA	2355	G	N9-C4-C5	5.71	107.68	105.40
54	BA	2626	C	N3-C2-O2	-5.71	117.91	121.90
21	AA	8	A	C4-C5-C6	-5.71	114.15	117.00
21	AA	1432	G	C8-N9-C4	-5.71	104.12	106.40
54	BA	343	C	N3-C2-O2	-5.71	117.91	121.90
54	BA	343	C	N3-C4-C5	5.71	124.18	121.90
54	BA	1519	G	C8-N9-C4	-5.71	104.12	106.40
54	BA	1738	G	N7-C8-N9	5.71	115.95	113.10
55	BB	88	C	N3-C2-O2	-5.71	117.91	121.90
21	AA	275	G	N9-C4-C5	5.71	107.68	105.40
21	AA	1465	A	N1-C6-N6	-5.71	115.18	118.60
54	BA	111	A	C5-C6-N1	5.71	120.55	117.70
54	BA	1073	A	C6-C5-N7	5.71	136.29	132.30
54	BA	1775	U	O4'-C1'-N1	5.71	112.76	108.20
21	AA	108	G	O4'-C1'-N9	5.70	112.76	108.20
21	AA	847	G	C5-C6-N1	5.70	114.35	111.50
21	AA	1061	G	C8-N9-C4	-5.70	104.12	106.40
21	AA	1472	U	N1-C2-N3	5.70	118.32	114.90
54	BA	93	G	N3-C4-C5	-5.70	125.75	128.60
54	BA	418	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	635	C	N1-C2-O2	5.70	122.32	118.90
54	BA	1320	C	N3-C4-C5	5.70	124.18	121.90
54	BA	2443	C	C5'-C4'-O4'	5.70	115.94	109.10
54	BA	2544	G	N3-C4-C5	-5.70	125.75	128.60
55	BB	81	G	C5-C6-N1	5.70	114.35	111.50
54	BA	1125	G	C5-C6-N1	5.70	114.35	111.50
21	AA	1141	C	N3-C4-C5	5.70	124.18	121.90
54	BA	83	A	C6-C5-N7	5.70	136.29	132.30
54	BA	601	C	N1-C2-O2	5.70	122.32	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2368	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	2428	G	C8-N9-C4	-5.70	104.12	106.40
21	AA	466	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	732	C	N1-C2-O2	5.70	122.32	118.90
22	A1	53	G	N1-C6-O6	-5.70	116.48	119.90
54	BA	359	G	N3-C4-C5	-5.70	125.75	128.60
54	BA	1430	G	C8-N9-C4	-5.70	104.12	106.40
26	BD	59	ARG	NE-CZ-NH2	-5.70	117.45	120.30
54	BA	1830	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	2611	C	C6-N1-C2	-5.70	118.02	120.30
55	BB	97	C	N1-C2-O2	5.70	122.32	118.90
21	AA	202	G	C5-C6-N1	5.70	114.35	111.50
21	AA	327	A	C5-C6-N1	5.70	120.55	117.70
54	BA	707	G	C5-C6-N1	5.70	114.35	111.50
54	BA	715	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2230	G	C5-C6-N1	5.70	114.35	111.50
21	AA	573	A	C6-C5-N7	5.69	136.29	132.30
21	AA	882	C	N1-C2-O2	5.69	122.32	118.90
38	BP	87	ARG	NE-CZ-NH1	5.69	123.15	120.30
54	BA	270	A	C6-C5-N7	5.69	136.29	132.30
54	BA	1633	G	N1-C6-O6	-5.69	116.48	119.90
21	AA	1500	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	1408	G	N1-C6-O6	-5.69	116.48	119.90
54	BA	2694	G	C5-C6-N1	5.69	114.35	111.50
2	AC	87	ARG	NE-CZ-NH1	5.69	123.14	120.30
21	AA	164	G	N1-C6-O6	-5.69	116.49	119.90
21	AA	391	G	N3-C4-C5	-5.69	125.75	128.60
21	AA	531	U	C5-C6-N1	-5.69	119.86	122.70
21	AA	1115	U	N1-C2-N3	5.69	118.31	114.90
21	AA	1156	G	N3-C4-C5	-5.69	125.75	128.60
32	BJ	34	ARG	NE-CZ-NH1	5.69	123.14	120.30
54	BA	584	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	652	U	N1-C2-N3	5.69	118.31	114.90
54	BA	2824	C	O4'-C1'-N1	5.69	112.75	108.20
54	BA	54	G	N3-C4-C5	-5.69	125.75	128.60
54	BA	1740	G	N1-C6-O6	-5.69	116.49	119.90
54	BA	2374	C	N3-C4-C5	5.69	124.18	121.90
54	BA	2638	G	N1-C6-O6	-5.69	116.49	119.90
21	AA	708	C	O4'-C1'-N1	5.69	112.75	108.20
54	BA	296	U	C5-C6-N1	-5.69	119.86	122.70
54	BA	1311	G	N1-C6-O6	-5.69	116.49	119.90
54	BA	2364	C	N1-C2-O2	5.69	122.31	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	416	G	C5-C6-N1	5.69	114.34	111.50
54	BA	1928	A	N1-C6-N6	-5.69	115.19	118.60
21	AA	372	C	N1-C2-O2	5.68	122.31	118.90
21	AA	815	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	923	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	1219	A	C4-C5-C6	-5.68	114.16	117.00
46	BX	56	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	277	G	O4'-C1'-N9	5.68	112.75	108.20
54	BA	1024	G	O4'-C1'-N9	5.68	112.75	108.20
54	BA	1081	U	N1-C2-N3	5.68	118.31	114.90
54	BA	2565	A	C5-C6-N1	5.68	120.54	117.70
54	BA	2566	A	N1-C6-N6	-5.68	115.19	118.60
55	BB	25	U	N1-C2-N3	5.68	118.31	114.90
13	AN	41	ARG	NE-CZ-NH2	-5.68	117.46	120.30
22	A1	57	G	C5-C6-N1	5.68	114.34	111.50
24	A3	7	G	N1-C6-O6	-5.68	116.49	119.90
30	BH	97	ARG	NE-CZ-NH1	5.68	123.14	120.30
40	BR	90	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	503	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	599	A	C6-C5-N7	5.68	136.28	132.30
54	BA	797	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	848	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	1005	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	1390	U	O4'-C1'-N1	5.68	112.75	108.20
54	BA	1790	C	N3-C2-O2	-5.68	117.92	121.90
8	AI	98	ARG	NH1-CZ-NH2	-5.68	113.15	119.40
21	AA	1533	C	P-O3'-C3'	5.68	126.52	119.70
54	BA	40	U	N1-C2-N3	5.68	118.31	114.90
54	BA	1496	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	660	C	N3-C2-O2	-5.68	117.92	121.90
21	AA	664	G	N1-C6-O6	-5.68	116.49	119.90
21	AA	754	C	N1-C2-O2	5.68	122.31	118.90
21	AA	1397	C	N1-C2-O2	5.68	122.31	118.90
21	AA	1428	A	C6-C5-N7	5.68	136.28	132.30
54	BA	577	G	C5-C6-N1	5.68	114.34	111.50
54	BA	1677	A	N7-C8-N9	5.68	116.64	113.80
54	BA	2233	U	O4'-C1'-N1	5.68	112.74	108.20
54	BA	2301	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	2702	G	N3-C2-N2	-5.68	115.92	119.90
54	BA	2738	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	735	C	N3-C2-O2	-5.68	117.93	121.90
21	AA	1014	A	C5-C6-N1	5.68	120.54	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1071	C	O4'-C1'-N1	5.68	112.74	108.20
21	AA	1487	G	N9-C4-C5	5.68	107.67	105.40
54	BA	25	U	C5-C6-N1	-5.68	119.86	122.70
54	BA	25	U	N3-C2-O2	-5.68	118.23	122.20
54	BA	316	C	O4'-C1'-N1	5.68	112.74	108.20
54	BA	650	C	N3-C2-O2	-5.68	117.93	121.90
54	BA	668	A	C5-C6-N1	5.68	120.54	117.70
54	BA	1147	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1267	U	O4'-C1'-N1	5.68	112.74	108.20
54	BA	2117	A	N1-C6-N6	-5.68	115.19	118.60
21	AA	1426	G	N7-C8-N9	5.67	115.94	113.10
22	A1	18	G	N3-C4-C5	-5.67	125.76	128.60
54	BA	1881	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	236	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	542	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	556	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	2473	U	O4'-C1'-N1	5.67	112.74	108.20
21	AA	1277	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	100	U	C5-C6-N1	-5.67	119.86	122.70
54	BA	409	G	N7-C8-N9	5.67	115.94	113.10
54	BA	915	C	N1-C2-O2	5.67	122.30	118.90
54	BA	2063	C	C2-N3-C4	-5.67	117.06	119.90
54	BA	2401	U	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2577	A	C5-C6-N1	5.67	120.54	117.70
21	AA	925	G	N3-C4-C5	-5.67	125.77	128.60
54	BA	31	C	N3-C4-C5	5.67	124.17	121.90
54	BA	2743	U	C5'-C4'-O4'	5.67	115.91	109.10
55	BB	117	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	1027	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	1046	A	C6-C5-N7	5.67	136.27	132.30
21	AA	1504	G	C1'-O4'-C4'	-5.67	105.36	109.90
54	BA	806	C	N1-C2-O2	5.67	122.30	118.90
54	BA	814	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	1817	G	N1-C6-O6	-5.67	116.50	119.90
54	BA	2862	G	N3-C4-C5	-5.67	125.77	128.60
21	AA	124	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	705	G	C6-C5-N7	5.67	133.80	130.40
21	AA	796	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2525	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	239	U	N3-C2-O2	-5.67	118.23	122.20
54	BA	2039	U	N3-C2-O2	-5.67	118.23	122.20
21	AA	496	A	C8-N9-C4	-5.66	103.53	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1624	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	1681	G	O4'-C1'-N9	5.66	112.73	108.20
54	BA	1864	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	1895	C	N1-C2-O2	5.66	122.30	118.90
24	A3	71	G	C8-N9-C4	-5.66	104.14	106.40
54	BA	2798	U	O4'-C1'-N1	5.66	112.73	108.20
21	AA	709	U	N1-C2-N3	5.66	118.30	114.90
21	AA	1041	G	N9-C4-C5	5.66	107.66	105.40
21	AA	1098	C	N1-C2-O2	5.66	122.30	118.90
21	AA	1434	A	C6-C5-N7	5.66	136.26	132.30
21	AA	1520	C	C6-N1-C2	-5.66	118.03	120.30
54	BA	237	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1946	U	C5-C6-N1	-5.66	119.87	122.70
54	BA	2074	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	2222	C	N3-C4-C5	5.66	124.16	121.90
54	BA	2903	U	O4'-C1'-N1	5.66	112.73	108.20
21	AA	1210	C	N1-C2-O2	5.66	122.30	118.90
46	BX	36	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	40	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	1319	C	N1-C2-O2	5.66	122.30	118.90
55	BB	71	C	O4'-C1'-N1	5.66	112.73	108.20
54	BA	1127	A	C5-C6-N1	5.66	120.53	117.70
55	BB	19	C	N3-C4-C5	5.66	124.16	121.90
21	AA	719	C	N1-C2-O2	5.66	122.29	118.90
21	AA	1416	G	N1-C6-O6	-5.66	116.51	119.90
54	BA	274	C	O4'-C1'-N1	5.66	112.72	108.20
54	BA	738	G	O4'-C1'-N9	5.66	112.72	108.20
54	BA	833	A	O4'-C1'-N9	5.66	112.72	108.20
54	BA	1237	A	C5-C6-N1	5.66	120.53	117.70
54	BA	1694	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	2802	G	C5-C6-N1	5.66	114.33	111.50
21	AA	559	A	O4'-C1'-N9	5.65	112.72	108.20
21	AA	586	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	760	G	N1-C6-O6	-5.65	116.51	119.90
21	AA	1411	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	2362	C	N1-C2-O2	5.65	122.29	118.90
21	AA	393	A	C5-C6-N1	5.65	120.53	117.70
21	AA	741	G	C8-N9-C4	-5.65	104.14	106.40
21	AA	901	A	C4-C5-C6	-5.65	114.17	117.00
34	BL	60	ARG	NE-CZ-NH1	5.65	123.13	120.30
51	B2	12	ARG	NE-CZ-NH1	5.65	123.13	120.30
54	BA	507	A	C4-C5-C6	-5.65	114.17	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	731	C	N1-C2-O2	5.65	122.29	118.90
54	BA	1647	U	N3-C2-O2	-5.65	118.24	122.20
54	BA	1747	U	C5-C6-N1	-5.65	119.87	122.70
54	BA	2291	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	2742	G	N1-C6-O6	-5.65	116.51	119.90
21	AA	356	A	C2-N3-C4	5.65	113.43	110.60
24	A3	41	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	123	G	N1-C6-O6	-5.65	116.51	119.90
54	BA	301	G	N1-C6-O6	-5.65	116.51	119.90
54	BA	1715	G	C5-C6-N1	5.65	114.33	111.50
54	BA	1836	C	C3'-C2'-C1'	5.65	106.02	101.50
55	BB	84	G	N3-C2-N2	-5.65	115.94	119.90
21	AA	582	C	N3-C2-O2	-5.65	117.95	121.90
54	BA	161	A	C6-C5-N7	5.65	136.25	132.30
54	BA	1234	U	C5-C6-N1	-5.65	119.88	122.70
54	BA	1419	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	2123	G	N9-C4-C5	5.65	107.66	105.40
54	BA	2324	U	N3-C2-O2	-5.65	118.25	122.20
21	AA	433	G	N3-C2-N2	-5.65	115.95	119.90
54	BA	358	U	N1-C2-N3	5.65	118.29	114.90
54	BA	718	A	C2-N3-C4	5.65	113.42	110.60
54	BA	1429	G	N7-C8-N9	5.65	115.92	113.10
54	BA	1667	G	N9-C4-C5	5.65	107.66	105.40
54	BA	1751	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	2056	G	C5-C6-N1	5.65	114.32	111.50
54	BA	2380	C	N1-C2-O2	5.65	122.29	118.90
21	AA	1066	C	N3-C4-C5	5.65	124.16	121.90
24	A3	64	G	N7-C8-N9	5.65	115.92	113.10
54	BA	1711	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	2708	G	N9-C4-C5	5.65	107.66	105.40
21	AA	429	U	C5-C6-N1	-5.64	119.88	122.70
21	AA	519	C	N1-C2-O2	5.64	122.29	118.90
21	AA	1441	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	8	C	O4'-C1'-N1	5.64	112.72	108.20
54	BA	153	U	O4'-C1'-N1	5.64	112.72	108.20
54	BA	1071	G	C5'-C4'-C3'	-5.64	106.97	116.00
54	BA	1253	A	C5'-C4'-C3'	-5.64	106.97	116.00
54	BA	1345	C	N3-C4-C5	5.64	124.16	121.90
54	BA	1579	A	N1-C6-N6	-5.64	115.21	118.60
54	BA	1992	G	C5-C6-N1	5.64	114.32	111.50
54	BA	2072	C	O4'-C1'-N1	5.64	112.72	108.20
21	AA	290	C	N1-C2-O2	5.64	122.29	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	295	C	C1'-O4'-C4'	-5.64	105.39	109.90
21	AA	1166	G	C3'-C2'-C1'	5.64	106.01	101.50
21	AA	1450	U	C5-C6-N1	-5.64	119.88	122.70
54	BA	315	G	N1-C6-O6	-5.64	116.51	119.90
54	BA	1490	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1738	G	C8-N9-C4	-5.64	104.14	106.40
54	BA	1767	G	N1-C6-O6	-5.64	116.52	119.90
54	BA	66	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1481	U	C5-C6-N1	-5.64	119.88	122.70
54	BA	2073	C	C5'-C4'-O4'	5.64	115.87	109.10
54	BA	2246	G	C5-C6-N1	5.64	114.32	111.50
21	AA	315	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	2731	G	N3-C4-C5	-5.64	125.78	128.60
54	BA	2751	G	N3-C4-C5	-5.64	125.78	128.60
55	BB	102	G	C5-C6-N1	5.64	114.32	111.50
55	BB	104	A	N1-C6-N6	-5.64	115.22	118.60
21	AA	1527	U	C5-C6-N1	-5.64	119.88	122.70
54	BA	382	A	O4'-C1'-N9	5.64	112.71	108.20
54	BA	1941	C	N1-C2-O2	5.64	122.28	118.90
21	AA	551	U	N3-C2-O2	-5.64	118.25	122.20
21	AA	689	C	O4'-C1'-N1	5.64	112.71	108.20
21	AA	1461	G	O4'-C1'-N9	5.64	112.71	108.20
22	A1	62	C	N1-C2-O2	5.64	122.28	118.90
54	BA	963	U	O4'-C1'-N1	5.64	112.71	108.20
54	BA	1925	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2095	A	C4'-C3'-C2'	-5.64	96.96	102.60
54	BA	2179	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2859	G	C5-C6-N1	5.64	114.32	111.50
55	BB	93	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	1524	G	C5-C6-N1	5.63	114.32	111.50
54	BA	1598	A	C4-C5-C6	-5.63	114.18	117.00
55	BB	71	C	N1-C2-O2	5.63	122.28	118.90
55	BB	111	U	C5-C6-N1	-5.63	119.88	122.70
21	AA	253	A	C4-C5-C6	-5.63	114.18	117.00
21	AA	385	C	C6-N1-C2	-5.63	118.05	120.30
21	AA	523	A	C6-C5-N7	5.63	136.24	132.30
24	A3	59	A	N1-C6-N6	-5.63	115.22	118.60
54	BA	218	A	C6-C5-N7	5.63	136.24	132.30
54	BA	2161	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	2263	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	2450	A	C4-C5-C6	-5.63	114.18	117.00
55	BB	60	C	O4'-C1'-N1	5.63	112.71	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1150	A	C5-C6-N1	5.63	120.52	117.70
21	AA	1333	A	C5-C6-N1	5.63	120.52	117.70
21	AA	1516	G	N3-C2-N2	-5.63	115.96	119.90
39	BQ	5	ARG	NE-CZ-NH1	5.63	123.12	120.30
54	BA	167	A	C5-C6-N1	5.63	120.52	117.70
54	BA	180	G	N9-C4-C5	5.63	107.65	105.40
54	BA	1694	C	N1-C2-O2	5.63	122.28	118.90
54	BA	2393	U	N3-C2-O2	-5.63	118.26	122.20
55	BB	59	A	C5-C6-N1	5.63	120.52	117.70
21	AA	292	G	C8-N9-C4	-5.63	104.15	106.40
23	A2	93	U	C5-C6-N1	-5.63	119.89	122.70
28	BF	29	ARG	NE-CZ-NH1	5.63	123.11	120.30
54	BA	1038	G	C5-C6-N1	5.63	114.31	111.50
54	BA	1574	C	N3-C2-O2	-5.63	117.96	121.90
21	AA	40	C	N1-C2-O2	5.63	122.28	118.90
21	AA	340	U	C3'-C2'-C1'	5.63	106.00	101.50
54	BA	724	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	893	C	O4'-C1'-N1	5.63	112.70	108.20
54	BA	1350	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	1402	U	N1-C2-N3	5.63	118.28	114.90
54	BA	2268	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	2895	G	C5-C6-N1	5.63	114.31	111.50
54	BA	1172	C	N1-C2-O2	5.63	122.28	118.90
54	BA	1410	G	C5-C6-N1	5.63	114.31	111.50
54	BA	2180	U	N1-C2-N3	5.63	118.28	114.90
54	BA	2279	G	N3-C2-N2	-5.63	115.96	119.90
21	AA	803	G	C5-C6-N1	5.62	114.31	111.50
54	BA	2508	G	C5-C6-N1	5.62	114.31	111.50
54	BA	2808	G	N3-C4-C5	-5.62	125.79	128.60
54	BA	2850	A	C5-C6-N1	5.62	120.51	117.70
21	AA	271	C	N1-C2-O2	5.62	122.27	118.90
21	AA	364	A	C6-C5-N7	5.62	136.24	132.30
21	AA	629	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	942	G	C5-C6-N1	5.62	114.31	111.50
54	BA	770	G	C5-C6-N1	5.62	114.31	111.50
54	BA	1346	G	N3-C2-N2	-5.62	115.96	119.90
54	BA	1766	G	O4'-C1'-N9	5.62	112.70	108.20
54	BA	2366	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2569	G	N1-C6-O6	-5.62	116.53	119.90
21	AA	490	C	N3-C4-C5	5.62	124.15	121.90
21	AA	1417	G	C5-C6-N1	5.62	114.31	111.50
24	A3	40	C	N3-C2-O2	-5.62	117.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	68	C	N3-C4-C5	5.62	124.15	121.90
54	BA	613	A	O4'-C1'-N9	5.62	112.70	108.20
54	BA	711	G	N1-C6-O6	-5.62	116.53	119.90
54	BA	1776	G	C5'-C4'-C3'	-5.62	107.01	116.00
21	AA	622	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	824	G	C8-N9-C4	-5.62	104.15	106.40
21	AA	1178	G	C5-C6-N1	5.62	114.31	111.50
34	BL	21	ARG	NE-CZ-NH1	5.62	123.11	120.30
54	BA	120	U	O4'-C1'-N1	5.62	112.70	108.20
21	AA	490	C	O4'-C1'-N1	5.62	112.70	108.20
21	AA	728	A	C6-C5-N7	5.62	136.23	132.30
21	AA	1105	A	C6-C5-N7	5.62	136.23	132.30
21	AA	1271	A	C4-C5-C6	-5.62	114.19	117.00
48	BZ	44	ARG	NE-CZ-NH1	5.62	123.11	120.30
54	BA	55	G	C5-C6-N1	5.62	114.31	111.50
54	BA	135	U	C5-C6-N1	-5.62	119.89	122.70
54	BA	1236	G	N3-C2-N2	-5.62	115.97	119.90
54	BA	1542	U	O4'-C1'-N1	5.62	112.69	108.20
54	BA	2545	G	N3-C4-C5	-5.62	125.79	128.60
54	BA	2802	G	N3-C4-C5	-5.62	125.79	128.60
21	AA	451	A	P-O3'-C3'	5.62	126.44	119.70
54	BA	1517	G	C5-C6-N1	5.62	114.31	111.50
21	AA	704	A	C5-C6-N1	5.62	120.51	117.70
21	AA	941	G	N3-C4-C5	-5.62	125.79	128.60
54	BA	820	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2140	G	N1-C6-O6	-5.62	116.53	119.90
21	AA	338	A	C5-C6-N1	5.61	120.51	117.70
21	AA	1070	U	N1-C2-N3	5.61	118.27	114.90
54	BA	1719	G	N3-C4-C5	-5.61	125.79	128.60
54	BA	1793	C	N1-C2-O2	5.61	122.27	118.90
54	BA	2185	U	O4'-C1'-N1	5.61	112.69	108.20
54	BA	2429	G	C5-C6-N1	5.61	114.31	111.50
54	BA	2630	G	C5-C6-N1	5.61	114.31	111.50
55	BB	17	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	923	A	C5-C6-N1	5.61	120.51	117.70
21	AA	975	A	N1-C6-N6	-5.61	115.23	118.60
54	BA	199	A	N1-C6-N6	-5.61	115.23	118.60
54	BA	2403	C	O4'-C1'-N1	5.61	112.69	108.20
24	A3	32	G	N1-C6-O6	-5.61	116.53	119.90
54	BA	346	A	O4'-C1'-N9	5.61	112.69	108.20
54	BA	394	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1960	A	C4-C5-C6	-5.61	114.20	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2385	C	N3-C4-C5	5.61	124.14	121.90
21	AA	97	G	C5-C6-N1	5.61	114.30	111.50
54	BA	203	A	C8-N9-C4	-5.61	103.56	105.80
54	BA	863	A	C5-C6-N1	5.61	120.50	117.70
21	AA	1306	A	N1-C6-N6	-5.61	115.24	118.60
22	A1	17	U	N1-C2-N3	5.61	118.26	114.90
53	B4	36	ARG	NE-CZ-NH2	-5.61	117.50	120.30
54	BA	159	G	N3-C4-C5	-5.61	125.80	128.60
54	BA	1478	G	N7-C8-N9	5.61	115.90	113.10
54	BA	1997	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	2455	G	N3-C4-C5	-5.61	125.80	128.60
54	BA	2547	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	787	A	C5-C6-N1	5.60	120.50	117.70
54	BA	792	A	C6-C5-N7	5.60	136.22	132.30
54	BA	2896	C	N3-C2-O2	-5.60	117.98	121.90
21	AA	19	A	C5-C6-N1	5.60	120.50	117.70
21	AA	193	C	N1-C2-O2	5.60	122.26	118.90
21	AA	1509	C	N3-C4-N4	-5.60	114.08	118.00
54	BA	240	C	N1-C2-O2	5.60	122.26	118.90
54	BA	1029	A	O4'-C1'-N9	5.60	112.68	108.20
54	BA	1036	G	N1-C6-O6	-5.60	116.54	119.90
54	BA	1943	U	O4'-C1'-N1	5.60	112.68	108.20
54	BA	2759	G	N3-C2-N2	-5.60	115.98	119.90
54	BA	2767	C	N1-C2-O2	5.60	122.26	118.90
54	BA	2829	A	C6-C5-N7	5.60	136.22	132.30
54	BA	786	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	2253	G	N3-C2-N2	-5.60	115.98	119.90
54	BA	2612	C	N1-C2-O2	5.60	122.26	118.90
54	BA	2721	A	O4'-C1'-N9	5.60	112.68	108.20
21	AA	453	G	N9-C4-C5	5.60	107.64	105.40
54	BA	239	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	1265	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	97	G	N1-C6-O6	-5.60	116.54	119.90
21	AA	490	C	C2-N3-C4	-5.60	117.10	119.90
21	AA	1191	A	C6-C5-N7	5.60	136.22	132.30
54	BA	1760	C	C2-N3-C4	-5.60	117.10	119.90
55	BB	54	G	C5-C6-N1	5.60	114.30	111.50
21	AA	1365	G	N7-C8-N9	5.60	115.90	113.10
54	BA	2092	U	C5-C6-N1	-5.60	119.90	122.70
54	BA	2499	C	N3-C2-O2	-5.60	117.98	121.90
21	AA	776	G	C8-N9-C4	-5.59	104.16	106.40
54	BA	321	U	O4'-C1'-N1	5.59	112.68	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	359	G	N1-C6-O6	-5.59	116.54	119.90
54	BA	1418	G	C5-C6-N1	5.59	114.30	111.50
54	BA	1795	C	N3-C2-O2	-5.59	117.98	121.90
54	BA	2482	A	C4-C5-C6	-5.59	114.20	117.00
3	AD	80	ARG	NE-CZ-NH1	5.59	123.10	120.30
54	BA	67	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	74	A	N1-C6-N6	-5.59	115.24	118.60
54	BA	1880	U	C5-C6-N1	-5.59	119.90	122.70
21	AA	172	A	C2-N3-C4	5.59	113.40	110.60
21	AA	1439	G	N1-C6-O6	-5.59	116.55	119.90
21	AA	1471	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	564	C	C5'-C4'-O4'	5.59	115.81	109.10
54	BA	627	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	1597	A	C4-C5-C6	-5.59	114.20	117.00
21	AA	426	U	N3-C2-O2	-5.59	118.29	122.20
21	AA	624	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	910	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	1043	C	N1-C2-O2	5.59	122.25	118.90
54	BA	1254	A	C3'-C2'-C1'	5.59	105.97	101.50
54	BA	1314	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	1442	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	1980	G	N1-C6-O6	-5.59	116.55	119.90
54	BA	2232	C	C5'-C4'-O4'	5.59	115.81	109.10
54	BA	2306	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2597	G	C8-N9-C4	-5.59	104.16	106.40
54	BA	2756	U	C5-C6-N1	-5.59	119.91	122.70
21	AA	831	A	C4-C5-C6	-5.59	114.21	117.00
21	AA	1121	U	N3-C2-O2	-5.59	118.29	122.20
30	BH	123	ARG	NE-CZ-NH1	5.59	123.09	120.30
54	BA	393	C	N1-C2-O2	5.59	122.25	118.90
54	BA	1933	G	N9-C4-C5	5.59	107.64	105.40
54	BA	2706	A	C4-C5-C6	-5.59	114.21	117.00
21	AA	106	C	O4'-C1'-N1	5.59	112.67	108.20
21	AA	198	G	C5-C6-N1	5.59	114.29	111.50
21	AA	568	G	C8-N9-C4	-5.59	104.17	106.40
54	BA	1992	G	N3-C4-C5	-5.59	125.81	128.60
54	BA	2014	A	C5-C6-N1	5.59	120.49	117.70
54	BA	2065	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2263	C	C6-N1-C2	-5.59	118.06	120.30
54	BA	2308	G	N3-C4-C5	-5.59	125.81	128.60
54	BA	2651	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1306	A	C4-C5-C6	-5.58	114.21	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	537	G	N3-C4-C5	-5.58	125.81	128.60
21	AA	94	G	O4'-C1'-N9	5.58	112.67	108.20
21	AA	1227	A	C5-C6-N1	5.58	120.49	117.70
54	BA	558	U	O4'-C1'-N1	5.58	112.67	108.20
54	BA	1215	G	N3-C2-N2	-5.58	115.99	119.90
54	BA	1583	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	123	U	O4'-C1'-N1	5.58	112.67	108.20
21	AA	1406	U	C5-C6-N1	-5.58	119.91	122.70
54	BA	274	C	N1-C2-O2	5.58	122.25	118.90
21	AA	535	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	1524	C	N3-C4-C5	5.58	124.13	121.90
22	A1	1	G	C8-N9-C4	-5.58	104.17	106.40
54	BA	728	G	N7-C8-N9	5.58	115.89	113.10
54	BA	1171	G	N1-C6-O6	-5.58	116.55	119.90
54	BA	1665	A	C6-C5-N7	5.58	136.20	132.30
54	BA	1692	U	N1-C2-N3	5.58	118.25	114.90
54	BA	2015	A	C5-C6-N1	5.58	120.49	117.70
54	BA	2462	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	2752	C	O4'-C1'-N1	5.58	112.66	108.20
55	BB	112	G	N1-C6-O6	-5.58	116.55	119.90
21	AA	84	U	O4'-C1'-N1	5.58	112.66	108.20
21	AA	1029	U	N1-C2-N3	5.58	118.25	114.90
21	AA	1170	A	C6-C5-N7	5.58	136.20	132.30
54	BA	741	U	C5-C6-N1	-5.58	119.91	122.70
54	BA	1989	G	N7-C8-N9	5.58	115.89	113.10
21	AA	455	G	C5-N7-C8	-5.58	101.51	104.30
54	BA	545	U	C5-C6-N1	-5.58	119.91	122.70
54	BA	585	G	N7-C8-N9	5.58	115.89	113.10
54	BA	1415	U	C5-C6-N1	-5.58	119.91	122.70
54	BA	1465	G	C5-C6-N1	5.58	114.29	111.50
54	BA	1630	A	C6-C5-N7	5.58	136.20	132.30
21	AA	157	U	N3-C2-O2	-5.57	118.30	122.20
21	AA	785	G	C5-C6-N1	5.57	114.29	111.50
21	AA	936	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	193	U	N1-C2-N3	5.57	118.24	114.90
54	BA	209	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	372	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	587	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	694	U	N3-C2-O2	-5.57	118.30	122.20
54	BA	775	G	O4'-C1'-N9	5.57	112.66	108.20
54	BA	1370	C	N1-C2-O2	5.57	122.25	118.90
54	BA	2323	G	C8-N9-C4	-5.57	104.17	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2538	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	2770	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	130	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	983	A	C4-C5-C6	-5.57	114.21	117.00
54	BA	1792	G	C5-C6-N1	5.57	114.29	111.50
54	BA	861	A	C6-C5-N7	5.57	136.20	132.30
54	BA	1259	G	C5-C6-N1	5.57	114.29	111.50
54	BA	1531	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	998	C	N1-C2-O2	5.57	122.24	118.90
22	A1	43	G	C5-C6-N1	5.57	114.28	111.50
54	BA	894	U	N3-C2-O2	-5.57	118.30	122.20
54	BA	2663	G	N3-C4-C5	-5.57	125.82	128.60
54	BA	2902	C	N1-C2-O2	5.57	122.24	118.90
23	A2	91	A	C6-C5-N7	5.57	136.20	132.30
54	BA	177	G	N7-C8-N9	5.57	115.88	113.10
54	BA	1208	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	1240	U	C3'-C2'-C1'	5.57	105.95	101.50
54	BA	2520	C	N1-C2-O2	5.57	122.24	118.90
55	BB	42	C	C6-N1-C2	-5.57	118.07	120.30
21	AA	1051	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	1069	C	O4'-C1'-N1	5.57	112.65	108.20
21	AA	1128	C	N1-C2-O2	5.57	122.24	118.90
54	BA	1097	U	C4-C5-C6	5.57	123.04	119.70
54	BA	2393	U	C5-C6-N1	-5.57	119.92	122.70
54	BA	2578	G	N3-C2-N2	-5.57	116.00	119.90
54	BA	2781	A	C6-C5-N7	5.57	136.20	132.30
54	BA	2785	C	N1-C2-O2	5.57	122.24	118.90
56	B5	9	ARG	NE-CZ-NH1	5.57	123.08	120.30
54	BA	53	A	C4'-C3'-C2'	-5.56	97.04	102.60
54	BA	1169	A	N1-C6-N6	-5.56	115.26	118.60
21	AA	312	C	O4'-C1'-N1	5.56	112.65	108.20
21	AA	1176	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	1311	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	1445	U	O4'-C1'-N1	5.56	112.65	108.20
21	AA	1458	G	C5-C6-N1	5.56	114.28	111.50
54	BA	556	A	O4'-C1'-N9	5.56	112.65	108.20
54	BA	873	C	N3-C4-C5	5.56	124.12	121.90
54	BA	1919	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	2802	G	C5'-C4'-O4'	5.56	115.77	109.10
21	AA	535	A	O4'-C4'-C3'	5.56	110.55	106.10
21	AA	605	U	N1-C2-N3	5.56	118.24	114.90
21	AA	1072	G	N1-C6-O6	-5.56	116.56	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BF	101	ARG	NE-CZ-NH1	5.56	123.08	120.30
21	AA	40	C	N3-C4-C5	5.56	124.12	121.90
21	AA	148	G	C2-N3-C4	5.56	114.68	111.90
21	AA	319	G	N1-C6-O6	-5.56	116.56	119.90
21	AA	975	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	1403	C	C6-N1-C2	-5.56	118.08	120.30
21	AA	1432	G	N3-C4-C5	-5.56	125.82	128.60
54	BA	96	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	551	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	867	C	O4'-C1'-N1	5.56	112.65	108.20
21	AA	360	G	N1-C6-O6	-5.56	116.57	119.90
21	AA	463	U	N3-C2-O2	-5.56	118.31	122.20
54	BA	1262	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1701	A	C5-C6-N1	5.56	120.48	117.70
21	AA	1221	G	N1-C6-O6	-5.56	116.57	119.90
54	BA	19	A	C6-C5-N7	5.56	136.19	132.30
54	BA	739	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1832	C	N1-C2-O2	5.56	122.23	118.90
11	AL	82	ARG	NE-CZ-NH2	-5.55	117.52	120.30
21	AA	236	A	C5-C6-N1	5.55	120.48	117.70
21	AA	1442	G	N3-C2-N2	-5.55	116.01	119.90
54	BA	603	A	N1-C6-N6	-5.55	115.27	118.60
54	BA	622	G	N3-C4-C5	-5.55	125.82	128.60
54	BA	679	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1590	A	C5-C6-N1	5.55	120.48	117.70
54	BA	2226	C	N3-C4-C5	5.55	124.12	121.90
54	BA	2480	C	N3-C2-O2	-5.55	118.01	121.90
21	AA	301	G	C5-C6-N1	5.55	114.28	111.50
21	AA	1319	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	286	U	C5-C6-N1	-5.55	119.92	122.70
54	BA	1591	A	N1-C6-N6	-5.55	115.27	118.60
54	BA	2176	A	C6-C5-N7	5.55	136.19	132.30
21	AA	868	C	N1-C2-O2	5.55	122.23	118.90
21	AA	1232	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	725	G	C5-C6-N1	5.55	114.28	111.50
54	BA	1265	A	C5-C6-N1	5.55	120.48	117.70
54	BA	1522	A	C5-C6-N1	5.55	120.48	117.70
54	BA	2349	G	C5-C6-N1	5.55	114.28	111.50
54	BA	2658	C	N1-C2-O2	5.55	122.23	118.90
21	AA	40	C	C2-N3-C4	-5.55	117.12	119.90
21	AA	250	A	C2-N3-C4	5.55	113.37	110.60
21	AA	419	C	N3-C2-O2	-5.55	118.02	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1450	U	N3-C2-O2	-5.55	118.31	122.20
22	A1	67	U	N3-C2-O2	-5.55	118.31	122.20
54	BA	34	U	N1-C2-N3	5.55	118.23	114.90
54	BA	126	A	C5'-C4'-C3'	-5.55	107.12	116.00
21	AA	993	G	N3-C4-C5	-5.55	125.83	128.60
25	BC	257	ARG	NE-CZ-NH1	5.55	123.07	120.30
54	BA	404	A	O4'-C1'-N9	5.55	112.64	108.20
54	BA	656	G	N7-C8-N9	5.55	115.87	113.10
54	BA	1153	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	2232	C	N1-C2-O2	5.55	122.23	118.90
21	AA	222	C	N3-C4-C5	5.55	124.12	121.90
21	AA	342	C	N3-C4-C5	5.55	124.12	121.90
24	A3	71	G	N9-C4-C5	5.55	107.62	105.40
54	BA	177	G	C8-N9-C4	-5.55	104.18	106.40
54	BA	1764	C	C6-N1-C2	-5.55	118.08	120.30
54	BA	2625	G	C5-C6-N1	5.55	114.27	111.50
54	BA	1088	A	C2-N3-C4	5.54	113.37	110.60
54	BA	1562	U	N3-C2-O2	-5.54	118.32	122.20
54	BA	2112	G	N3-C2-N2	-5.54	116.02	119.90
54	BA	2395	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	2879	A	O4'-C1'-N9	5.54	112.64	108.20
21	AA	102	G	C5-C6-N1	5.54	114.27	111.50
21	AA	918	A	C5-C6-N1	5.54	120.47	117.70
21	AA	1169	A	C6-C5-N7	5.54	136.18	132.30
54	BA	752	A	C1'-O4'-C4'	-5.54	105.47	109.90
54	BA	2441	U	C5'-C4'-O4'	5.54	115.75	109.10
21	AA	418	C	N1-C2-O2	5.54	122.22	118.90
54	BA	402	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	1538	G	N3-C4-C5	-5.54	125.83	128.60
54	BA	1797	G	N1-C6-O6	-5.54	116.58	119.90
54	BA	2326	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	2894	G	N1-C6-O6	-5.54	116.58	119.90
55	BB	39	A	C4-C5-C6	-5.54	114.23	117.00
2	AC	125	ARG	NE-CZ-NH1	5.54	123.07	120.30
21	AA	296	U	N1-C2-N3	5.54	118.22	114.90
54	BA	380	G	C4'-C3'-C2'	-5.54	97.06	102.60
54	BA	925	A	C5-C6-N1	5.54	120.47	117.70
54	BA	1326	U	O4'-C1'-N1	5.54	112.63	108.20
21	AA	377	G	N1-C6-O6	-5.54	116.58	119.90
21	AA	1113	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	443	A	O4'-C1'-N9	5.54	112.63	108.20
54	BA	997	G	N1-C6-O6	-5.54	116.58	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1381	G	N3-C2-N2	-5.54	116.02	119.90
54	BA	1512	C	N3-C4-C5	5.54	124.12	121.90
54	BA	1704	C	N3-C4-C5	5.54	124.11	121.90
54	BA	2286	G	C3'-C2'-C1'	5.54	105.93	101.50
55	BB	116	G	N9-C4-C5	5.54	107.62	105.40
21	AA	1482	G	N3-C4-C5	-5.54	125.83	128.60
54	BA	687	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	2587	A	O4'-C1'-N9	5.54	112.63	108.20
54	BA	2686	G	N3-C4-C5	-5.54	125.83	128.60
21	AA	344	A	N1-C6-N6	-5.54	115.28	118.60
21	AA	1056	U	N1-C2-N3	5.54	118.22	114.90
23	A2	92	U	O4'-C1'-N1	5.54	112.63	108.20
54	BA	657	U	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1779	U	C5-C6-N1	-5.54	119.93	122.70
54	BA	2030	A	O4'-C1'-N9	5.54	112.63	108.20
54	BA	2526	G	N1-C6-O6	-5.54	116.58	119.90
21	AA	377	G	C5-C6-N1	5.53	114.27	111.50
21	AA	993	G	C5'-C4'-C3'	-5.53	107.15	116.00
21	AA	1067	A	N1-C6-N6	-5.53	115.28	118.60
21	AA	1517	G	C8-N9-C4	-5.53	104.19	106.40
54	BA	623	C	N3-C4-C5	5.53	124.11	121.90
54	BA	1064	C	C6-N1-C2	-5.53	118.09	120.30
54	BA	1104	C	C6-N1-C2	-5.53	118.09	120.30
54	BA	2162	G	N9-C4-C5	5.53	107.61	105.40
54	BA	2785	C	N3-C4-C5	5.53	124.11	121.90
21	AA	164	G	N9-C4-C5	5.53	107.61	105.40
21	AA	254	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	541	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	2089	C	C2-N3-C4	-5.53	117.13	119.90
55	BB	49	C	N3-C2-O2	-5.53	118.03	121.90
8	AI	48	ARG	NE-CZ-NH1	5.53	123.06	120.30
21	AA	773	G	N1-C6-O6	-5.53	116.58	119.90
24	A3	35	C	N1-C2-O2	5.53	122.22	118.90
44	BV	19	ARG	NE-CZ-NH2	-5.53	117.53	120.30
54	BA	296	U	O4'-C1'-N1	5.53	112.62	108.20
54	BA	651	G	N3-C4-C5	-5.53	125.83	128.60
54	BA	1799	G	N1-C6-O6	-5.53	116.58	119.90
21	AA	68	G	O4'-C1'-N9	5.53	112.62	108.20
21	AA	327	A	C4-C5-C6	-5.53	114.24	117.00
21	AA	927	G	C5-C6-N1	5.53	114.27	111.50
21	AA	1078	U	N3-C2-O2	-5.53	118.33	122.20
54	BA	348	A	C4-C5-C6	-5.53	114.23	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1968	G	C8-N9-C4	-5.53	104.19	106.40
54	BA	2503	A	C1'-O4'-C4'	-5.53	105.48	109.90
54	BA	2687	U	N1-C2-N3	5.53	118.22	114.90
21	AA	434	U	C5-C6-N1	-5.53	119.94	122.70
21	AA	848	C	N1-C2-O2	5.53	122.22	118.90
48	BZ	29	ARG	NE-CZ-NH1	5.53	123.06	120.30
54	BA	654	A	C2-N3-C4	5.53	113.36	110.60
54	BA	662	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	830	G	C5-C6-N1	5.53	114.26	111.50
54	BA	1446	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	1539	U	C5-C6-N1	-5.53	119.94	122.70
54	BA	1732	C	N3-C4-C5	5.53	124.11	121.90
54	BA	2716	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	2894	G	C5-C6-N1	5.53	114.26	111.50
21	AA	1203	C	O4'-C1'-N1	5.53	112.62	108.20
21	AA	1218	C	N1-C2-O2	5.53	122.22	118.90
21	AA	1382	C	N3-C4-C5	5.53	124.11	121.90
54	BA	1365	A	O4'-C1'-N9	5.53	112.62	108.20
54	BA	1579	A	C5'-C4'-O4'	5.53	115.73	109.10
54	BA	1962	C	N3-C4-N4	-5.53	114.13	118.00
54	BA	2061	G	C8-N9-C4	-5.53	104.19	106.40
54	BA	411	G	P-O3'-C3'	5.52	126.33	119.70
54	BA	1608	A	C5-C6-N1	5.52	120.46	117.70
54	BA	2746	U	O4'-C1'-N1	5.52	112.62	108.20
21	AA	253	A	C5-C6-N1	5.52	120.46	117.70
21	AA	368	U	C1'-O4'-C4'	-5.52	105.48	109.90
21	AA	757	U	O4'-C1'-N1	5.52	112.62	108.20
54	BA	190	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	900	A	C6-C5-N7	5.52	136.17	132.30
21	AA	179	A	C5-C6-N1	5.52	120.46	117.70
21	AA	522	C	N3-C4-N4	-5.52	114.14	118.00
54	BA	1037	G	C5-C6-N1	5.52	114.26	111.50
54	BA	1547	C	O4'-C1'-N1	5.52	112.62	108.20
21	AA	199	A	C4-C5-C6	-5.52	114.24	117.00
24	A3	5	G	C8-N9-C4	-5.52	104.19	106.40
54	BA	253	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	417	C	O4'-C1'-N1	5.52	112.61	108.20
54	BA	1525	A	C5-C6-N1	5.52	120.46	117.70
54	BA	2892	G	C5-C6-N1	5.52	114.26	111.50
14	AO	88	ARG	NE-CZ-NH1	5.52	123.06	120.30
21	AA	1050	G	C5-C6-N1	5.52	114.26	111.50
54	BA	872	U	O4'-C1'-N1	5.52	112.61	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1954	G	C8-N9-C4	-5.52	104.19	106.40
54	BA	2723	C	C5'-C4'-O4'	5.52	115.72	109.10
54	BA	2865	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	24	G	O4'-C1'-N9	5.51	112.61	108.20
54	BA	364	C	N1-C2-O2	5.51	122.21	118.90
54	BA	1759	A	N7-C8-N9	5.51	116.56	113.80
54	BA	2067	G	N1-C6-O6	-5.51	116.59	119.90
54	BA	2812	G	C8-N9-C4	-5.51	104.19	106.40
21	AA	556	C	C6-N1-C2	-5.51	118.09	120.30
21	AA	1145	A	C4-C5-C6	-5.51	114.24	117.00
37	BO	81	ARG	NE-CZ-NH1	5.51	123.06	120.30
54	BA	1537	G	C8-N9-C4	-5.51	104.19	106.40
54	BA	2669	G	N1-C6-O6	-5.51	116.59	119.90
54	BA	2771	C	N1-C2-O2	5.51	122.21	118.90
21	AA	321	A	C5-C6-N1	5.51	120.46	117.70
21	AA	1429	A	C5'-C4'-O4'	5.51	115.71	109.10
54	BA	884	U	C5-C6-N1	-5.51	119.94	122.70
54	BA	1758	U	N3-C2-O2	-5.51	118.34	122.20
21	AA	403	C	N3-C4-C5	5.51	124.10	121.90
21	AA	862	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	973	G	C5-C6-N1	5.51	114.25	111.50
54	BA	331	C	O4'-C1'-N1	5.51	112.61	108.20
54	BA	1064	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	1468	U	N1-C2-N3	5.51	118.21	114.90
54	BA	2147	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	2717	C	C2-N3-C4	-5.51	117.14	119.90
54	BA	2779	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	2160	C	N3-C4-C5	5.51	124.10	121.90
54	BA	2339	C	N1-C2-O2	5.51	122.20	118.90
9	AJ	5	ARG	NE-CZ-NH1	5.51	123.05	120.30
21	AA	63	C	N1-C2-O2	5.51	122.20	118.90
21	AA	353	A	C2-N3-C4	5.51	113.35	110.60
21	AA	484	G	N9-C4-C5	5.51	107.60	105.40
21	AA	1385	G	O4'-C1'-N9	5.51	112.61	108.20
24	A3	69	C	N1-C2-O2	5.51	122.20	118.90
54	BA	812	C	N1-C2-O2	5.51	122.20	118.90
54	BA	1146	C	O4'-C1'-N1	5.51	112.61	108.20
54	BA	1206	G	C5-N7-C8	-5.51	101.55	104.30
23	A2	92	U	C5-C6-N1	-5.50	119.95	122.70
24	A3	38	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	474	G	C8-N9-C4	-5.50	104.20	106.40
54	BA	1275	A	N1-C6-N6	-5.50	115.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	375	U	O4'-C1'-N1	5.50	112.60	108.20
21	AA	949	A	C6-C5-N7	5.50	136.15	132.30
21	AA	1064	G	N3-C2-N2	-5.50	116.05	119.90
21	AA	1243	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	205	G	C8-N9-C4	-5.50	104.20	106.40
54	BA	1378	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1452	G	C8-N9-C4	-5.50	104.20	106.40
54	BA	1475	G	N3-C4-C5	-5.50	125.85	128.60
54	BA	2454	G	C8-N9-C4	-5.50	104.20	106.40
21	AA	686	U	N1-C2-N3	5.50	118.20	114.90
54	BA	2103	C	N1-C2-O2	5.50	122.20	118.90
21	AA	272	C	C1'-O4'-C4'	-5.50	105.50	109.90
21	AA	369	G	N1-C6-O6	-5.50	116.60	119.90
21	AA	847	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	1146	C	N1-C2-O2	5.50	122.20	118.90
54	BA	2597	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	2610	C	N1-C2-O2	5.50	122.20	118.90
54	BA	2773	C	N3-C2-O2	-5.50	118.05	121.90
12	AM	69	ARG	NE-CZ-NH1	5.50	123.05	120.30
21	AA	71	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	139	U	C5-C6-N1	-5.50	119.95	122.70
54	BA	144	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1539	U	C1'-O4'-C4'	-5.50	105.50	109.90
1	AB	94	ARG	NE-CZ-NH1	5.50	123.05	120.30
21	AA	447	G	C8-N9-C4	-5.50	104.20	106.40
21	AA	833	G	C5-C6-N1	5.50	114.25	111.50
21	AA	974	A	O4'-C1'-N9	5.50	112.60	108.20
54	BA	1476	U	N1-C2-N3	5.50	118.20	114.90
54	BA	2084	C	N1-C2-O2	5.50	122.20	118.90
54	BA	2240	U	C5-C6-N1	-5.50	119.95	122.70
54	BA	2241	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	2748	A	C5-C6-N1	5.50	120.45	117.70
21	AA	822	U	C1'-O4'-C4'	-5.49	105.50	109.90
21	AA	849	G	C5-C6-N1	5.49	114.25	111.50
21	AA	1157	A	C5-C6-N1	5.49	120.45	117.70
24	A3	50	G	C5-C6-N1	5.49	114.25	111.50
54	BA	723	C	C4'-C3'-C2'	-5.49	97.11	102.60
55	BB	7	G	N9-C4-C5	5.49	107.60	105.40
21	AA	205	A	O4'-C4'-C3'	5.49	110.49	106.10
21	AA	1146	A	C5-C6-N1	5.49	120.45	117.70
21	AA	1197	A	C3'-C2'-C1'	5.49	105.89	101.50
21	AA	1262	C	N3-C2-O2	-5.49	118.06	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	537	G	C5-C6-N1	5.49	114.25	111.50
54	BA	2638	G	N9-C4-C5	5.49	107.60	105.40
21	AA	107	G	N1-C6-O6	-5.49	116.61	119.90
21	AA	187	G	C5-C6-N1	5.49	114.25	111.50
54	BA	1	G	N7-C8-N9	5.49	115.84	113.10
54	BA	361	G	N3-C2-N2	-5.49	116.06	119.90
54	BA	1826	G	N1-C6-O6	-5.49	116.61	119.90
54	BA	2087	G	O4'-C1'-N9	5.49	112.59	108.20
54	BA	2828	G	N1-C6-O6	-5.49	116.61	119.90
21	AA	314	C	N1-C2-O2	5.49	122.19	118.90
21	AA	341	C	N1-C2-O2	5.49	122.19	118.90
54	BA	250	G	N1-C6-O6	-5.49	116.61	119.90
54	BA	492	A	C5-C6-N1	5.49	120.44	117.70
54	BA	1035	U	N1-C2-N3	5.49	118.19	114.90
54	BA	1775	U	C4'-C3'-C2'	-5.49	97.11	102.60
54	BA	2328	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	295	G	N7-C8-N9	5.49	115.84	113.10
54	BA	2376	A	C4-C5-C6	-5.49	114.26	117.00
22	A1	28	C	N1-C2-O2	5.49	122.19	118.90
54	BA	496	G	O4'-C1'-N9	5.49	112.59	108.20
54	BA	577	G	N3-C4-C5	-5.49	125.86	128.60
54	BA	1209	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	1409	U	C5-C6-N1	-5.49	119.96	122.70
21	AA	1375	A	C2-N3-C4	5.48	113.34	110.60
21	AA	1495	U	N3-C2-O2	-5.48	118.36	122.20
28	BF	149	ARG	NE-CZ-NH1	5.48	123.04	120.30
21	AA	328	C	O4'-C1'-N1	5.48	112.59	108.20
21	AA	546	A	C6-C5-N7	5.48	136.14	132.30
21	AA	1498	U	O4'-C1'-N1	5.48	112.59	108.20
30	BH	51	ARG	NE-CZ-NH1	5.48	123.04	120.30
54	BA	1290	C	N3-C4-C5	5.48	124.09	121.90
54	BA	1560	G	N3-C2-N2	-5.48	116.06	119.90
21	AA	1465	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1112	G	N3-C4-C5	-5.48	125.86	128.60
54	BA	1404	C	N3-C4-N4	-5.48	114.16	118.00
55	BB	66	A	C5-C6-N1	5.48	120.44	117.70
55	BB	91	C	N1-C2-O2	5.48	122.19	118.90
54	BA	620	G	N3-C4-C5	-5.48	125.86	128.60
54	BA	806	C	N3-C4-C5	5.48	124.09	121.90
54	BA	1325	U	N1-C1'-C2'	5.48	121.12	114.00
54	BA	2127	G	N9-C4-C5	5.48	107.59	105.40
21	AA	71	A	N1-C6-N6	-5.48	115.31	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1833	C	N3-C4-C5	5.48	124.09	121.90
54	BA	1981	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2289	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	2628	C	N3-C4-C5	5.48	124.09	121.90
21	AA	170	U	N3-C2-O2	-5.48	118.37	122.20
21	AA	958	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	403	U	O4'-C1'-N1	5.48	112.58	108.20
21	AA	391	G	N1-C6-O6	-5.47	116.61	119.90
21	AA	1300	G	N1-C6-O6	-5.47	116.61	119.90
54	BA	1403	A	N1-C6-N6	-5.47	115.31	118.60
54	BA	1461	C	N3-C2-O2	-5.47	118.07	121.90
54	BA	1508	A	C4-C5-C6	-5.47	114.26	117.00
54	BA	1533	C	N1-C2-O2	5.47	122.19	118.90
54	BA	2042	A	C4-C5-C6	-5.47	114.26	117.00
21	AA	1314	C	N1-C2-O2	5.47	122.18	118.90
21	AA	1388	C	N3-C4-C5	5.47	124.09	121.90
21	AA	1438	G	C8-N9-C4	-5.47	104.21	106.40
54	BA	51	G	C8-N9-C4	-5.47	104.21	106.40
54	BA	296	U	N1-C2-N3	5.47	118.18	114.90
54	BA	1297	C	C6-N1-C2	-5.47	118.11	120.30
54	BA	2757	A	C4-C5-C6	-5.47	114.26	117.00
55	BB	3	C	N1-C2-O2	5.47	122.18	118.90
21	AA	566	G	N1-C6-O6	-5.47	116.62	119.90
21	AA	859	G	C5-C6-N1	5.47	114.23	111.50
21	AA	1055	A	C5-C6-N1	5.47	120.44	117.70
24	A3	62	C	N3-C4-C5	5.47	124.09	121.90
54	BA	144	A	C6-C5-N7	5.47	136.13	132.30
54	BA	517	C	N1-C2-O2	5.47	122.18	118.90
54	BA	1560	G	N7-C8-N9	5.47	115.84	113.10
54	BA	2293	G	C8-N9-C4	-5.47	104.21	106.40
54	BA	2384	U	N1-C2-N3	5.47	118.18	114.90
21	AA	1138	G	C5-C6-N1	5.47	114.23	111.50
21	AA	1416	G	N9-C4-C5	5.47	107.59	105.40
54	BA	1634	A	P-O3'-C3'	5.47	126.26	119.70
54	BA	1846	G	C3'-C2'-C1'	5.47	105.88	101.50
54	BA	2296	U	N3-C2-O2	-5.47	118.37	122.20
54	BA	2344	U	N3-C2-O2	-5.47	118.37	122.20
24	A3	2	G	C5-C6-N1	5.47	114.23	111.50
21	AA	650	G	N1-C6-O6	-5.47	116.62	119.90
21	AA	851	G	N7-C8-N9	5.47	115.83	113.10
54	BA	688	U	O4'-C1'-N1	5.47	112.57	108.20
54	BA	2018	G	C5-C6-N1	5.47	114.23	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2295	C	O4'-C1'-N1	5.47	112.57	108.20
54	BA	2342	C	O4'-C1'-N1	5.47	112.57	108.20
21	AA	117	G	C5-C6-N1	5.46	114.23	111.50
21	AA	152	A	O4'-C1'-N9	5.46	112.57	108.20
21	AA	819	A	C6-C5-N7	5.46	136.12	132.30
54	BA	1178	C	N1-C2-O2	5.46	122.18	118.90
54	BA	1616	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1950	G	C8-N9-C4	-5.46	104.21	106.40
21	AA	131	A	C6-C5-N7	5.46	136.12	132.30
21	AA	403	C	O4'-C1'-N1	5.46	112.57	108.20
22	A1	36	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	1719	G	C5-C6-N1	5.46	114.23	111.50
54	BA	1748	C	N1-C2-O2	5.46	122.18	118.90
21	AA	96	U	C5-C6-N1	-5.46	119.97	122.70
21	AA	711	G	N1-C6-O6	-5.46	116.62	119.90
21	AA	1211	U	O4'-C4'-C3'	5.46	110.47	106.10
21	AA	1526	G	N9-C4-C5	5.46	107.58	105.40
54	BA	138	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	198	C	N1-C2-O2	5.46	122.18	118.90
54	BA	769	U	C5'-C4'-O4'	5.46	115.65	109.10
54	BA	1037	G	N1-C6-O6	-5.46	116.62	119.90
54	BA	1099	G	N3-C2-N2	-5.46	116.08	119.90
54	BA	1556	C	N3-C4-C5	5.46	124.08	121.90
54	BA	2053	G	C8-N9-C4	-5.46	104.22	106.40
51	B2	39	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	60	G	N3-C4-C5	-5.46	125.87	128.60
54	BA	592	A	C5-C6-N1	5.46	120.43	117.70
54	BA	748	G	N1-C6-O6	-5.46	116.62	119.90
54	BA	1135	C	O4'-C1'-N1	5.46	112.57	108.20
54	BA	2286	G	C1'-O4'-C4'	-5.46	105.53	109.90
54	BA	2397	G	N1-C6-O6	-5.46	116.62	119.90
21	AA	110	C	C1'-O4'-C4'	-5.46	105.53	109.90
21	AA	290	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	482	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	1512	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	100	U	C4-C5-C6	5.46	122.97	119.70
54	BA	1448	G	C5-C6-N1	5.46	114.23	111.50
54	BA	1509	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1607	C	N1-C2-O2	5.46	122.17	118.90
54	BA	2087	G	N3-C2-N2	-5.46	116.08	119.90
21	AA	955	U	C5-C6-N1	-5.46	119.97	122.70
54	BA	567	U	O4'-C1'-N1	5.46	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1343	G	C8-N9-C4	-5.46	104.22	106.40
54	BA	2127	G	C8-N9-C4	-5.46	104.22	106.40
54	BA	2311	A	C6-C5-N7	5.46	136.12	132.30
54	BA	2355	G	C8-N9-C4	-5.46	104.22	106.40
54	BA	2715	C	O4'-C1'-N1	5.46	112.56	108.20
23	A2	90	U	C5-C6-N1	-5.46	119.97	122.70
54	BA	752	A	C2-N3-C4	5.46	113.33	110.60
54	BA	1348	C	C2-N3-C4	-5.46	117.17	119.90
54	BA	1672	A	N1-C6-N6	-5.46	115.33	118.60
55	BB	15	A	C2-N3-C4	5.46	113.33	110.60
21	AA	453	G	N1-C6-O6	-5.45	116.63	119.90
21	AA	469	C	C6-N1-C2	-5.45	118.12	120.30
21	AA	1162	C	C6-N1-C2	-5.45	118.12	120.30
21	AA	1390	U	O4'-C1'-N1	5.45	112.56	108.20
54	BA	287	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	417	C	N3-C2-O2	-5.45	118.08	121.90
54	BA	1726	C	N3-C2-O2	-5.45	118.08	121.90
54	BA	2095	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	2430	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	2722	G	C5-C6-N1	5.45	114.23	111.50
54	BA	2862	G	C5-C6-N1	5.45	114.23	111.50
54	BA	2870	C	N3-C4-C5	5.45	124.08	121.90
21	AA	233	C	N3-C4-C5	5.45	124.08	121.90
54	BA	11	C	N3-C2-O2	-5.45	118.08	121.90
54	BA	1351	C	N3-C2-O2	-5.45	118.08	121.90
54	BA	1396	U	N3-C2-O2	-5.45	118.39	122.20
21	AA	139	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	194	C	C3'-C2'-C1'	5.45	105.86	101.50
21	AA	553	A	C2-N3-C4	5.45	113.32	110.60
21	AA	1059	C	N3-C2-O2	-5.45	118.08	121.90
25	BC	188	ARG	NE-CZ-NH1	5.45	123.02	120.30
54	BA	71	A	C6-C5-N7	5.45	136.11	132.30
54	BA	943	A	C5'-C4'-O4'	5.45	115.64	109.10
54	BA	1314	C	N1-C2-O2	5.45	122.17	118.90
54	BA	1782	U	N1-C2-N3	5.45	118.17	114.90
54	BA	1928	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	1534	A	C5'-C4'-O4'	5.45	115.64	109.10
54	BA	2597	G	N9-C4-C5	5.45	107.58	105.40
54	BA	1890	A	C4-C5-C6	-5.45	114.28	117.00
24	A3	20	G	N3-C4-C5	-5.44	125.88	128.60
54	BA	514	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	700	G	O4'-C1'-N9	5.44	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2300	C	O4'-C1'-N1	5.44	112.56	108.20
21	AA	890	G	C8-N9-C4	-5.44	104.22	106.40
54	BA	262	A	C5-C6-N1	5.44	120.42	117.70
54	BA	1069	A	C5-C6-N1	5.44	120.42	117.70
54	BA	1291	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	2242	G	C5-C6-N1	5.44	114.22	111.50
54	BA	2628	C	N1-C2-O2	5.44	122.17	118.90
54	BA	2760	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	30	U	N3-C2-O2	-5.44	118.39	122.20
21	AA	825	A	C6-C5-N7	5.44	136.11	132.30
21	AA	1527	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	295	G	N9-C4-C5	5.44	107.58	105.40
54	BA	1339	G	C8-N9-C4	-5.44	104.22	106.40
54	BA	1965	C	C2-N3-C4	-5.44	117.18	119.90
54	BA	2411	A	C6-C5-N7	5.44	136.11	132.30
21	AA	120	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	277	G	C5-C6-N1	5.44	114.22	111.50
54	BA	1900	A	C6-C5-N7	5.44	136.11	132.30
54	BA	2584	U	C4'-C3'-C2'	-5.44	97.16	102.60
54	BA	2902	C	C4'-C3'-C2'	-5.44	97.16	102.60
21	AA	129	A	C6-C5-N7	5.44	136.11	132.30
54	BA	1385	A	C1'-O4'-C4'	-5.44	105.55	109.90
54	BA	1594	U	N3-C2-O2	-5.44	118.39	122.20
54	BA	2406	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	2756	U	N1-C2-N3	5.44	118.16	114.90
55	BB	14	U	N3-C2-O2	-5.44	118.39	122.20
21	AA	159	G	C5-C6-N1	5.44	114.22	111.50
21	AA	384	G	N7-C8-N9	5.44	115.82	113.10
21	AA	444	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	366	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	623	C	N1-C2-O2	5.44	122.16	118.90
54	BA	1564	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	1836	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	1970	A	C6-C5-N7	5.44	136.10	132.30
54	BA	2080	A	O4'-C1'-N9	5.44	112.55	108.20
54	BA	2743	U	N3-C2-O2	-5.44	118.39	122.20
21	AA	275	G	N3-C2-N2	-5.43	116.10	119.90
21	AA	383	A	C2-N3-C4	5.43	113.32	110.60
21	AA	1359	C	N3-C2-O2	-5.43	118.09	121.90
54	BA	286	U	C4-C5-C6	5.43	122.96	119.70
54	BA	466	A	N1-C6-N6	-5.43	115.34	118.60
54	BA	1287	A	C4-C5-C6	-5.43	114.28	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	545	U	N3-C2-O2	-5.43	118.40	122.20
54	BA	762	U	P-O3'-C3'	5.43	126.22	119.70
54	BA	1325	U	O4'-C1'-C2'	-5.43	100.37	105.80
54	BA	1471	G	C5-C6-N1	5.43	114.22	111.50
21	AA	1202	U	O4'-C1'-N1	5.43	112.55	108.20
21	AA	1210	C	N3-C4-C5	5.43	124.07	121.90
54	BA	234	U	N3-C2-O2	-5.43	118.40	122.20
54	BA	523	C	N1-C2-O2	5.43	122.16	118.90
54	BA	2209	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	2255	G	C5-C6-N1	5.43	114.22	111.50
21	AA	369	G	C8-N9-C4	-5.43	104.23	106.40
21	AA	1067	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	602	A	C5-C6-N1	5.43	120.42	117.70
54	BA	2229	U	C5-C6-N1	-5.43	119.98	122.70
54	BA	2314	A	C4-C5-C6	-5.43	114.28	117.00
55	BB	63	C	O4'-C1'-N1	5.43	112.54	108.20
21	AA	977	A	O4'-C1'-N9	5.43	112.54	108.20
22	A1	17	U	C5-C6-N1	-5.43	119.99	122.70
54	BA	1426	G	N9-C4-C5	5.43	107.57	105.40
21	AA	185	U	N1-C2-N3	5.43	118.16	114.90
21	AA	331	G	C8-N9-C4	-5.43	104.23	106.40
21	AA	1069	C	C6-N1-C2	-5.43	118.13	120.30
21	AA	1497	G	C5-C6-N1	5.43	114.21	111.50
54	BA	704	G	N3-C4-C5	-5.43	125.89	128.60
54	BA	961	C	C6-N1-C2	-5.43	118.13	120.30
54	BA	1152	C	O4'-C1'-N1	5.43	112.54	108.20
54	BA	1429	G	C8-N9-C4	-5.43	104.23	106.40
54	BA	1538	G	C5-C6-N1	5.43	114.21	111.50
54	BA	2161	C	N1-C2-O2	5.43	122.16	118.90
54	BA	2687	U	N3-C2-O2	-5.43	118.40	122.20
54	BA	2867	G	C5-C6-N1	5.43	114.21	111.50
21	AA	206	C	N3-C2-O2	-5.42	118.10	121.90
21	AA	655	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	1184	G	N1-C6-O6	-5.42	116.64	119.90
49	B0	49	ARG	NE-CZ-NH1	5.42	123.01	120.30
54	BA	291	G	N9-C4-C5	5.42	107.57	105.40
54	BA	431	U	C4-C5-C6	5.42	122.95	119.70
54	BA	485	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	923	G	N1-C6-O6	-5.42	116.64	119.90
54	BA	1703	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	1807	G	N1-C6-O6	-5.42	116.64	119.90
4	AE	19	ARG	NE-CZ-NH1	5.42	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	247	G	C4-C5-N7	-5.42	108.63	110.80
21	AA	473	U	C4-C5-C6	5.42	122.95	119.70
21	AA	1201	A	C5'-C4'-C3'	-5.42	107.32	116.00
54	BA	130	C	N3-C4-C5	5.42	124.07	121.90
54	BA	2603	G	C5-C6-N1	5.42	114.21	111.50
21	AA	1143	G	C8-N9-C4	-5.42	104.23	106.40
21	AA	1368	A	C6-C5-N7	5.42	136.09	132.30
54	BA	1739	A	C5-C6-N1	5.42	120.41	117.70
54	BA	2699	C	N1-C2-O2	5.42	122.15	118.90
54	BA	2821	A	C5-C6-N1	5.42	120.41	117.70
55	BB	27	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	438	U	N1-C2-N3	5.42	118.15	114.90
21	AA	477	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	1431	A	C5-C6-N1	5.42	120.41	117.70
54	BA	1376	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	2104	C	N1-C2-O2	5.42	122.15	118.90
55	BB	109	A	C1'-O4'-C4'	-5.42	105.56	109.90
21	AA	917	G	N7-C8-N9	5.42	115.81	113.10
54	BA	1503	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2269	G	C8-N9-C4	-5.42	104.23	106.40
54	BA	2652	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	580	C	N3-C4-C5	5.42	124.07	121.90
21	AA	1331	G	C8-N9-C4	-5.42	104.23	106.40
24	A3	1	C	N3-C4-N4	-5.42	114.21	118.00
54	BA	423	A	C2-N3-C4	5.42	113.31	110.60
54	BA	1373	A	C5-C6-N1	5.42	120.41	117.70
54	BA	1675	C	C2-N3-C4	-5.42	117.19	119.90
54	BA	2524	G	O4'-C1'-N9	5.42	112.53	108.20
24	A3	67	C	O4'-C1'-N1	5.42	112.53	108.20
54	BA	211	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	405	U	N3-C2-O2	-5.42	118.41	122.20
55	BB	16	G	N7-C8-N9	5.42	115.81	113.10
21	AA	115	G	N3-C4-C5	-5.41	125.89	128.60
21	AA	251	G	C3'-C2'-C1'	5.41	105.83	101.50
21	AA	497	G	C5-C6-N1	5.41	114.21	111.50
21	AA	818	G	C5-C6-N1	5.41	114.21	111.50
21	AA	1009	U	O4'-C1'-N1	5.41	112.53	108.20
21	AA	1127	G	C5-C6-N1	5.41	114.21	111.50
21	AA	1441	A	C6-C5-N7	5.41	136.09	132.30
24	A3	69	C	C5'-C4'-C3'	-5.41	107.34	116.00
54	BA	423	A	C6-C5-N7	5.41	136.09	132.30
54	BA	720	U	O4'-C1'-N1	5.41	112.53	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2772	C	N3-C2-O2	-5.41	118.11	121.90
21	AA	165	G	C5-C6-N1	5.41	114.21	111.50
54	BA	305	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	2368	C	N3-C4-C5	5.41	124.06	121.90
21	AA	720	C	N3-C2-O2	-5.41	118.11	121.90
21	AA	1223	C	N3-C2-O2	-5.41	118.11	121.90
22	A1	69	A	C5-C6-N1	5.41	120.41	117.70
54	BA	1618	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	2847	U	C5-C6-N1	-5.41	120.00	122.70
21	AA	753	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	925	G	N1-C6-O6	-5.41	116.66	119.90
21	AA	1028	C	N3-C2-O2	-5.41	118.11	121.90
21	AA	1078	U	C5-C6-N1	-5.41	120.00	122.70
49	B0	51	ARG	NE-CZ-NH1	5.41	123.00	120.30
54	BA	601	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	815	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	1655	A	C6-C5-N7	5.41	136.09	132.30
54	BA	2130	U	C4-C5-C6	5.41	122.94	119.70
54	BA	2853	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	338	G	C5-C6-N1	5.41	114.20	111.50
54	BA	455	C	O4'-C4'-C3'	5.41	110.43	106.10
54	BA	825	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	1236	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1281	G	O4'-C1'-N9	5.41	112.52	108.20
54	BA	1571	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1758	U	C3'-C2'-C1'	-5.41	97.18	101.50
54	BA	1958	C	N3-C2-O2	-5.41	118.12	121.90
54	BA	2098	U	N3-C2-O2	-5.41	118.42	122.20
54	BA	2211	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	2699	C	N3-C4-C5	5.41	124.06	121.90
54	BA	1241	A	C2-N3-C4	5.40	113.30	110.60
54	BA	2178	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	2227	A	C6-C5-N7	5.40	136.08	132.30
21	AA	342	C	N1-C2-O2	5.40	122.14	118.90
21	AA	1150	A	C6-C5-N7	5.40	136.08	132.30
21	AA	1207	G	C8-N9-C4	-5.40	104.24	106.40
21	AA	1293	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	44	A	C5-C6-N1	5.40	120.40	117.70
54	BA	677	A	C5-N7-C8	-5.40	101.20	103.90
54	BA	832	U	C5-C6-N1	-5.40	120.00	122.70
54	BA	2025	C	N3-C4-C5	5.40	124.06	121.90
54	BA	2881	U	N3-C2-O2	-5.40	118.42	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1207	G	N9-C4-C5	5.40	107.56	105.40
54	BA	207	A	C5-C6-N1	5.40	120.40	117.70
54	BA	646	U	O4'-C1'-N1	5.40	112.52	108.20
54	BA	901	C	N3-C4-C5	5.40	124.06	121.90
54	BA	1307	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1315	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	1981	A	O4'-C4'-C3'	5.40	110.42	106.10
54	BA	2617	U	C5'-C4'-O4'	5.40	115.58	109.10
4	AE	28	ARG	CD-NE-CZ	5.40	131.16	123.60
21	AA	114	U	N1-C2-N3	5.40	118.14	114.90
21	AA	125	U	C1'-O4'-C4'	-5.40	105.58	109.90
21	AA	765	G	N3-C4-C5	-5.40	125.90	128.60
54	BA	1098	A	C6-C5-N7	5.40	136.08	132.30
54	BA	2050	C	N3-C4-C5	5.40	124.06	121.90
21	AA	164	G	C1'-O4'-C4'	-5.40	105.58	109.90
21	AA	837	U	N1-C2-N3	5.40	118.14	114.90
21	AA	1328	C	N1-C2-O2	5.40	122.14	118.90
54	BA	20	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	39	G	C8-N9-C4	-5.40	104.24	106.40
54	BA	705	A	C5-C6-N1	5.40	120.40	117.70
54	BA	1370	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	2373	G	N1-C6-O6	-5.40	116.66	119.90
54	BA	2698	U	N3-C2-O2	-5.40	118.42	122.20
7	AH	79	ARG	NE-CZ-NH1	5.40	123.00	120.30
21	AA	173	U	C1'-O4'-C4'	-5.40	105.58	109.90
21	AA	539	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	1056	U	O4'-C1'-N1	5.40	112.52	108.20
21	AA	1092	A	C5-C6-N1	5.40	120.40	117.70
54	BA	2162	G	N3-C2-N2	-5.40	116.12	119.90
54	BA	2861	U	N1-C2-N3	5.40	118.14	114.90
21	AA	730	G	C8-N9-C4	-5.39	104.24	106.40
21	AA	831	A	C5-C6-N1	5.39	120.40	117.70
54	BA	257	C	O4'-C1'-N1	5.39	112.52	108.20
54	BA	1232	G	N3-C2-N2	-5.39	116.12	119.90
54	BA	1530	G	N7-C8-N9	5.39	115.80	113.10
54	BA	1701	A	O4'-C1'-N9	5.39	112.52	108.20
54	BA	1915	U	O4'-C1'-N1	5.39	112.52	108.20
54	BA	2722	G	N1-C6-O6	-5.39	116.66	119.90
54	BA	2745	C	N3-C2-O2	-5.39	118.12	121.90
54	BA	557	C	N3-C2-O2	-5.39	118.12	121.90
55	BB	22	U	N1-C2-N3	5.39	118.14	114.90
21	AA	967	C	N1-C2-O2	5.39	122.13	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A2	90	U	N3-C2-O2	-5.39	118.43	122.20
54	BA	409	G	C8-N9-C4	-5.39	104.24	106.40
54	BA	1197	G	N1-C6-O6	-5.39	116.67	119.90
54	BA	1340	U	N3-C2-O2	-5.39	118.43	122.20
21	AA	52	C	N3-C4-C5	5.39	124.06	121.90
21	AA	64	G	O4'-C1'-N9	5.39	112.51	108.20
24	A3	65	G	N3-C2-N2	-5.39	116.13	119.90
24	A3	67	C	C2-N3-C4	-5.39	117.20	119.90
54	BA	543	G	N1-C6-O6	-5.39	116.67	119.90
54	BA	906	U	C5-C6-N1	-5.39	120.01	122.70
54	BA	1091	G	C5-C6-N1	5.39	114.19	111.50
54	BA	1282	U	C5-C6-N1	-5.39	120.00	122.70
54	BA	1432	G	C5-C6-N1	5.39	114.19	111.50
54	BA	2574	G	C5-C6-N1	5.39	114.19	111.50
55	BB	60	C	N1-C2-O2	5.39	122.13	118.90
21	AA	242	G	N1-C6-O6	-5.39	116.67	119.90
21	AA	764	C	N3-C2-O2	-5.39	118.13	121.90
54	BA	116	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	401	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	2614	A	C6-C5-N7	5.39	136.07	132.30
54	BA	2634	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	2745	C	N3-C4-C5	5.39	124.06	121.90
55	BB	18	G	O4'-C1'-N9	5.39	112.51	108.20
21	AA	358	U	C3'-C2'-C1'	5.39	105.81	101.50
21	AA	512	U	C5-C6-N1	-5.39	120.01	122.70
22	A1	40	G	N7-C8-N9	5.39	115.79	113.10
46	BX	27	ARG	NE-CZ-NH1	5.39	122.99	120.30
54	BA	420	C	C6-N1-C2	-5.39	118.14	120.30
54	BA	455	C	C3'-C2'-C1'	5.39	105.81	101.50
54	BA	1352	U	C4-C5-C6	5.39	122.93	119.70
54	BA	1476	U	N3-C2-O2	-5.39	118.43	122.20
54	BA	2380	C	N3-C4-C5	5.39	124.06	121.90
54	BA	2783	U	O4'-C1'-N1	5.39	112.51	108.20
21	AA	716	A	O4'-C1'-N9	5.38	112.51	108.20
21	AA	1057	G	C5-C6-N1	5.38	114.19	111.50
22	A1	48	C	N3-C2-O2	-5.38	118.13	121.90
54	BA	385	C	N1-C2-O2	5.38	122.13	118.90
54	BA	1319	C	C1'-O4'-C4'	-5.38	105.59	109.90
54	BA	1677	A	C8-N9-C4	-5.38	103.65	105.80
54	BA	1826	G	C2'-C3'-O3'	5.38	122.31	113.70
54	BA	2828	G	C5-C6-N1	5.38	114.19	111.50
55	BB	109	A	O4'-C1'-N9	5.38	112.51	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	861	G	N7-C8-N9	5.38	115.79	113.10
21	AA	1184	G	C5-C6-N1	5.38	114.19	111.50
54	BA	805	G	C5-C6-N1	5.38	114.19	111.50
54	BA	2371	G	O4'-C1'-N9	5.38	112.51	108.20
21	AA	387	U	C5-C6-N1	-5.38	120.01	122.70
21	AA	1153	G	C5-C6-N1	5.38	114.19	111.50
54	BA	33	C	N3-C2-O2	-5.38	118.13	121.90
54	BA	385	C	N3-C4-C5	5.38	124.05	121.90
54	BA	1011	G	O4'-C1'-N9	5.38	112.51	108.20
54	BA	1090	A	C6-C5-N7	5.38	136.07	132.30
54	BA	1256	G	C8-N9-C4	-5.38	104.25	106.40
54	BA	1973	G	N9-C4-C5	5.38	107.55	105.40
54	BA	2389	G	N3-C2-N2	-5.38	116.13	119.90
54	BA	372	G	N3-C4-C5	-5.38	125.91	128.60
21	AA	9	G	C5-C6-N1	5.38	114.19	111.50
21	AA	309	A	C5-C6-N1	5.38	120.39	117.70
21	AA	560	A	C6-C5-N7	5.38	136.06	132.30
21	AA	1234	C	N1-C2-O2	5.38	122.13	118.90
54	BA	76	C	N1-C2-O2	5.38	122.13	118.90
54	BA	278	A	C5-C6-N1	5.38	120.39	117.70
54	BA	841	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	1543	G	N3-C4-C5	-5.38	125.91	128.60
54	BA	2683	C	O4'-C1'-N1	5.38	112.50	108.20
21	AA	70	U	O4'-C4'-C3'	5.38	110.40	106.10
21	AA	77	A	C5-C6-N1	5.38	120.39	117.70
21	AA	625	U	N1-C2-N3	5.38	118.13	114.90
21	AA	995	C	C1'-O4'-C4'	-5.38	105.60	109.90
22	A1	31	C	N3-C2-O2	-5.38	118.14	121.90
54	BA	1	G	C8-N9-C4	-5.38	104.25	106.40
54	BA	774	G	C8-N9-C4	-5.38	104.25	106.40
54	BA	2339	C	N3-C4-C5	5.38	124.05	121.90
54	BA	2389	G	C8-N9-C4	-5.38	104.25	106.40
55	BB	18	G	C5-C6-N1	5.38	114.19	111.50
21	AA	1477	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	13	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	374	A	C6-C5-N7	5.38	136.06	132.30
21	AA	1526	G	N3-C4-C5	-5.37	125.91	128.60
54	BA	134	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	386	G	N3-C4-C5	-5.37	125.91	128.60
54	BA	540	C	N1-C2-O2	5.37	122.12	118.90
54	BA	736	C	N1-C2-O2	5.37	122.12	118.90
54	BA	863	A	C4-C5-C6	-5.37	114.31	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	946	C	N1-C2-O2	5.37	122.12	118.90
1	AB	62	ARG	NE-CZ-NH2	-5.37	117.61	120.30
21	AA	525	C	N1-C2-O2	5.37	122.12	118.90
21	AA	1031	C	C1'-O4'-C4'	-5.37	105.60	109.90
21	AA	1355	G	N1-C6-O6	-5.37	116.68	119.90
36	BN	103	ARG	NE-CZ-NH1	5.37	122.99	120.30
54	BA	548	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	974	G	N3-C4-C5	-5.37	125.91	128.60
54	BA	1121	C	C4'-C3'-C2'	-5.37	97.23	102.60
54	BA	1465	G	P-O3'-C3'	5.37	126.15	119.70
54	BA	1945	G	C8-N9-C4	-5.37	104.25	106.40
54	BA	2526	G	O4'-C1'-N9	5.37	112.50	108.20
21	AA	1486	G	C5-C6-N1	5.37	114.19	111.50
54	BA	1037	G	N3-C4-C5	-5.37	125.92	128.60
54	BA	1489	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	2325	G	N1-C6-O6	-5.37	116.68	119.90
8	AI	123	ARG	NE-CZ-NH1	5.37	122.98	120.30
21	AA	893	C	C6-N1-C2	-5.37	118.15	120.30
22	A1	17	U	C4-C5-C6	5.37	122.92	119.70
54	BA	746	U	N3-C2-O2	-5.37	118.44	122.20
54	BA	1261	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	1345	C	O4'-C1'-N1	5.37	112.50	108.20
54	BA	2030	A	C6-C5-N7	5.37	136.06	132.30
54	BA	2161	C	N3-C4-C5	5.37	124.05	121.90
21	AA	340	U	C5-C6-N1	-5.37	120.02	122.70
21	AA	653	U	O4'-C1'-N1	5.37	112.49	108.20
21	AA	1495	U	N1-C2-N3	5.37	118.12	114.90
54	BA	70	G	C8-N9-C4	-5.37	104.25	106.40
54	BA	199	A	C4-C5-C6	-5.37	114.32	117.00
54	BA	501	A	C4-C5-C6	-5.37	114.32	117.00
54	BA	2324	U	C3'-C2'-C1'	5.37	105.79	101.50
55	BB	9	G	N3-C4-C5	-5.37	125.92	128.60
21	AA	417	G	C5-C6-N1	5.37	114.18	111.50
21	AA	932	C	N1-C2-O2	5.37	122.12	118.90
54	BA	2	G	C8-N9-C4	-5.37	104.25	106.40
54	BA	756	A	C4-C5-C6	-5.37	114.32	117.00
54	BA	1101	U	C5-C6-N1	-5.37	120.02	122.70
54	BA	1305	C	O4'-C1'-N1	5.37	112.49	108.20
54	BA	1799	G	C5-C6-N1	5.37	114.18	111.50
54	BA	1940	U	O4'-C1'-N1	5.37	112.49	108.20
54	BA	2136	G	N9-C4-C5	5.37	107.55	105.40
54	BA	2422	C	N3-C4-C5	5.37	124.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	57	G	N1-C6-O6	-5.36	116.68	119.90
25	BC	79	ARG	NE-CZ-NH1	5.36	122.98	120.30
54	BA	121	G	N3-C2-N2	-5.36	116.15	119.90
54	BA	721	A	C6-C5-N7	5.36	136.06	132.30
54	BA	1128	G	N1-C6-O6	-5.36	116.68	119.90
54	BA	1370	C	N3-C4-C5	5.36	124.05	121.90
54	BA	1464	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	1501	G	N3-C2-N2	-5.36	116.15	119.90
54	BA	1685	C	C4'-C3'-C2'	-5.36	97.24	102.60
54	BA	1822	C	N3-C4-C5	5.36	124.05	121.90
54	BA	1244	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	1558	C	N3-C4-N4	-5.36	114.25	118.00
54	BA	1945	G	N3-C2-N2	-5.36	116.15	119.90
54	BA	2822	G	C5-C6-N1	5.36	114.18	111.50
21	AA	264	C	O4'-C1'-N1	5.36	112.49	108.20
21	AA	1332	A	C4-C5-C6	-5.36	114.32	117.00
22	A1	41	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	830	G	N1-C6-O6	-5.36	116.69	119.90
54	BA	1569	A	C5-C6-N1	5.36	120.38	117.70
54	BA	2271	G	N9-C4-C5	5.36	107.54	105.40
21	AA	84	U	C5-C6-N1	-5.36	120.02	122.70
21	AA	976	G	C8-N9-C4	-5.36	104.26	106.40
21	AA	1002	G	C8-N9-C4	-5.36	104.26	106.40
21	AA	1217	C	N1-C2-O2	5.36	122.11	118.90
21	AA	1517	G	N1-C6-O6	-5.36	116.69	119.90
54	BA	1277	G	C5-C6-N1	5.36	114.18	111.50
54	BA	1541	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	1588	G	N1-C6-O6	-5.36	116.69	119.90
54	BA	1607	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	1643	G	O4'-C1'-N9	5.36	112.49	108.20
54	BA	1931	U	N3-C2-O2	-5.36	118.45	122.20
54	BA	2356	U	N3-C2-O2	-5.36	118.45	122.20
54	BA	2687	U	C5-C6-N1	-5.36	120.02	122.70
55	BB	6	G	C4'-C3'-C2'	-5.36	97.24	102.60
21	AA	71	A	C3'-C2'-C1'	5.36	105.78	101.50
21	AA	874	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	233	A	C6-C5-N7	5.36	136.05	132.30
54	BA	653	U	N3-C2-O2	-5.36	118.45	122.20
54	BA	996	A	C6-C5-N7	5.36	136.05	132.30
54	BA	1185	G	N3-C2-N2	-5.36	116.15	119.90
54	BA	1470	A	C5-C6-N1	5.36	120.38	117.70
54	BA	2153	C	N3-C2-O2	-5.36	118.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2494	G	O4'-C1'-N9	5.36	112.48	108.20
54	BA	2890	G	N3-C4-C5	-5.36	125.92	128.60
33	BK	105	ARG	NE-CZ-NH1	5.35	122.98	120.30
54	BA	58	G	C8-N9-C4	-5.35	104.26	106.40
54	BA	528	A	C6-C5-N7	5.35	136.05	132.30
54	BA	1065	U	O4'-C1'-N1	5.35	112.48	108.20
21	AA	1058	G	C3'-C2'-C1'	5.35	105.78	101.50
54	BA	684	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	885	C	N3-C4-C5	5.35	124.04	121.90
54	BA	2239	G	N7-C8-N9	5.35	115.78	113.10
54	BA	2307	G	C5-C6-N1	5.35	114.18	111.50
54	BA	2680	U	N1-C2-N3	5.35	118.11	114.90
21	AA	248	C	O4'-C1'-N1	5.35	112.48	108.20
21	AA	968	A	O4'-C1'-N9	5.35	112.48	108.20
54	BA	341	C	C2-N3-C4	-5.35	117.22	119.90
54	BA	675	A	C4'-C3'-C2'	-5.35	97.25	102.60
54	BA	984	A	O4'-C4'-C3'	5.35	110.38	106.10
54	BA	2002	G	N3-C4-C5	-5.35	125.92	128.60
55	BB	110	C	N1-C2-O2	5.35	122.11	118.90
21	AA	575	G	P-O3'-C3'	5.35	126.12	119.70
21	AA	929	G	N7-C8-N9	5.35	115.77	113.10
54	BA	116	C	N3-C4-C5	5.35	124.04	121.90
54	BA	143	C	C6-N1-C2	-5.35	118.16	120.30
54	BA	291	G	C8-N9-C4	-5.35	104.26	106.40
54	BA	360	U	C5-C6-N1	-5.35	120.03	122.70
54	BA	1097	U	N1-C2-N3	5.35	118.11	114.90
54	BA	2669	G	O4'-C1'-N9	5.35	112.48	108.20
21	AA	170	U	N1-C2-N3	5.35	118.11	114.90
21	AA	392	C	N3-C4-C5	5.35	124.04	121.90
21	AA	874	G	C5-C6-N1	5.35	114.17	111.50
54	BA	1887	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	2089	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	2155	U	O4'-C1'-N1	5.35	112.48	108.20
54	BA	2325	G	C5-C6-N1	5.35	114.17	111.50
21	AA	1367	C	N1-C2-O2	5.35	122.11	118.90
54	BA	2069	G	C5-C6-N1	5.35	114.17	111.50
54	BA	2684	U	O4'-C1'-N1	5.35	112.48	108.20
55	BB	94	A	C5-C6-N6	5.35	127.98	123.70
21	AA	247	G	C8-N9-C4	-5.34	104.26	106.40
21	AA	1172	C	O4'-C1'-N1	5.34	112.47	108.20
23	A2	92	U	N1-C2-N3	5.34	118.11	114.90
35	BM	18	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BN	90	ARG	NE-CZ-NH1	5.34	122.97	120.30
54	BA	182	A	O4'-C1'-N9	5.34	112.48	108.20
54	BA	2174	C	N3-C4-C5	5.34	124.04	121.90
54	BA	2730	C	N3-C2-O2	-5.34	118.16	121.90
55	BB	104	A	C5-C6-N1	5.34	120.37	117.70
21	AA	917	G	C8-N9-C4	-5.34	104.26	106.40
21	AA	1038	C	N3-C4-C5	5.34	124.04	121.90
21	AA	1423	G	C2-N3-C4	5.34	114.57	111.90
54	BA	279	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	280	U	N3-C2-O2	-5.34	118.46	122.20
54	BA	605	G	C8-N9-C4	-5.34	104.26	106.40
54	BA	1612	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1727	C	O4'-C1'-N1	5.34	112.47	108.20
55	BB	76	G	C5-C6-N1	5.34	114.17	111.50
9	AJ	62	ARG	NE-CZ-NH1	5.34	122.97	120.30
21	AA	864	A	C5-C6-N1	5.34	120.37	117.70
54	BA	79	C	N1-C2-O2	5.34	122.11	118.90
54	BA	938	G	C5-C6-N1	5.34	114.17	111.50
54	BA	94	A	C6-C5-N7	5.34	136.04	132.30
54	BA	605	G	N3-C4-C5	-5.34	125.93	128.60
54	BA	1443	U	N3-C2-O2	-5.34	118.46	122.20
54	BA	1995	U	N1-C2-N3	5.34	118.10	114.90
54	BA	2554	U	C4-C5-C6	5.34	122.90	119.70
54	BA	1121	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1636	U	N1-C2-N3	5.34	118.10	114.90
54	BA	2035	G	N3-C2-N2	-5.34	116.16	119.90
54	BA	2876	G	N1-C6-O6	-5.34	116.70	119.90
20	AU	47	ALA	C-N-CA	5.34	135.04	121.70
21	AA	1257	A	C5-C6-N1	5.34	120.37	117.70
21	AA	1524	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	779	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	885	C	N1-C2-O2	5.34	122.10	118.90
54	BA	1770	G	N3-C2-N2	-5.34	116.16	119.90
54	BA	2146	C	O4'-C1'-N1	5.34	112.47	108.20
21	AA	152	A	C6-C5-N7	5.33	136.03	132.30
3	AD	80	ARG	NE-CZ-NH2	-5.33	117.63	120.30
21	AA	759	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	1138	G	N1-C6-O6	-5.33	116.70	119.90
41	BS	92	ARG	NH1-CZ-NH2	-5.33	113.53	119.40
54	BA	1299	G	O4'-C1'-N9	5.33	112.47	108.20
54	BA	1522	A	C4-C5-C6	-5.33	114.33	117.00
54	BA	2574	G	N1-C6-O6	-5.33	116.70	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2848	G	N1-C6-O6	-5.33	116.70	119.90
21	AA	1177	G	O4'-C1'-N9	5.33	112.47	108.20
24	A3	29	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	97	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	201	C	N3-C4-C5	5.33	124.03	121.90
54	BA	640	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	781	A	C5-C6-N1	5.33	120.37	117.70
54	BA	1155	A	C4-C5-C6	-5.33	114.33	117.00
54	BA	2427	C	C2-N3-C4	-5.33	117.23	119.90
54	BA	2497	A	N1-C6-N6	-5.33	115.40	118.60
54	BA	2807	U	N3-C2-O2	-5.33	118.47	122.20
21	AA	1357	A	C6-C5-N7	5.33	136.03	132.30
54	BA	574	A	C5-C6-N1	5.33	120.36	117.70
54	BA	1318	U	C5-C6-N1	-5.33	120.03	122.70
54	BA	2342	C	N1-C2-O2	5.33	122.10	118.90
55	BB	105	G	N1-C6-O6	-5.33	116.70	119.90
55	BB	108	A	N1-C6-N6	-5.33	115.40	118.60
1	AB	20	ARG	NE-CZ-NH1	5.33	122.97	120.30
21	AA	748	G	C8-N9-C4	-5.33	104.27	106.40
21	AA	777	A	N1-C6-N6	-5.33	115.40	118.60
41	BS	92	ARG	NE-CZ-NH2	5.33	122.96	120.30
54	BA	30	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	213	A	O4'-C1'-N9	5.33	112.46	108.20
54	BA	1271	G	C5-C6-N1	5.33	114.16	111.50
54	BA	1647	U	N1-C2-N3	5.33	118.10	114.90
54	BA	2822	G	N9-C4-C5	5.33	107.53	105.40
21	AA	494	G	N3-C4-C5	-5.33	125.94	128.60
54	BA	292	U	N3-C2-O2	-5.33	118.47	122.20
54	BA	1391	U	N3-C2-O2	-5.33	118.47	122.20
21	AA	407	U	N1-C2-N3	5.33	118.09	114.90
22	A1	13	C	N3-C2-O2	-5.33	118.17	121.90
48	BZ	37	ARG	NH1-CZ-NH2	-5.33	113.54	119.40
54	BA	598	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	720	U	N3-C2-O2	-5.33	118.47	122.20
54	BA	1195	G	N3-C2-N2	-5.33	116.17	119.90
54	BA	1228	G	C5-C6-N1	5.33	114.16	111.50
54	BA	1390	U	N1-C2-N3	5.33	118.10	114.90
54	BA	2095	A	C5-C6-N1	5.33	120.36	117.70
54	BA	2287	A	C2-N3-C4	5.33	113.26	110.60
54	BA	2465	C	O4'-C1'-N1	5.33	112.46	108.20
54	BA	2570	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	2626	C	N3-C4-C5	5.33	124.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	234	C	N3-C4-C5	5.32	124.03	121.90
21	AA	658	C	O4'-C1'-N1	5.32	112.46	108.20
21	AA	1421	G	N1-C6-O6	-5.32	116.70	119.90
54	BA	1942	C	N1-C2-O2	5.32	122.09	118.90
54	BA	2279	G	C4'-C3'-C2'	-5.32	97.28	102.60
21	AA	96	U	O4'-C1'-N1	5.32	112.46	108.20
21	AA	396	C	N1-C2-O2	5.32	122.09	118.90
26	BD	179	ARG	NE-CZ-NH1	5.32	122.96	120.30
54	BA	599	A	O4'-C1'-N9	5.32	112.46	108.20
54	BA	1561	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	2091	C	N3-C4-C5	5.32	124.03	121.90
21	AA	386	C	N1-C2-O2	5.32	122.09	118.90
21	AA	446	G	C5-C6-N1	5.32	114.16	111.50
21	AA	1150	A	C5-C6-N6	5.32	127.96	123.70
21	AA	1529	G	N3-C4-C5	-5.32	125.94	128.60
22	A1	16	C	N1-C2-O2	5.32	122.09	118.90
54	BA	196	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	397	U	C5-C6-N1	-5.32	120.04	122.70
54	BA	1776	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	2175	C	N1-C2-O2	5.32	122.09	118.90
54	BA	2762	C	N1-C2-O2	5.32	122.09	118.90
55	BB	76	G	N1-C6-O6	-5.32	116.71	119.90
55	BB	95	U	C5-C6-N1	-5.32	120.04	122.70
21	AA	1468	A	C6-C5-N7	5.32	136.02	132.30
54	BA	1671	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	1869	G	O4'-C1'-N9	5.32	112.46	108.20
21	AA	57	G	N3-C4-C5	-5.32	125.94	128.60
21	AA	1286	U	C5-C6-N1	-5.32	120.04	122.70
54	BA	1161	C	N1-C2-O2	5.32	122.09	118.90
54	BA	1564	C	N1-C2-O2	5.32	122.09	118.90
54	BA	1607	C	C6-N1-C2	-5.32	118.17	120.30
54	BA	2201	G	O4'-C1'-N9	5.32	112.45	108.20
54	BA	2676	C	N3-C4-C5	5.32	124.03	121.90
54	BA	2843	G	C5-C6-N1	5.32	114.16	111.50
20	AU	44	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
21	AA	845	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	868	C	N3-C2-O2	-5.32	118.18	121.90
21	AA	1076	U	N3-C2-O2	-5.32	118.48	122.20
22	A1	38	A	C6-C5-N7	5.32	136.02	132.30
24	A3	9	G	N3-C4-C5	-5.32	125.94	128.60
54	BA	111	A	C5'-C4'-O4'	5.32	115.48	109.10
54	BA	114	U	O4'-C1'-N1	5.32	112.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2893	A	C5-C6-N1	5.32	120.36	117.70
55	BB	24	G	C3'-C2'-C1'	5.32	105.75	101.50
21	AA	354	G	N1-C6-O6	-5.31	116.71	119.90
21	AA	493	A	C6-C5-N7	5.31	136.02	132.30
21	AA	945	G	C5-C6-N1	5.31	114.16	111.50
21	AA	1251	A	C6-C5-N7	5.31	136.02	132.30
24	A3	6	G	N9-C4-C5	5.31	107.53	105.40
28	BF	124	ARG	NE-CZ-NH2	-5.31	117.64	120.30
54	BA	2226	C	O4'-C1'-N1	5.31	112.45	108.20
20	AU	44	ARG	NE-CZ-NH2	5.31	122.96	120.30
21	AA	943	U	C5-C6-N1	-5.31	120.04	122.70
21	AA	1160	G	N3-C2-N2	-5.31	116.18	119.90
21	AA	1189	U	N3-C2-O2	-5.31	118.48	122.20
54	BA	937	C	O4'-C1'-N1	5.31	112.45	108.20
21	AA	469	C	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1514	G	N9-C4-C5	5.31	107.52	105.40
54	BA	2712	C	N1-C2-O2	5.31	122.09	118.90
21	AA	68	G	N3-C4-C5	-5.31	125.94	128.60
21	AA	504	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	956	G	N3-C2-N2	-5.31	116.18	119.90
54	BA	1795	C	C4'-C3'-C2'	-5.31	97.29	102.60
54	BA	2309	A	C4-C5-C6	-5.31	114.34	117.00
21	AA	330	C	N1-C2-O2	5.31	122.08	118.90
21	AA	1467	C	C2-N3-C4	-5.31	117.25	119.90
25	BC	211	ARG	NE-CZ-NH2	-5.31	117.65	120.30
54	BA	399	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	797	G	C5-C6-N1	5.31	114.15	111.50
54	BA	1602	U	N3-C2-O2	-5.31	118.48	122.20
54	BA	1813	G	N1-C6-O6	-5.31	116.72	119.90
54	BA	2556	C	N1-C2-O2	5.31	122.08	118.90
55	BB	87	U	N3-C2-O2	-5.31	118.48	122.20
22	A1	14	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	323	C	C3'-C2'-C1'	5.31	105.75	101.50
54	BA	1739	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	2216	G	N1-C6-O6	-5.31	116.72	119.90
54	BA	2848	G	O4'-C1'-N9	5.31	112.44	108.20
21	AA	1041	G	C8-N9-C4	-5.30	104.28	106.40
21	AA	1407	C	N3-C4-C5	5.30	124.02	121.90
54	BA	40	U	C4-C5-C6	5.30	122.88	119.70
54	BA	56	A	C6-C5-N7	5.30	136.01	132.30
54	BA	414	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	1192	G	C5-C6-N1	5.30	114.15	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1782	U	N3-C2-O2	-5.30	118.49	122.20
54	BA	2021	C	N3-C4-C5	5.30	124.02	121.90
55	BB	50	A	C5-C6-N1	5.30	120.35	117.70
21	AA	349	A	C6-C5-N7	5.30	136.01	132.30
54	BA	145	C	N1-C2-O2	5.30	122.08	118.90
54	BA	353	C	N3-C4-N4	-5.30	114.29	118.00
54	BA	1154	G	N7-C8-N9	5.30	115.75	113.10
54	BA	2391	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	152	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	1221	G	C5-C6-N1	5.30	114.15	111.50
24	A3	7	G	C5-C6-N1	5.30	114.15	111.50
54	BA	379	G	C5-C6-N1	5.30	114.15	111.50
54	BA	775	G	N3-C2-N2	-5.30	116.19	119.90
54	BA	1317	G	N9-C4-C5	5.30	107.52	105.40
54	BA	1369	G	N3-C4-C5	-5.30	125.95	128.60
54	BA	2872	A	C6-C5-N7	5.30	136.01	132.30
21	AA	494	G	N9-C4-C5	5.30	107.52	105.40
21	AA	657	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	1031	C	O4'-C1'-N1	5.30	112.44	108.20
21	AA	1284	C	N3-C2-O2	-5.30	118.19	121.90
21	AA	1379	G	C5-C6-N1	5.30	114.15	111.50
54	BA	192	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	737	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	759	G	N3-C2-N2	-5.30	116.19	119.90
54	BA	809	G	C4'-C3'-C2'	-5.30	97.30	102.60
54	BA	1894	C	N1-C2-O2	5.30	122.08	118.90
54	BA	2444	G	C5-C6-N1	5.30	114.15	111.50
21	AA	938	A	C1'-O4'-C4'	-5.30	105.66	109.90
21	AA	673	A	C4-C5-C6	-5.30	114.35	117.00
22	A1	2	G	C5-C6-N1	5.30	114.15	111.50
54	BA	498	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	1332	G	C1'-O4'-C4'	-5.30	105.66	109.90
54	BA	1526	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	1678	A	O4'-C1'-N9	5.30	112.44	108.20
54	BA	2101	A	C5-C6-N1	5.30	120.35	117.70
54	BA	2280	G	O4'-C1'-N9	5.30	112.44	108.20
55	BB	79	G	C8-N9-C4	-5.30	104.28	106.40
21	AA	526	C	N3-C4-C5	5.29	124.02	121.90
21	AA	1182	G	C5-C6-N1	5.29	114.15	111.50
54	BA	337	C	N3-C4-N4	-5.29	114.29	118.00
54	BA	704	G	N7-C8-N9	5.29	115.75	113.10
54	BA	1702	G	C5-C6-N1	5.29	114.15	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2000	C	N1-C2-O2	5.29	122.08	118.90
21	AA	545	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	184	C	N3-C4-C5	5.29	124.02	121.90
54	BA	442	G	N7-C8-N9	5.29	115.75	113.10
54	BA	1154	G	C8-N9-C4	-5.29	104.28	106.40
54	BA	2794	C	N1-C2-O2	5.29	122.08	118.90
21	AA	13	U	N1-C2-N3	5.29	118.08	114.90
21	AA	426	U	C5-C6-N1	-5.29	120.06	122.70
21	AA	478	A	C4-C5-C6	-5.29	114.36	117.00
21	AA	744	C	N1-C2-O2	5.29	122.08	118.90
21	AA	1432	G	N9-C4-C5	5.29	107.52	105.40
54	BA	16	C	N1-C2-O2	5.29	122.08	118.90
54	BA	48	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	1092	C	N3-C2-O2	-5.29	118.20	121.90
54	BA	1720	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1874	C	N1-C2-O2	5.29	122.07	118.90
54	BA	1976	U	C5-C6-N1	-5.29	120.05	122.70
54	BA	2788	C	C4'-C3'-C2'	-5.29	97.31	102.60
21	AA	51	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	621	A	C5-C6-N1	5.29	120.34	117.70
21	AA	383	A	C6-C5-N7	5.29	136.00	132.30
21	AA	1363	A	O4'-C1'-N9	5.29	112.43	108.20
21	AA	1504	G	N1-C6-O6	-5.29	116.73	119.90
24	A3	54	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	713	G	N3-C2-N2	-5.29	116.20	119.90
54	BA	975	A	C5-C6-N6	5.29	127.93	123.70
54	BA	2112	G	N9-C4-C5	5.29	107.52	105.40
21	AA	852	G	C8-N9-C4	-5.29	104.28	106.40
54	BA	451	U	N3-C2-O2	-5.29	118.50	122.20
21	AA	22	G	N3-C4-C5	-5.29	125.96	128.60
21	AA	234	C	N3-C2-O2	-5.29	118.20	121.90
21	AA	576	C	O4'-C1'-N1	5.29	112.43	108.20
21	AA	1516	G	O4'-C4'-C3'	5.29	110.33	106.10
24	A3	7	G	N3-C4-C5	-5.29	125.96	128.60
54	BA	160	A	C5'-C4'-O4'	5.29	115.44	109.10
54	BA	984	A	C6-C5-N7	5.29	136.00	132.30
54	BA	1084	A	C6-C5-N7	5.29	136.00	132.30
54	BA	1115	G	C5-C6-N1	5.29	114.14	111.50
54	BA	2008	C	N1-C2-O2	5.29	122.07	118.90
54	BA	2019	A	N1-C6-N6	-5.29	115.43	118.60
54	BA	2226	C	C2-N3-C4	-5.29	117.26	119.90
54	BA	2356	U	O4'-C1'-N1	5.29	112.43	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	5	U	C1'-O4'-C4'	-5.28	105.67	109.90
21	AA	524	G	C5-C6-N1	5.28	114.14	111.50
22	A1	2	G	N1-C6-O6	-5.28	116.73	119.90
22	A1	47	U	C3'-C2'-C1'	5.28	105.73	101.50
54	BA	1356	G	C8-N9-C4	-5.28	104.29	106.40
54	BA	1549	A	C6-C5-N7	5.28	136.00	132.30
54	BA	1947	C	N1-C2-O2	5.28	122.07	118.90
54	BA	2310	C	N1-C2-O2	5.28	122.07	118.90
21	AA	1383	C	N3-C2-O2	-5.28	118.20	121.90
54	BA	578	G	C5-C6-N1	5.28	114.14	111.50
54	BA	907	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	1585	C	N1-C2-O2	5.28	122.07	118.90
54	BA	1636	U	C4-C5-C6	5.28	122.87	119.70
21	AA	602	A	C5-C6-N1	5.28	120.34	117.70
21	AA	614	C	N3-C4-C5	5.28	124.01	121.90
21	AA	1173	U	N3-C2-O2	-5.28	118.50	122.20
21	AA	1452	C	N3-C4-C5	5.28	124.01	121.90
21	AA	1487	G	N7-C8-N9	5.28	115.74	113.10
54	BA	1128	G	C1'-O4'-C4'	-5.28	105.68	109.90
54	BA	1290	C	C4'-C3'-C2'	-5.28	97.32	102.60
54	BA	1963	U	N3-C2-O2	-5.28	118.50	122.20
54	BA	2267	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	1152	A	C6-C5-N7	5.28	136.00	132.30
54	BA	2427	C	N1-C2-O2	5.28	122.07	118.90
54	BA	2793	C	O4'-C1'-N1	5.28	112.42	108.20
21	AA	275	G	N3-C4-C5	-5.28	125.96	128.60
21	AA	639	G	C5-C6-N1	5.28	114.14	111.50
21	AA	892	A	C6-C5-N7	5.28	136.00	132.30
22	A1	33	U	N3-C2-O2	-5.28	118.50	122.20
54	BA	193	U	O4'-C1'-N1	5.28	112.42	108.20
54	BA	362	A	C5'-C4'-C3'	-5.28	107.55	116.00
54	BA	677	A	C5-C6-N1	5.28	120.34	117.70
54	BA	910	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1221	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	1633	G	O4'-C1'-N9	5.28	112.42	108.20
54	BA	1723	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	2363	G	N3-C4-N9	5.28	129.17	126.00
54	BA	2709	G	C5-C6-N1	5.28	114.14	111.50
55	BB	106	G	N3-C4-C5	-5.28	125.96	128.60
54	BA	99	U	N3-C2-O2	-5.28	118.51	122.20
54	BA	309	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	574	A	C4-C5-C6	-5.28	114.36	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1347	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1433	A	N1-C6-N6	-5.28	115.44	118.60
54	BA	2044	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2200	C	N3-C2-O2	-5.28	118.21	121.90
54	BA	2236	U	N3-C2-O2	-5.28	118.51	122.20
54	BA	229	C	N1-C2-O2	5.27	122.06	118.90
54	BA	521	U	C5-C6-N1	-5.27	120.06	122.70
54	BA	1418	G	N3-C4-C5	-5.27	125.96	128.60
54	BA	1815	A	C5-C6-N1	5.27	120.34	117.70
54	BA	2618	G	N3-C4-C5	-5.27	125.96	128.60
21	AA	821	G	N3-C4-C5	-5.27	125.96	128.60
21	AA	1045	C	N1-C2-O2	5.27	122.06	118.90
54	BA	2442	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2556	C	N3-C4-N4	-5.27	114.31	118.00
54	BA	1272	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	2726	A	O4'-C1'-C2'	-5.27	100.53	105.80
54	BA	2804	U	O4'-C1'-N1	5.27	112.42	108.20
21	AA	1066	C	N3-C2-O2	-5.27	118.21	121.90
21	AA	1216	A	C4'-C3'-C2'	-5.27	97.33	102.60
21	AA	1500	A	C5-C6-N1	5.27	120.33	117.70
54	BA	113	U	C5-C6-N1	-5.27	120.06	122.70
54	BA	439	A	C2-N3-C4	5.27	113.23	110.60
54	BA	505	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	1086	A	C4-C5-C6	-5.27	114.37	117.00
54	BA	2300	C	N1-C2-O2	5.27	122.06	118.90
56	B5	60	ARG	NE-CZ-NH1	5.27	122.94	120.30
21	AA	57	G	C5-C6-N1	5.27	114.13	111.50
21	AA	331	G	N7-C8-N9	5.27	115.73	113.10
21	AA	658	C	N3-C4-C5	5.27	124.01	121.90
21	AA	1232	U	N1-C2-N3	5.27	118.06	114.90
24	A3	48	U	C5'-C4'-C3'	-5.27	107.57	116.00
39	BQ	91	ARG	NH1-CZ-NH2	-5.27	113.61	119.40
54	BA	35	G	C5-C6-N1	5.27	114.13	111.50
54	BA	234	U	O4'-C1'-N1	5.27	112.41	108.20
54	BA	243	U	O4'-C1'-N1	5.27	112.41	108.20
54	BA	437	U	N1-C2-N3	5.27	118.06	114.90
54	BA	817	C	N1-C2-O2	5.27	122.06	118.90
54	BA	1167	C	O4'-C1'-N1	5.27	112.41	108.20
54	BA	1210	G	C8-N9-C4	-5.27	104.29	106.40
54	BA	2276	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	139	U	N1-C2-N3	5.27	118.06	114.90
54	BA	440	C	N3-C2-O2	-5.27	118.21	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	575	A	C5-C6-N1	5.27	120.33	117.70
54	BA	583	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	2038	G	N3-C4-C5	-5.27	125.97	128.60
54	BA	2038	G	C8-N9-C4	-5.27	104.29	106.40
21	AA	82	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	111	G	N3-C4-C5	-5.26	125.97	128.60
21	AA	1038	C	N1-C2-O2	5.26	122.06	118.90
21	AA	1056	U	N3-C2-O2	-5.26	118.52	122.20
21	AA	1070	U	C5-C6-N1	-5.26	120.07	122.70
24	A3	77	A	C4-C5-C6	-5.26	114.37	117.00
36	BN	46	ARG	NE-CZ-NH2	-5.26	117.67	120.30
54	BA	1831	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	2619	C	N1-C2-O2	5.26	122.06	118.90
54	BA	2709	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	2767	C	O4'-C1'-N1	5.26	112.41	108.20
55	BB	47	C	N3-C2-O2	-5.26	118.22	121.90
10	AK	35	ASP	CB-CG-OD2	5.26	123.04	118.30
21	AA	147	G	O4'-C1'-N9	5.26	112.41	108.20
54	BA	67	U	N1-C2-N3	5.26	118.06	114.90
55	BB	98	G	N7-C8-N9	5.26	115.73	113.10
55	BB	105	G	N9-C4-C5	5.26	107.50	105.40
21	AA	1071	C	C2-N3-C4	-5.26	117.27	119.90
22	A1	71	C	N1-C2-O2	5.26	122.06	118.90
24	A3	3	C	N1-C2-O2	5.26	122.06	118.90
54	BA	87	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	89	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	652	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	1761	C	C2-N3-C4	-5.26	117.27	119.90
17	AR	56	ARG	NH1-CZ-NH2	-5.26	113.61	119.40
54	BA	125	A	C2-N3-C4	5.26	113.23	110.60
54	BA	607	U	C5-C6-N1	-5.26	120.07	122.70
54	BA	745	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	784	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	2239	G	C8-N9-C4	-5.26	104.30	106.40
54	BA	2707	U	N1-C2-N3	5.26	118.06	114.90
55	BB	4	C	N1-C2-O2	5.26	122.06	118.90
21	AA	1208	C	O4'-C1'-N1	5.26	112.41	108.20
54	BA	188	G	C5-C6-N1	5.26	114.13	111.50
21	AA	38	G	C5-C6-N1	5.26	114.13	111.50
21	AA	348	G	N3-C4-C5	-5.26	125.97	128.60
21	AA	795	C	N1-C2-O2	5.26	122.05	118.90
21	AA	1389	C	N3-C2-O2	-5.26	118.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1405	G	C4-C5-N7	-5.26	108.70	110.80
54	BA	396	G	C5-C6-N1	5.26	114.13	111.50
54	BA	536	G	C8-N9-C4	-5.26	104.30	106.40
54	BA	1389	G	O4'-C1'-N9	5.26	112.41	108.20
54	BA	1848	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	2334	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	2588	G	N3-C2-N2	-5.26	116.22	119.90
54	BA	2683	C	N1-C2-O2	5.26	122.05	118.90
21	AA	1427	C	C6-N1-C2	-5.25	118.20	120.30
24	A3	49	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2049	G	C5-C6-N1	5.25	114.13	111.50
54	BA	2672	U	O4'-C1'-N1	5.25	112.40	108.20
21	AA	1367	C	C2-N3-C4	-5.25	117.27	119.90
25	BC	100	ARG	NE-CZ-NH1	5.25	122.93	120.30
54	BA	209	C	N1-C2-O2	5.25	122.05	118.90
54	BA	371	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	431	U	N1-C2-N3	5.25	118.05	114.90
54	BA	1045	C	N3-C4-C5	5.25	124.00	121.90
54	BA	2425	A	C5-C6-N1	5.25	120.33	117.70
21	AA	8	A	O4'-C1'-N9	5.25	112.40	108.20
21	AA	993	G	O4'-C1'-N9	5.25	112.40	108.20
21	AA	1066	C	N1-C2-O2	5.25	122.05	118.90
24	A3	29	C	N1-C2-O2	5.25	122.05	118.90
54	BA	113	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	363	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	867	C	N3-C2-O2	-5.25	118.22	121.90
54	BA	1171	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	2554	U	C5'-C4'-C3'	-5.25	107.60	116.00
8	AI	32	ARG	NE-CZ-NH1	5.25	122.92	120.30
21	AA	305	G	C4-C5-N7	-5.25	108.70	110.80
21	AA	227	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	349	A	O4'-C1'-N9	5.25	112.40	108.20
21	AA	359	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	509	A	C2-N3-C4	5.25	113.22	110.60
54	BA	877	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	1449	G	C4'-C3'-C2'	-5.25	97.35	102.60
54	BA	1582	C	N1-C2-O2	5.25	122.05	118.90
54	BA	1729	U	C4-C5-C6	5.25	122.85	119.70
54	BA	1972	G	N7-C8-N9	5.25	115.72	113.10
21	AA	292	G	N7-C8-N9	5.25	115.72	113.10
21	AA	517	G	O4'-C1'-N9	5.25	112.40	108.20
21	AA	1406	U	O4'-C1'-N1	5.25	112.40	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	68	C	C1'-O4'-C4'	-5.25	105.70	109.90
54	BA	2041	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2282	G	N9-C4-C5	5.25	107.50	105.40
21	AA	883	C	N3-C2-O2	-5.25	118.23	121.90
21	AA	1519	A	C6-C5-N7	5.25	135.97	132.30
54	BA	1063	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	1323	C	N1-C2-O2	5.25	122.05	118.90
54	BA	1481	U	N3-C2-O2	-5.25	118.53	122.20
21	AA	151	A	C5-C6-N1	5.24	120.32	117.70
21	AA	792	A	C1'-O4'-C4'	-5.24	105.71	109.90
21	AA	1346	A	C6-C5-N7	5.24	135.97	132.30
21	AA	1524	C	N1-C2-O2	5.24	122.05	118.90
24	A3	64	G	C5-N7-C8	-5.24	101.68	104.30
54	BA	693	A	C6-C5-N7	5.24	135.97	132.30
54	BA	2699	C	C2-N3-C4	-5.24	117.28	119.90
54	BA	2820	A	N1-C6-N6	-5.24	115.45	118.60
21	AA	6	G	N7-C8-N9	5.24	115.72	113.10
21	AA	741	G	N7-C8-N9	5.24	115.72	113.10
21	AA	793	U	N3-C2-O2	-5.24	118.53	122.20
20	AU	16	ARG	NE-CZ-NH1	5.24	122.92	120.30
21	AA	222	C	N1-C2-O2	5.24	122.04	118.90
21	AA	304	U	C5-C6-N1	-5.24	120.08	122.70
21	AA	643	C	N3-C2-O2	-5.24	118.23	121.90
21	AA	709	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	1243	C	C6-N1-C2	-5.24	118.20	120.30
21	AA	1472	U	C4-C5-C6	5.24	122.84	119.70
23	A2	93	U	N3-C2-O2	-5.24	118.53	122.20
54	BA	973	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	1346	G	C4'-C3'-C2'	-5.24	97.36	102.60
54	BA	1555	G	C5-C6-N1	5.24	114.12	111.50
54	BA	1611	C	N1-C2-O2	5.24	122.04	118.90
54	BA	2080	A	C2-N3-C4	5.24	113.22	110.60
54	BA	2164	C	N1-C2-O2	5.24	122.04	118.90
55	BB	56	G	O4'-C4'-C3'	5.24	110.29	106.10
21	AA	1085	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	1108	G	C8-N9-C4	-5.24	104.31	106.40
21	AA	1312	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	467	G	N9-C4-C5	5.24	107.50	105.40
54	BA	1094	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	1531	C	O4'-C1'-N1	5.24	112.39	108.20
55	BB	100	G	N7-C8-N9	5.24	115.72	113.10
54	BA	731	C	O4'-C1'-N1	5.24	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1736	U	C5-C6-N1	-5.24	120.08	122.70
54	BA	2042	A	C5-C6-N1	5.24	120.32	117.70
21	AA	1345	U	O4'-C1'-N1	5.24	112.39	108.20
21	AA	1503	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	1521	G	C5-C6-N1	5.24	114.12	111.50
54	BA	1925	C	N3-C4-C5	5.24	124.00	121.90
10	AK	121	ARG	NE-CZ-NH2	5.23	122.92	120.30
21	AA	73	C	N1-C2-O2	5.23	122.04	118.90
54	BA	792	A	C2-N3-C4	5.23	113.22	110.60
54	BA	1185	G	O4'-C1'-N9	5.23	112.39	108.20
54	BA	2140	G	O4'-C1'-N9	5.23	112.39	108.20
54	BA	2790	U	C5-C6-N1	-5.23	120.08	122.70
21	AA	220	G	C8-N9-C4	-5.23	104.31	106.40
21	AA	1203	C	N1-C2-O2	5.23	122.04	118.90
54	BA	201	C	N1-C2-O2	5.23	122.04	118.90
54	BA	268	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	836	G	N3-C2-N2	-5.23	116.24	119.90
54	BA	969	G	C8-N9-C4	-5.23	104.31	106.40
54	BA	991	C	C6-N1-C2	-5.23	118.21	120.30
54	BA	1454	C	N3-C4-C5	5.23	123.99	121.90
54	BA	2759	G	C8-N9-C4	-5.23	104.31	106.40
21	AA	191	G	N3-C4-C5	-5.23	125.98	128.60
21	AA	216	U	N3-C2-O2	-5.23	118.54	122.20
21	AA	382	A	C6-C5-N7	5.23	135.96	132.30
54	BA	147	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	1118	C	N1-C2-O2	5.23	122.04	118.90
54	BA	1462	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	2209	G	C5-C6-N1	5.23	114.11	111.50
55	BB	46	A	C6-C5-N7	5.23	135.96	132.30
54	BA	2330	G	O4'-C1'-N9	5.23	112.38	108.20
21	AA	509	A	C6-C5-N7	5.23	135.96	132.30
21	AA	682	G	C5-C6-N1	5.23	114.11	111.50
21	AA	885	G	C5-C6-N1	5.23	114.11	111.50
21	AA	1183	U	N3-C2-O2	-5.23	118.54	122.20
21	AA	1355	G	N9-C4-C5	5.23	107.49	105.40
54	BA	358	U	N3-C2-O2	-5.23	118.54	122.20
54	BA	1826	G	P-O3'-C3'	5.23	125.97	119.70
54	BA	2050	C	O4'-C1'-N1	5.23	112.38	108.20
54	BA	2154	A	O4'-C1'-N9	5.23	112.38	108.20
54	BA	2256	G	N7-C8-N9	5.23	115.71	113.10
54	BA	2839	G	N3-C4-C5	-5.23	125.99	128.60
55	BB	76	G	O4'-C1'-N9	5.23	112.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1401	G	N3-C4-N9	5.23	129.14	126.00
54	BA	1556	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	2715	C	C6-N1-C2	-5.23	118.21	120.30
54	BA	2893	A	C4-C5-C6	-5.23	114.39	117.00
55	BB	114	C	N3-C4-C5	5.23	123.99	121.90
21	AA	83	C	O4'-C1'-N1	5.22	112.38	108.20
21	AA	1355	G	N3-C4-C5	-5.22	125.99	128.60
54	BA	104	A	C6-C5-N7	5.22	135.96	132.30
54	BA	208	C	C2-N3-C4	-5.22	117.29	119.90
54	BA	607	U	N3-C2-O2	-5.22	118.54	122.20
54	BA	617	G	N3-C4-C5	-5.22	125.99	128.60
54	BA	968	C	N3-C2-O2	-5.22	118.24	121.90
54	BA	998	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1345	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1707	G	C5-C6-N1	5.22	114.11	111.50
54	BA	1746	A	C6-C5-N7	5.22	135.96	132.30
21	AA	634	C	N1-C2-O2	5.22	122.03	118.90
21	AA	686	U	C4-C5-C6	5.22	122.83	119.70
21	AA	820	U	N1-C2-N3	5.22	118.03	114.90
21	AA	1192	C	N3-C2-O2	-5.22	118.24	121.90
21	AA	1269	A	C4-C5-C6	-5.22	114.39	117.00
22	A1	59	U	C3'-C2'-C1'	5.22	105.68	101.50
54	BA	608	A	C2-N3-C4	5.22	113.21	110.60
54	BA	1180	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	2527	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2620	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	2886	A	C8-N9-C4	-5.22	103.71	105.80
21	AA	444	G	N3-C4-C5	-5.22	125.99	128.60
21	AA	661	G	N3-C2-N2	-5.22	116.25	119.90
54	BA	10	A	O4'-C1'-N9	5.22	112.38	108.20
54	BA	509	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1194	A	N1-C6-N6	-5.22	115.47	118.60
54	BA	2201	G	N9-C4-C5	5.22	107.49	105.40
54	BA	659	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	772	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	810	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	1288	G	N3-C4-C5	-5.22	125.99	128.60
54	BA	2059	A	C5-C6-N1	5.22	120.31	117.70
54	BA	2337	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	2642	G	C4'-C3'-C2'	-5.22	97.38	102.60
54	BA	2807	U	N1-C2-N3	5.22	118.03	114.90
13	AN	65	ARG	NE-CZ-NH1	5.22	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	886	G	O4'-C1'-N9	5.22	112.37	108.20
21	AA	1391	U	N3-C2-O2	-5.22	118.55	122.20
54	BA	607	U	C5'-C4'-O4'	5.22	115.36	109.10
54	BA	2071	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	2175	C	O4'-C1'-N1	5.22	112.37	108.20
55	BB	35	C	N1-C2-O2	5.22	122.03	118.90
21	AA	419	C	C1'-O4'-C4'	-5.22	105.73	109.90
21	AA	595	A	C3'-C2'-C1'	5.22	105.67	101.50
21	AA	722	G	O4'-C1'-N9	5.22	112.37	108.20
21	AA	1298	U	O4'-C1'-N1	5.22	112.37	108.20
21	AA	1375	A	C6-C5-N7	5.22	135.95	132.30
54	BA	4	U	N3-C2-O2	-5.22	118.55	122.20
54	BA	64	A	C6-C5-N7	5.22	135.95	132.30
54	BA	287	G	C5-C6-N1	5.22	114.11	111.50
54	BA	637	A	C5-C6-N1	5.22	120.31	117.70
54	BA	823	C	N3-C2-O2	-5.22	118.25	121.90
54	BA	891	G	C8-N9-C4	-5.22	104.31	106.40
54	BA	2301	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2675	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	2818	U	N3-C2-O2	-5.22	118.55	122.20
21	AA	746	A	C5-C6-N1	5.21	120.31	117.70
42	BT	3	ARG	NE-CZ-NH2	-5.21	117.69	120.30
54	BA	658	U	N3-C2-O2	-5.21	118.55	122.20
54	BA	883	G	C5-C6-N1	5.21	114.11	111.50
54	BA	1777	U	N3-C2-O2	-5.21	118.55	122.20
21	AA	243	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	813	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1056	G	C5-C6-N1	5.21	114.11	111.50
54	BA	1087	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	1237	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	2426	A	C6-C5-N7	5.21	135.95	132.30
21	AA	420	U	N1-C2-N3	5.21	118.03	114.90
21	AA	474	G	C5-C6-N1	5.21	114.11	111.50
54	BA	247	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	452	G	C5'-C4'-O4'	5.21	115.35	109.10
54	BA	1364	G	C5-C6-N1	5.21	114.11	111.50
54	BA	1879	C	N1-C2-O2	5.21	122.03	118.90
54	BA	2563	U	N1-C2-N3	5.21	118.03	114.90
55	BB	85	G	N7-C8-N9	5.21	115.70	113.10
21	AA	33	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	127	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	1002	G	O4'-C1'-N9	5.21	112.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1081	U	N3-C2-O2	-5.21	118.55	122.20
54	BA	1219	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2331	G	N1-C6-O6	-5.21	116.77	119.90
21	AA	1043	G	N3-C4-C5	-5.21	126.00	128.60
21	AA	1056	U	C4-C5-C6	5.21	122.83	119.70
21	AA	1080	A	N7-C8-N9	5.21	116.40	113.80
21	AA	1458	G	N3-C4-C5	-5.21	126.00	128.60
24	A3	45	A	C6-C5-N7	5.21	135.94	132.30
54	BA	584	C	N1-C2-O2	5.21	122.03	118.90
54	BA	1289	C	N1-C2-O2	5.21	122.03	118.90
54	BA	1835	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	2005	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	2240	U	N1-C2-N3	5.21	118.03	114.90
54	BA	2584	U	O4'-C1'-N1	5.21	112.37	108.20
55	BB	65	U	O4'-C1'-N1	5.21	112.37	108.20
14	AO	76	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
21	AA	641	U	N3-C2-O2	-5.21	118.56	122.20
21	AA	1116	U	N3-C2-O2	-5.21	118.56	122.20
54	BA	62	U	C4-C5-C6	5.21	122.82	119.70
54	BA	1008	A	C4-C5-C6	-5.21	114.40	117.00
54	BA	1286	A	C4-C5-C6	-5.21	114.40	117.00
54	BA	1529	G	C5-C6-N1	5.21	114.10	111.50
54	BA	1552	A	C1'-O4'-C4'	-5.21	105.73	109.90
54	BA	2221	G	N3-C4-C5	-5.21	126.00	128.60
54	BA	2321	U	C4-C5-C6	5.21	122.82	119.70
54	BA	2388	A	N1-C6-N6	-5.21	115.48	118.60
54	BA	2856	A	C6-C5-N7	5.21	135.94	132.30
54	BA	285	G	O4'-C1'-N9	5.21	112.36	108.20
54	BA	1658	C	N1-C2-O2	5.21	122.02	118.90
54	BA	1798	U	O4'-C1'-N1	5.21	112.36	108.20
54	BA	2099	U	N3-C2-O2	-5.21	118.56	122.20
21	AA	882	C	N3-C4-C5	5.20	123.98	121.90
21	AA	1206	G	N7-C8-N9	5.20	115.70	113.10
21	AA	1448	C	N3-C2-O2	-5.20	118.26	121.90
49	B0	39	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
54	BA	97	C	C5'-C4'-O4'	5.20	115.34	109.10
54	BA	1933	G	N7-C8-N9	5.20	115.70	113.10
54	BA	1996	C	N3-C4-C5	5.20	123.98	121.90
54	BA	2078	C	C5'-C4'-O4'	5.20	115.34	109.10
54	BA	2729	G	N3-C2-N2	-5.20	116.26	119.90
21	AA	590	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	232	G	N3-C4-C5	-5.20	126.00	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	764	A	O4'-C1'-N9	5.20	112.36	108.20
54	BA	987	C	N3-C2-O2	-5.20	118.26	121.90
21	AA	58	C	N3-C4-C5	5.20	123.98	121.90
21	AA	1458	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	212	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	594	U	C5-C6-N1	-5.20	120.10	122.70
54	BA	1256	G	N3-C2-N2	-5.20	116.26	119.90
55	BB	34	A	C4-C5-C6	-5.20	114.40	117.00
55	BB	54	G	N3-C4-C5	-5.20	126.00	128.60
21	AA	34	C	N3-C4-C5	5.20	123.98	121.90
21	AA	824	G	N3-C2-N2	-5.20	116.26	119.90
21	AA	1026	G	N1-C6-O6	-5.20	116.78	119.90
21	AA	1231	G	N3-C2-N2	-5.20	116.26	119.90
21	AA	1231	G	C8-N9-C4	-5.20	104.32	106.40
21	AA	1392	G	N1-C6-O6	-5.20	116.78	119.90
21	AA	1435	G	C5-C6-N1	5.20	114.10	111.50
54	BA	116	C	N3-C4-N4	-5.20	114.36	118.00
54	BA	346	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	2544	G	N7-C8-N9	5.20	115.70	113.10
54	BA	618	G	C5-C6-N1	5.20	114.10	111.50
54	BA	1122	G	N7-C8-N9	5.20	115.70	113.10
54	BA	2591	C	N1-C2-O2	5.20	122.02	118.90
54	BA	2610	C	N3-C4-C5	5.20	123.98	121.90
54	BA	2725	A	C5-C6-N1	5.20	120.30	117.70
21	AA	36	C	N1-C2-O2	5.20	122.02	118.90
21	AA	1182	G	N9-C4-C5	5.20	107.48	105.40
54	BA	114	U	N1-C2-N3	5.20	118.02	114.90
54	BA	544	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	586	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	1407	G	C4'-C3'-C2'	-5.20	97.41	102.60
54	BA	389	G	N9-C4-C5	5.19	107.48	105.40
54	BA	1068	G	C5-C6-N1	5.19	114.10	111.50
54	BA	1214	A	C4-C5-C6	-5.19	114.40	117.00
54	BA	1651	G	O4'-C1'-N9	5.19	112.36	108.20
54	BA	1712	U	N3-C2-O2	-5.19	118.56	122.20
54	BA	2142	A	C6-C5-N7	5.19	135.94	132.30
54	BA	2198	A	C6-C5-N7	5.19	135.94	132.30
54	BA	2372	U	C5'-C4'-O4'	5.19	115.33	109.10
21	AA	1099	G	C5-C6-N1	5.19	114.10	111.50
21	AA	1318	A	C6-C5-N7	5.19	135.94	132.30
21	AA	1488	G	N1-C6-O6	-5.19	116.78	119.90
54	BA	67	U	C5-C6-N1	-5.19	120.10	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1585	C	N3-C4-C5	5.19	123.98	121.90
21	AA	129	A	C3'-C2'-C1'	5.19	105.65	101.50
54	BA	123	G	O4'-C1'-N9	5.19	112.35	108.20
54	BA	908	C	N3-C4-C5	5.19	123.98	121.90
54	BA	1312	U	N3-C2-O2	-5.19	118.57	122.20
54	BA	2289	G	N3-C4-C5	-5.19	126.00	128.60
54	BA	2366	A	C5-C6-N1	5.19	120.30	117.70
54	BA	2806	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	2623	G	C8-N9-C4	-5.19	104.32	106.40
54	BA	2664	G	C5-C6-N1	5.19	114.09	111.50
21	AA	498	A	C2-N3-C4	5.19	113.19	110.60
21	AA	605	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	33	C	N1-C2-O2	5.19	122.01	118.90
54	BA	58	G	N9-C4-C5	5.19	107.47	105.40
54	BA	837	C	C6-N1-C2	-5.19	118.22	120.30
54	BA	1335	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	1671	U	C5-C6-N1	-5.19	120.11	122.70
54	BA	2255	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	2398	U	N3-C2-O2	-5.19	118.57	122.20
54	BA	2554	U	N1-C2-N3	5.19	118.01	114.90
21	AA	827	U	C5-C6-N1	-5.19	120.11	122.70
54	BA	129	C	N1-C2-O2	5.19	122.01	118.90
54	BA	510	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	1207	C	N3-C2-O2	-5.19	118.27	121.90
21	AA	220	G	N3-C4-C5	-5.18	126.01	128.60
21	AA	522	C	C2-N3-C4	-5.18	117.31	119.90
21	AA	564	C	N1-C2-O2	5.18	122.01	118.90
21	AA	1049	U	N3-C2-O2	-5.18	118.57	122.20
21	AA	1063	C	N1-C2-O2	5.18	122.01	118.90
54	BA	322	A	C2-N3-C4	5.18	113.19	110.60
54	BA	844	A	C5-C6-N1	5.18	120.29	117.70
54	BA	1023	U	N3-C2-O2	-5.18	118.57	122.20
54	BA	1674	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	1759	A	N9-C4-C5	5.18	107.87	105.80
54	BA	2362	C	C2-N3-C4	-5.18	117.31	119.90
21	AA	79	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	123	U	N3-C2-O2	-5.18	118.57	122.20
21	AA	310	G	N3-C2-N2	-5.18	116.27	119.90
21	AA	527	G	N3-C4-C5	-5.18	126.01	128.60
21	AA	1261	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	100	U	N3-C2-O2	-5.18	118.57	122.20
54	BA	325	G	N3-C4-C5	-5.18	126.01	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	352	A	N9-C4-C5	5.18	107.87	105.80
54	BA	1930	G	C5-C6-N1	5.18	114.09	111.50
54	BA	2671	G	C5-C6-N1	5.18	114.09	111.50
55	BB	36	C	N1-C2-O2	5.18	122.01	118.90
55	BB	81	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	2459	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2708	G	N3-C4-C5	-5.18	126.01	128.60
21	AA	370	C	C2-N3-C4	-5.18	117.31	119.90
21	AA	518	C	N1-C2-O2	5.18	122.01	118.90
21	AA	675	A	C5-C6-N1	5.18	120.29	117.70
21	AA	755	G	O4'-C4'-C3'	5.18	110.24	106.10
21	AA	1371	G	N3-C2-N2	-5.18	116.28	119.90
21	AA	1489	G	N3-C4-C5	-5.18	126.01	128.60
54	BA	1359	A	O4'-C1'-N9	5.18	112.34	108.20
54	BA	2066	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	447	A	C6-C5-N7	5.18	135.93	132.30
54	BA	784	G	P-O3'-C3'	5.18	125.91	119.70
54	BA	1246	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	288	A	O4'-C1'-N9	5.18	112.34	108.20
21	AA	328	C	N3-C4-C5	5.18	123.97	121.90
21	AA	346	G	C2-N3-C4	5.18	114.49	111.90
54	BA	307	G	C5-C6-N1	5.18	114.09	111.50
54	BA	389	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	604	G	C8-N9-C4	-5.18	104.33	106.40
54	BA	1464	G	C5-C6-N1	5.18	114.09	111.50
55	BB	35	C	N3-C4-C5	5.18	123.97	121.90
21	AA	1487	G	N3-C2-N2	-5.17	116.28	119.90
54	BA	299	A	C2-N3-C4	5.17	113.19	110.60
54	BA	600	G	N3-C4-C5	-5.17	126.01	128.60
54	BA	1255	U	C1'-O4'-C4'	-5.17	105.76	109.90
54	BA	1745	A	C4-C5-C6	-5.17	114.41	117.00
54	BA	1895	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	2371	G	C8-N9-C4	-5.17	104.33	106.40
54	BA	2411	A	O4'-C1'-N9	5.17	112.34	108.20
54	BA	2716	C	C5'-C4'-O4'	5.17	115.31	109.10
54	BA	2882	A	C6-C5-N7	5.17	135.92	132.30
54	BA	1767	G	O4'-C1'-N9	5.17	112.34	108.20
54	BA	1808	A	C6-C5-N7	5.17	135.92	132.30
54	BA	1843	C	N3-C2-O2	-5.17	118.28	121.90
21	AA	38	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	128	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	580	C	N1-C2-O2	5.17	122.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1049	U	C4-C5-C6	5.17	122.80	119.70
21	AA	1411	C	N1-C2-O2	5.17	122.00	118.90
54	BA	62	U	N1-C2-N3	5.17	118.00	114.90
54	BA	913	U	O4'-C1'-N1	5.17	112.34	108.20
54	BA	1363	C	C5'-C4'-O4'	5.17	115.31	109.10
54	BA	1582	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	1663	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1813	G	O4'-C1'-N9	5.17	112.34	108.20
54	BA	2103	C	C2-N3-C4	-5.17	117.31	119.90
54	BA	2685	G	N3-C2-N2	-5.17	116.28	119.90
35	BM	114	ARG	NE-CZ-NH2	-5.17	117.72	120.30
54	BA	1756	G	C5-C6-N1	5.17	114.08	111.50
54	BA	1766	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	2079	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	2654	A	C6-C5-N7	5.17	135.92	132.30
21	AA	20	U	O4'-C1'-N1	5.17	112.33	108.20
21	AA	465	A	N7-C8-N9	5.17	116.39	113.80
21	AA	491	G	C5-C6-N1	5.17	114.08	111.50
21	AA	920	U	C5-C6-N1	-5.17	120.12	122.70
21	AA	1064	G	N7-C8-N9	5.17	115.68	113.10
21	AA	1467	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1446	C	C6-N1-C2	-5.17	118.23	120.30
54	BA	2053	G	N9-C4-C5	5.17	107.47	105.40
36	BN	2	ARG	NE-CZ-NH1	5.17	122.88	120.30
54	BA	37	C	N1-C2-O2	5.17	122.00	118.90
54	BA	148	U	O4'-C1'-N1	5.17	112.33	108.20
54	BA	851	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	1873	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	2104	C	N3-C4-N4	-5.17	114.38	118.00
54	BA	2109	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	2163	A	C4-C5-C6	-5.17	114.42	117.00
54	BA	2501	C	N3-C2-O2	-5.17	118.28	121.90
5	AF	91	ARG	NE-CZ-NH1	5.17	122.88	120.30
21	AA	520	A	C5-C6-N1	5.17	120.28	117.70
21	AA	1192	C	N3-C4-C5	5.17	123.97	121.90
54	BA	1613	G	N3-C2-N2	-5.17	116.28	119.90
54	BA	2225	A	C5-C6-N1	5.17	120.28	117.70
54	BA	2686	G	C8-N9-C4	-5.17	104.33	106.40
21	AA	908	A	N1-C6-N6	-5.16	115.50	118.60
39	BQ	2	ARG	NE-CZ-NH1	5.16	122.88	120.30
54	BA	109	C	O4'-C1'-N1	5.16	112.33	108.20
54	BA	264	C	N1-C2-O2	5.16	122.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	267	C	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1317	G	C4-C5-N7	-5.16	108.73	110.80
54	BA	2506	U	C5-C6-N1	-5.16	120.12	122.70
54	BA	2539	C	N1-C2-O2	5.16	122.00	118.90
21	AA	596	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	1031	C	N3-C4-N4	-5.16	114.39	118.00
54	BA	525	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	765	C	O4'-C1'-N1	5.16	112.33	108.20
54	BA	2580	U	O4'-C1'-N1	5.16	112.33	108.20
55	BB	62	C	N3-C2-O2	-5.16	118.29	121.90
55	BB	82	U	O4'-C1'-N1	5.16	112.33	108.20
21	AA	516	U	O4'-C1'-N1	5.16	112.33	108.20
22	A1	3	G	C5-C6-N1	5.16	114.08	111.50
54	BA	98	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	545	U	N1-C2-N3	5.16	118.00	114.90
54	BA	1148	U	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1963	U	C5-C6-N1	-5.16	120.12	122.70
54	BA	2403	C	N1-C2-O2	5.16	122.00	118.90
54	BA	2818	U	N1-C2-N3	5.16	118.00	114.90
21	AA	1176	A	C5-C6-N1	5.16	120.28	117.70
54	BA	337	C	N1-C2-O2	5.16	122.00	118.90
54	BA	1468	U	C5-C6-N1	-5.16	120.12	122.70
55	BB	62	C	N1-C2-O2	5.16	122.00	118.90
21	AA	574	A	C4-C5-C6	-5.16	114.42	117.00
32	BJ	116	ARG	NE-CZ-NH2	-5.16	117.72	120.30
54	BA	1645	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	1970	A	O4'-C1'-N9	5.16	112.33	108.20
21	AA	575	G	N3-C4-C5	-5.16	126.02	128.60
21	AA	852	G	N9-C4-C5	5.16	107.46	105.40
21	AA	1294	G	N7-C8-N9	5.16	115.68	113.10
21	AA	1336	C	C2-N3-C4	-5.16	117.32	119.90
22	A1	60	C	N3-C4-C5	5.16	123.96	121.90
54	BA	251	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	467	G	O4'-C1'-N9	5.16	112.33	108.20
54	BA	1097	U	C5-C6-N1	-5.16	120.12	122.70
54	BA	1543	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	2557	G	C8-N9-C4	-5.16	104.34	106.40
54	BA	2587	A	C6-C5-N7	5.16	135.91	132.30
55	BB	93	C	C4'-C3'-C2'	-5.16	97.44	102.60
21	AA	863	U	N1-C2-N3	5.15	117.99	114.90
54	BA	2578	G	C4'-C3'-C2'	-5.15	97.45	102.60
55	BB	118	C	O4'-C1'-N1	5.15	112.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	267	C	N1-C2-O2	5.15	121.99	118.90
21	AA	470	C	N3-C4-C5	5.15	123.96	121.90
21	AA	518	C	N3-C4-N4	-5.15	114.39	118.00
21	AA	532	A	O4'-C1'-N9	5.15	112.32	108.20
21	AA	1136	C	N3-C4-C5	5.15	123.96	121.90
21	AA	1490	U	N3-C2-O2	-5.15	118.59	122.20
21	AA	1528	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2	G	N3-C4-C5	-5.15	126.02	128.60
54	BA	67	U	N3-C2-O2	-5.15	118.59	122.20
54	BA	477	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	620	G	C8-N9-C4	-5.15	104.34	106.40
54	BA	954	G	C5-C6-N1	5.15	114.08	111.50
54	BA	1169	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	2710	C	N1-C2-O2	5.15	121.99	118.90
55	BB	90	C	O4'-C1'-N1	5.15	112.32	108.20
55	BB	114	C	N1-C2-O2	5.15	121.99	118.90
21	AA	1092	A	N1-C6-N6	-5.15	115.51	118.60
21	AA	1409	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	63	A	C6-C5-N7	5.15	135.91	132.30
54	BA	163	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	586	A	C5-C6-N1	5.15	120.28	117.70
54	BA	758	C	C4'-C3'-C2'	-5.15	97.45	102.60
54	BA	1256	G	N7-C8-N9	5.15	115.68	113.10
54	BA	1493	C	N1-C2-O2	5.15	121.99	118.90
54	BA	1726	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	1979	U	C5-C6-N1	-5.15	120.12	122.70
54	BA	1981	A	C6-C5-N7	5.15	135.91	132.30
54	BA	2598	A	C6-C5-N7	5.15	135.91	132.30
21	AA	335	C	O4'-C1'-N1	5.15	112.32	108.20
21	AA	1439	G	C5-C6-N1	5.15	114.07	111.50
54	BA	317	G	C5-C6-N1	5.15	114.07	111.50
54	BA	2703	C	N3-C2-O2	-5.15	118.30	121.90
21	AA	295	C	N3-C2-O2	-5.15	118.30	121.90
21	AA	818	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	48	G	N3-C4-C5	-5.15	126.03	128.60
54	BA	584	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	956	G	C5-C6-N1	5.15	114.07	111.50
54	BA	2238	G	P-O3'-C3'	5.15	125.88	119.70
54	BA	2851	A	C6-C5-N7	5.15	135.90	132.30
54	BA	2853	C	N3-C2-O2	-5.15	118.30	121.90
21	AA	44	A	O4'-C1'-N9	5.15	112.32	108.20
21	AA	191	G	N1-C6-O6	-5.15	116.81	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	797	G	O4'-C1'-N9	5.15	112.32	108.20
54	BA	1947	C	N3-C4-C5	5.15	123.96	121.90
55	BB	8	C	N1-C2-O2	5.15	121.99	118.90
21	AA	46	G	C5-C6-N1	5.14	114.07	111.50
21	AA	68	G	C5-C6-N1	5.14	114.07	111.50
21	AA	266	G	N3-C2-N2	-5.14	116.30	119.90
21	AA	419	C	N1-C2-O2	5.14	121.99	118.90
21	AA	1022	A	C6-C5-N7	5.14	135.90	132.30
21	AA	1108	G	N1-C6-O6	-5.14	116.81	119.90
24	A3	13	C	O4'-C1'-N1	5.14	112.31	108.20
25	BC	216	ARG	NH1-CZ-NH2	-5.14	113.74	119.40
25	BC	269	ARG	NE-CZ-NH2	-5.14	117.73	120.30
26	BD	33	ARG	NE-CZ-NH1	5.14	122.87	120.30
54	BA	318	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	543	G	C5'-C4'-O4'	5.14	115.27	109.10
54	BA	825	A	C6-C5-N7	5.14	135.90	132.30
54	BA	1232	G	C8-N9-C4	-5.14	104.34	106.40
2	AC	178	ARG	NE-CZ-NH1	5.14	122.87	120.30
21	AA	119	A	C5-C6-N1	5.14	120.27	117.70
21	AA	679	C	O4'-C1'-N1	5.14	112.31	108.20
21	AA	713	G	N1-C6-O6	-5.14	116.81	119.90
21	AA	1164	G	C5-C6-N1	5.14	114.07	111.50
54	BA	515	A	C6-C5-N7	5.14	135.90	132.30
54	BA	1068	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	1560	G	C8-N9-C4	-5.14	104.34	106.40
54	BA	2313	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2679	A	C4-C5-C6	-5.14	114.43	117.00
55	BB	114	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	2073	C	C2-N3-C4	-5.14	117.33	119.90
54	BA	2179	C	O4'-C1'-N1	5.14	112.31	108.20
13	AN	81	ARG	NE-CZ-NH1	5.14	122.87	120.30
21	AA	177	G	O4'-C1'-N9	5.14	112.31	108.20
21	AA	457	G	N9-C4-C5	5.14	107.46	105.40
21	AA	554	A	C5-C6-N1	5.14	120.27	117.70
25	BC	176	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
54	BA	583	G	O4'-C1'-N9	5.14	112.31	108.20
54	BA	626	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	931	U	N3-C2-O2	-5.14	118.60	122.20
54	BA	942	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	1264	A	C6-C5-N7	5.14	135.90	132.30
54	BA	2817	U	N1-C2-N3	5.14	117.98	114.90
21	AA	956	U	C5-C6-N1	-5.14	120.13	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1124	G	C1'-O4'-C4'	-5.14	105.79	109.90
36	BN	8	ARG	NE-CZ-NH1	5.14	122.87	120.30
54	BA	394	C	C4'-C3'-C2'	-5.14	97.46	102.60
54	BA	1295	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	2680	U	C4-C5-C6	5.14	122.78	119.70
19	AT	28	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
21	AA	83	C	N1-C2-O2	5.14	121.98	118.90
21	AA	1422	G	C8-N9-C4	-5.14	104.34	106.40
42	BT	6	ARG	NE-CZ-NH1	5.14	122.87	120.30
54	BA	666	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	1469	A	N1-C6-N6	-5.14	115.52	118.60
54	BA	1720	U	C5-C6-N1	-5.14	120.13	122.70
54	BA	1822	C	N1-C2-O2	5.14	121.98	118.90
21	AA	454	G	N3-C4-C5	-5.13	126.03	128.60
21	AA	1406	U	C4-C5-C6	5.13	122.78	119.70
54	BA	193	U	N3-C2-O2	-5.13	118.61	122.20
54	BA	295	G	C5'-C4'-C3'	-5.13	107.78	116.00
54	BA	370	G	C5-C6-N1	5.13	114.07	111.50
54	BA	1128	G	C8-N9-C4	-5.13	104.35	106.40
54	BA	1427	A	C6-C5-N7	5.13	135.89	132.30
54	BA	1580	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	1903	G	N3-C2-N2	-5.13	116.31	119.90
54	BA	2497	A	C5-N7-C8	-5.13	101.33	103.90
21	AA	1488	G	C4-C5-N7	-5.13	108.75	110.80
21	AA	1518	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	1735	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	1954	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2122	U	O4'-C1'-N1	5.13	112.31	108.20
21	AA	76	G	N7-C8-N9	5.13	115.67	113.10
54	BA	49	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	160	A	C4'-C3'-C2'	-5.13	97.47	102.60
54	BA	341	C	N1-C2-O2	5.13	121.98	118.90
54	BA	406	G	C5-C6-N1	5.13	114.07	111.50
54	BA	684	G	C8-N9-C4	-5.13	104.35	106.40
54	BA	745	G	N3-C2-N2	-5.13	116.31	119.90
54	BA	1972	G	C8-N9-C4	-5.13	104.35	106.40
12	AM	91	ARG	NE-CZ-NH2	-5.13	117.73	120.30
21	AA	908	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	974	A	C3'-C2'-C1'	5.13	105.60	101.50
21	AA	1292	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	73	A	C1'-O4'-C4'	-5.13	105.80	109.90
54	BA	254	G	N1-C6-O6	-5.13	116.82	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	419	U	N1-C2-N3	5.13	117.98	114.90
54	BA	709	U	C4'-C3'-C2'	-5.13	97.47	102.60
54	BA	1100	C	C6-N1-C2	-5.13	118.25	120.30
54	BA	1713	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	1943	U	N3-C2-O2	-5.13	118.61	122.20
54	BA	2397	G	C5-C6-N1	5.13	114.06	111.50
21	AA	25	C	N1-C2-O2	5.13	121.98	118.90
21	AA	1114	C	N3-C2-O2	-5.13	118.31	121.90
52	B3	29	ARG	NE-CZ-NH1	5.13	122.86	120.30
54	BA	701	G	N3-C4-C5	-5.13	126.03	128.60
54	BA	1569	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	1230	C	N3-C2-O2	-5.13	118.31	121.90
21	AA	1512	U	C5-C6-N1	-5.13	120.14	122.70
54	BA	62	U	O4'-C1'-N1	5.13	112.30	108.20
54	BA	1007	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	1247	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	1505	A	C6-C5-N7	5.13	135.89	132.30
54	BA	1679	A	C6-C5-N7	5.13	135.89	132.30
54	BA	2604	U	N3-C2-O2	-5.13	118.61	122.20
21	AA	289	G	C5-C6-N1	5.12	114.06	111.50
21	AA	363	A	N9-C4-C5	5.12	107.85	105.80
54	BA	437	U	C5-C6-N1	-5.12	120.14	122.70
54	BA	1401	G	N3-C4-C5	-5.12	126.04	128.60
54	BA	2087	G	N7-C8-N9	5.12	115.66	113.10
54	BA	2368	C	C2-N3-C4	-5.12	117.34	119.90
54	BA	2641	G	C5-C6-N1	5.12	114.06	111.50
21	AA	355	C	O4'-C1'-N1	5.12	112.30	108.20
21	AA	604	G	C8-N9-C4	-5.12	104.35	106.40
22	A1	20	G	N3-C4-C5	-5.12	126.04	128.60
54	BA	541	A	C4'-C3'-C2'	-5.12	97.48	102.60
54	BA	651	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1639	C	N3-C4-C5	5.12	123.95	121.90
54	BA	1695	G	N7-C8-N9	5.12	115.66	113.10
54	BA	2260	C	N3-C2-O2	-5.12	118.31	121.90
54	BA	2391	G	N3-C4-C5	-5.12	126.04	128.60
54	BA	2635	A	C6-C5-N7	5.12	135.89	132.30
54	BA	2718	G	C5-C6-N1	5.12	114.06	111.50
21	AA	122	G	C5-C6-N1	5.12	114.06	111.50
54	BA	141	G	N7-C8-N9	5.12	115.66	113.10
54	BA	2016	U	C5-C6-N1	-5.12	120.14	122.70
21	AA	291	U	O4'-C1'-N1	5.12	112.30	108.20
21	AA	978	A	C4-C5-C6	-5.12	114.44	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	172	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	1968	G	N7-C8-N9	5.12	115.66	113.10
54	BA	2031	A	O4'-C1'-N9	5.12	112.30	108.20
21	AA	21	G	C5-C6-N1	5.12	114.06	111.50
21	AA	621	A	O4'-C1'-N9	5.12	112.30	108.20
54	BA	203	A	C5-C6-N1	5.12	120.26	117.70
54	BA	1249	U	C5-C6-N1	-5.12	120.14	122.70
54	BA	1975	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	2092	U	O4'-C1'-N1	5.12	112.29	108.20
21	AA	1503	A	C5-C6-N1	5.12	120.26	117.70
54	BA	957	C	N3-C4-C5	5.12	123.95	121.90
54	BA	2052	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2372	U	N1-C2-N3	5.12	117.97	114.90
21	AA	705	G	C4-C5-N7	-5.12	108.75	110.80
54	BA	121	G	C8-N9-C4	-5.12	104.35	106.40
54	BA	267	C	N3-C2-O2	-5.12	118.32	121.90
54	BA	396	G	N3-C4-C5	-5.12	126.04	128.60
54	BA	458	G	C8-N9-C4	-5.12	104.35	106.40
54	BA	1520	U	O4'-C1'-N1	5.12	112.29	108.20
54	BA	2116	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	2177	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	2381	A	N1-C2-N3	-5.12	126.74	129.30
54	BA	2614	A	C2-N3-C4	5.12	113.16	110.60
54	BA	2753	A	C5-C6-N1	5.12	120.26	117.70
13	AN	9	ARG	CD-NE-CZ	5.11	130.76	123.60
21	AA	727	G	C5-C6-N1	5.11	114.06	111.50
21	AA	800	G	N7-C8-N9	5.11	115.66	113.10
21	AA	1140	C	N3-C4-C5	5.11	123.95	121.90
21	AA	1161	C	N3-C2-O2	-5.11	118.32	121.90
54	BA	45	G	N3-C4-C5	-5.11	126.04	128.60
54	BA	116	C	N1-C2-O2	5.11	121.97	118.90
54	BA	135	U	N3-C2-O2	-5.11	118.62	122.20
54	BA	1033	U	N3-C2-O2	-5.11	118.62	122.20
54	BA	1991	U	N1-C2-N3	5.11	117.97	114.90
2	AC	106	ARG	NE-CZ-NH1	5.11	122.86	120.30
21	AA	520	A	C5-C6-N6	5.11	127.79	123.70
21	AA	959	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	2039	U	N1-C2-N3	5.11	117.97	114.90
9	AJ	9	ARG	NE-CZ-NH1	5.11	122.86	120.30
21	AA	314	C	N3-C2-O2	-5.11	118.32	121.90
52	B3	39	ARG	NE-CZ-NH1	5.11	122.86	120.30
54	BA	393	C	N3-C2-O2	-5.11	118.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	798	G	C5-C6-N1	5.11	114.06	111.50
54	BA	1050	A	C5'-C4'-O4'	5.11	115.23	109.10
54	BA	1750	G	C8-N9-C4	-5.11	104.36	106.40
54	BA	1971	U	C5'-C4'-C3'	-5.11	107.82	116.00
56	B5	122	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
21	AA	34	C	C3'-C2'-C1'	5.11	105.59	101.50
49	B0	16	ARG	NE-CZ-NH1	5.11	122.85	120.30
54	BA	755	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	1751	U	N1-C2-N3	5.11	117.97	114.90
54	BA	1959	G	C4-C5-N7	-5.11	108.76	110.80
54	BA	2203	U	C5-C6-N1	-5.11	120.15	122.70
54	BA	2475	C	N3-C2-O2	-5.11	118.33	121.90
55	BB	24	G	C8-N9-C4	-5.11	104.36	106.40
21	AA	249	U	C3'-C2'-C1'	5.11	105.58	101.50
21	AA	1194	U	N3-C2-O2	-5.11	118.63	122.20
54	BA	113	U	C3'-C2'-C1'	5.11	105.58	101.50
54	BA	161	A	C2-N3-C4	5.11	113.15	110.60
54	BA	567	U	N1-C2-N3	5.11	117.96	114.90
54	BA	1746	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	2021	C	C2-N3-C4	-5.11	117.35	119.90
21	AA	1177	G	N3-C2-N2	-5.10	116.33	119.90
54	BA	2192	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	2366	A	N1-C6-N6	-5.10	115.54	118.60
54	BA	2649	C	N1-C2-O2	5.10	121.96	118.90
54	BA	2696	U	O4'-C1'-N1	5.10	112.28	108.20
9	AJ	72	ARG	CD-NE-CZ	5.10	130.75	123.60
21	AA	1360	A	C6-C5-N7	5.10	135.87	132.30
22	A1	71	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	703	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	984	A	P-O3'-C3'	5.10	125.82	119.70
54	BA	1995	U	C4-C5-C6	5.10	122.76	119.70
54	BA	2367	G	N9-C4-C5	5.10	107.44	105.40
54	BA	2573	C	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1405	G	O4'-C1'-N9	5.10	112.28	108.20
54	BA	343	C	N1-C2-O2	5.10	121.96	118.90
21	AA	454	G	N1-C6-O6	-5.10	116.84	119.90
21	AA	1216	A	C4-C5-C6	-5.10	114.45	117.00
21	AA	1300	G	O4'-C1'-N9	5.10	112.28	108.20
21	AA	1352	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1494	G	N7-C8-N9	5.10	115.65	113.10
54	BA	61	C	N3-C4-C5	5.10	123.94	121.90
54	BA	141	G	N3-C2-N2	-5.10	116.33	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	632	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	735	A	C6-C5-N7	5.10	135.87	132.30
54	BA	2006	C	N1-C2-O2	5.10	121.96	118.90
54	BA	2783	U	C5-C6-N1	-5.10	120.15	122.70
54	BA	2794	C	O4'-C1'-N1	5.10	112.28	108.20
55	BB	18	G	N9-C4-C5	5.10	107.44	105.40
21	AA	194	C	O4'-C4'-C3'	5.10	110.18	106.10
21	AA	1070	U	C4-C5-C6	5.10	122.76	119.70
21	AA	1119	C	N3-C2-O2	-5.10	118.33	121.90
24	A3	48	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	1662	U	C5-C6-N1	-5.10	120.15	122.70
54	BA	2119	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2266	A	C4-C5-C6	-5.10	114.45	117.00
55	BB	5	U	C4'-C3'-C2'	-5.10	97.50	102.60
21	AA	701	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	357	C	N3-C2-O2	-5.10	118.33	121.90
54	BA	1263	U	C5-C6-N1	-5.10	120.15	122.70
54	BA	1442	U	N1-C2-N3	5.10	117.96	114.90
54	BA	1914	C	N1-C2-O2	5.10	121.96	118.90
54	BA	2074	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	2235	G	N3-C4-C5	-5.10	126.05	128.60
9	AJ	41	PRO	C-N-CA	5.09	134.44	121.70
14	AO	63	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
21	AA	318	G	N1-C6-O6	-5.09	116.84	119.90
21	AA	832	G	C5-C6-N1	5.09	114.05	111.50
21	AA	924	C	O4'-C1'-N1	5.09	112.28	108.20
54	BA	86	G	O4'-C1'-N9	5.09	112.28	108.20
54	BA	438	G	N3-C4-C5	-5.09	126.05	128.60
54	BA	1729	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	2032	G	N3-C4-C5	-5.09	126.05	128.60
54	BA	2495	G	C5'-C4'-C3'	-5.09	107.85	116.00
21	AA	593	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	559	G	N7-C8-N9	5.09	115.65	113.10
54	BA	653	U	C3'-C2'-C1'	5.09	105.57	101.50
54	BA	1646	C	N1-C2-O2	5.09	121.96	118.90
54	BA	2035	G	O4'-C1'-N9	5.09	112.27	108.20
54	BA	2416	C	N1-C2-O2	5.09	121.96	118.90
21	AA	153	C	N1-C2-O2	5.09	121.95	118.90
21	AA	1086	U	N3-C2-O2	-5.09	118.64	122.20
21	AA	1300	G	C5-C6-N1	5.09	114.05	111.50
21	AA	1448	C	O4'-C4'-C3'	5.09	110.17	106.10
54	BA	384	A	C4-C5-C6	-5.09	114.45	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1536	C	N3-C2-O2	-5.09	118.34	121.90
54	BA	1831	G	C5-C6-N1	5.09	114.05	111.50
54	BA	2492	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	2589	A	O4'-C1'-N9	5.09	112.27	108.20
55	BB	89	U	N1-C2-N3	5.09	117.95	114.90
21	AA	117	G	N1-C6-O6	-5.09	116.85	119.90
54	BA	715	A	C6-C5-N7	5.09	135.86	132.30
54	BA	1071	G	N3-C4-C5	-5.09	126.06	128.60
54	BA	1380	G	N1-C6-O6	-5.09	116.85	119.90
54	BA	1528	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	1636	U	C5-C6-N1	-5.09	120.16	122.70
54	BA	2186	G	C5-C6-N1	5.09	114.05	111.50
54	BA	73	A	C5-C6-N1	5.09	120.24	117.70
54	BA	313	G	N3-C2-N2	-5.09	116.34	119.90
54	BA	1075	C	N3-C4-C5	5.09	123.94	121.90
54	BA	1234	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2178	C	N3-C2-O2	-5.09	118.34	121.90
2	AC	39	ARG	NE-CZ-NH2	-5.09	117.76	120.30
21	AA	175	C	N3-C4-N4	-5.09	114.44	118.00
21	AA	948	C	O4'-C1'-N1	5.09	112.27	108.20
22	A1	61	C	N1-C2-O2	5.09	121.95	118.90
54	BA	621	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	1638	C	N1-C2-O2	5.09	121.95	118.90
54	BA	1980	G	N3-C4-C5	-5.09	126.06	128.60
54	BA	2277	G	C5-C6-N1	5.09	114.04	111.50
54	BA	2395	C	C6-N1-C2	-5.09	118.27	120.30
6	AG	2	ARG	NE-CZ-NH1	5.08	122.84	120.30
21	AA	671	G	C5-C6-N1	5.08	114.04	111.50
21	AA	1476	A	C5-C6-N1	5.08	120.24	117.70
54	BA	620	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	2532	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	56	U	N3-C2-O2	-5.08	118.64	122.20
21	AA	129	A	O4'-C1'-N9	5.08	112.27	108.20
21	AA	162	A	N1-C2-N3	-5.08	126.76	129.30
21	AA	942	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	1528	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	1358	G	C5-C6-N1	5.08	114.04	111.50
54	BA	2825	G	C2-N3-C4	5.08	114.44	111.90
55	BB	70	C	C5'-C4'-O4'	5.08	115.20	109.10
21	AA	619	U	N1-C2-N3	5.08	117.95	114.90
21	AA	1240	U	C5-C6-N1	-5.08	120.16	122.70
21	AA	1293	C	O4'-C1'-N1	5.08	112.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	162	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	277	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1451	C	C1'-O4'-C4'	-5.08	105.83	109.90
54	BA	2180	U	C4-C5-C6	5.08	122.75	119.70
54	BA	2271	G	C8-N9-C4	-5.08	104.37	106.40
54	BA	2376	A	O4'-C1'-N9	5.08	112.27	108.20
54	BA	2752	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2807	U	C5-C6-N1	-5.08	120.16	122.70
21	AA	839	C	N1-C2-O2	5.08	121.95	118.90
21	AA	1341	U	N1-C2-N3	5.08	117.95	114.90
54	BA	437	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1566	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	2842	G	N1-C6-O6	-5.08	116.85	119.90
55	BB	37	C	O4'-C1'-N1	5.08	112.26	108.20
21	AA	183	C	O4'-C1'-N1	5.08	112.26	108.20
21	AA	335	C	C2-N3-C4	-5.08	117.36	119.90
54	BA	685	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	784	G	C3'-C2'-C1'	5.08	105.56	101.50
54	BA	1349	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	2177	C	N3-C2-O2	-5.08	118.34	121.90
55	BB	18	G	C6-C5-N7	5.08	133.45	130.40
21	AA	1527	U	N1-C2-N3	5.08	117.95	114.90
54	BA	412	A	C5-C6-N1	5.08	120.24	117.70
54	BA	476	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1111	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1792	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	37	U	O4'-C1'-N1	5.08	112.26	108.20
21	AA	734	G	N7-C8-N9	5.08	115.64	113.10
21	AA	808	C	C1'-O4'-C4'	-5.08	105.84	109.90
54	BA	33	C	N3-C4-C5	5.08	123.93	121.90
54	BA	71	A	C2-N3-C4	5.08	113.14	110.60
54	BA	465	G	N3-C2-N2	-5.08	116.35	119.90
54	BA	1105	U	N1-C2-N3	5.08	117.95	114.90
54	BA	1478	G	C5-N7-C8	-5.08	101.76	104.30
54	BA	1774	C	N3-C4-C5	5.08	123.93	121.90
54	BA	1864	U	C5-C6-N1	-5.08	120.16	122.70
54	BA	2347	C	N3-C2-O2	-5.08	118.35	121.90
54	BA	2420	C	N3-C4-C5	5.08	123.93	121.90
54	BA	2559	C	N1-C2-O2	5.08	121.94	118.90
55	BB	31	C	N3-C2-O2	-5.08	118.35	121.90
21	AA	155	A	C5-C6-N1	5.07	120.24	117.70
21	AA	175	C	N3-C4-C5	5.07	123.93	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	287	U	O4'-C1'-N1	5.07	112.26	108.20
21	AA	1446	A	C5-C6-N1	5.07	120.24	117.70
54	BA	288	U	C5-C6-N1	-5.07	120.16	122.70
54	BA	336	C	N3-C2-O2	-5.07	118.35	121.90
54	BA	446	G	C3'-C2'-C1'	5.07	105.56	101.50
54	BA	1899	A	C4-C5-C6	-5.07	114.46	117.00
54	BA	2124	G	C4-C5-N7	-5.07	108.77	110.80
54	BA	2267	A	C2-N3-C4	5.07	113.14	110.60
54	BA	2361	G	O4'-C1'-N9	5.07	112.26	108.20
54	BA	2870	C	O4'-C1'-N1	5.07	112.26	108.20
54	BA	2891	U	N3-C2-O2	-5.07	118.65	122.20
55	BB	109	A	C6-C5-N7	5.07	135.85	132.30
21	AA	454	G	C5-C6-N1	5.07	114.04	111.50
21	AA	777	A	C4-C5-C6	-5.07	114.46	117.00
21	AA	1006	G	C5-C6-N1	5.07	114.04	111.50
54	BA	107	G	N9-C4-C5	5.07	107.43	105.40
54	BA	2768	U	C4'-C3'-C2'	-5.07	97.53	102.60
21	AA	1003	G	N1-C6-O6	-5.07	116.86	119.90
21	AA	1103	C	C6-N1-C2	-5.07	118.27	120.30
21	AA	1228	C	N3-C2-O2	-5.07	118.35	121.90
54	BA	1451	C	C6-N1-C2	-5.07	118.27	120.30
54	BA	1824	G	C5-C6-N1	5.07	114.03	111.50
21	AA	912	C	N1-C2-O2	5.07	121.94	118.90
54	BA	2734	A	C6-C5-N7	5.07	135.85	132.30
21	AA	282	A	C5'-C4'-C3'	-5.07	107.89	116.00
21	AA	1294	G	C8-N9-C4	-5.07	104.37	106.40
34	BL	132	ARG	NE-CZ-NH1	5.07	122.83	120.30
35	BM	10	ARG	NE-CZ-NH1	5.07	122.83	120.30
54	BA	1310	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1732	C	N3-C4-N4	-5.07	114.45	118.00
54	BA	1846	G	C5-C6-N1	5.07	114.03	111.50
55	BB	68	C	N3-C2-O2	-5.07	118.35	121.90
55	BB	116	G	N7-C8-N9	5.07	115.63	113.10
11	AL	85	ARG	NH1-CZ-NH2	-5.07	113.83	119.40
54	BA	479	A	P-O3'-C3'	5.07	125.78	119.70
54	BA	741	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	1633	G	N3-C4-C5	-5.07	126.07	128.60
54	BA	1681	G	C8-N9-C4	-5.07	104.37	106.40
54	BA	2083	G	C8-N9-C4	-5.07	104.37	106.40
21	AA	61	G	C5-C6-N1	5.06	114.03	111.50
21	AA	680	C	N1-C2-O2	5.06	121.94	118.90
21	AA	1184	G	N3-C4-C5	-5.06	126.07	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	607	U	N1-C2-N3	5.06	117.94	114.90
54	BA	1397	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	1835	G	C5-C6-N1	5.06	114.03	111.50
54	BA	2250	G	C3'-C2'-C1'	5.06	105.55	101.50
54	BA	2662	A	C5-C6-N1	5.06	120.23	117.70
21	AA	177	G	N3-C4-N9	5.06	129.04	126.00
21	AA	911	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	1082	A	C6-C5-N7	5.06	135.84	132.30
21	AA	1390	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	310	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	325	G	C5-C6-N1	5.06	114.03	111.50
54	BA	330	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	965	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	982	C	C6-N1-C1'	-5.06	114.72	120.80
54	BA	1236	G	N9-C4-C5	5.06	107.42	105.40
54	BA	1765	U	C5-C6-N1	-5.06	120.17	122.70
54	BA	2805	C	N1-C2-O2	5.06	121.94	118.90
56	B5	71	ARG	NE-CZ-NH2	-5.06	117.77	120.30
3	AD	127	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
25	BC	86	ARG	CD-NE-CZ	5.06	130.69	123.60
54	BA	228	C	N1-C2-O2	5.06	121.94	118.90
54	BA	1708	C	N3-C2-O2	-5.06	118.36	121.90
54	BA	2184	A	C5-C6-N1	5.06	120.23	117.70
54	BA	2538	C	O4'-C1'-N1	5.06	112.25	108.20
21	AA	641	U	P-O3'-C3'	5.06	125.77	119.70
30	BH	68	ARG	NE-CZ-NH2	-5.06	117.77	120.30
54	BA	297	G	N3-C4-C5	-5.06	126.07	128.60
54	BA	664	G	C5-C6-N1	5.06	114.03	111.50
54	BA	1763	G	N9-C1'-C2'	-5.06	106.44	112.00
54	BA	1935	G	C5-C6-N1	5.06	114.03	111.50
54	BA	2150	C	N1-C2-O2	5.06	121.94	118.90
55	BB	33	G	N3-C2-N2	-5.06	116.36	119.90
21	AA	802	A	C5-C6-N1	5.06	120.23	117.70
21	AA	1033	G	C5-C6-N1	5.06	114.03	111.50
54	BA	528	A	O4'-C1'-N9	5.06	112.25	108.20
54	BA	651	G	N9-C4-C5	5.06	107.42	105.40
54	BA	1964	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	2124	G	C5-C6-N1	5.06	114.03	111.50
54	BA	2592	G	C5-C6-N1	5.06	114.03	111.50
54	BA	2692	G	C8-N9-C4	-5.06	104.38	106.40
54	BA	2759	G	N9-C4-C5	5.06	107.42	105.40
21	AA	22	G	C5-C6-N1	5.06	114.03	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1042	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	355	U	C1'-O4'-C4'	-5.06	105.86	109.90
54	BA	952	G	N9-C4-C5	5.06	107.42	105.40
54	BA	2524	G	N1-C6-O6	-5.06	116.87	119.90
54	BA	2686	G	C4'-C3'-C2'	-5.06	97.54	102.60
7	AH	53	ASP	C-N-CA	5.05	134.34	121.70
21	AA	103	U	C1'-O4'-C4'	-5.05	105.86	109.90
21	AA	212	G	C5-C6-N1	5.05	114.03	111.50
21	AA	226	G	N9-C4-C5	5.05	107.42	105.40
21	AA	490	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1070	U	N3-C2-O2	-5.05	118.66	122.20
54	BA	1008	A	C6-C5-N7	5.05	135.84	132.30
54	BA	1202	G	C5-C6-N1	5.05	114.03	111.50
54	BA	1435	G	C8-N9-C4	-5.05	104.38	106.40
54	BA	1456	G	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	1793	C	C5'-C4'-O4'	5.05	115.17	109.10
54	BA	2130	U	N3-C2-O2	-5.05	118.66	122.20
54	BA	2406	A	C6-C5-N7	5.05	135.84	132.30
54	BA	2794	C	N3-C4-C5	5.05	123.92	121.90
54	BA	2841	C	O4'-C1'-N1	5.05	112.24	108.20
7	AH	116	ARG	NE-CZ-NH2	-5.05	117.77	120.30
21	AA	180	U	N3-C2-O2	-5.05	118.66	122.20
21	AA	481	G	N9-C4-C5	5.05	107.42	105.40
24	A3	53	G	C8-N9-C4	-5.05	104.38	106.40
54	BA	1795	C	O4'-C1'-N1	5.05	112.24	108.20
21	AA	30	U	C5-C6-N1	-5.05	120.17	122.70
21	AA	141	G	N3-C4-C5	-5.05	126.07	128.60
21	AA	1512	U	N1-C2-N3	5.05	117.93	114.90
54	BA	750	A	C6-C5-N7	5.05	135.84	132.30
54	BA	1313	U	N3-C2-O2	-5.05	118.66	122.20
54	BA	2703	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2710	C	N3-C4-C5	5.05	123.92	121.90
55	BB	23	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	150	U	O4'-C4'-C3'	5.05	110.14	106.10
54	BA	288	U	N3-C2-O2	-5.05	118.67	122.20
54	BA	652	U	C4-C5-C6	5.05	122.73	119.70
54	BA	1227	G	C5-C6-N1	5.05	114.03	111.50
54	BA	1301	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	2195	U	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	2360	G	C5-N7-C8	-5.05	101.78	104.30
54	BA	2248	C	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	2745	C	N1-C2-O2	5.05	121.93	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	169	C	N3-C2-O2	-5.05	118.37	121.90
21	AA	545	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1052	U	C1'-O4'-C4'	-5.05	105.86	109.90
21	AA	1422	G	N3-C4-C5	-5.05	126.08	128.60
54	BA	364	C	N3-C4-C5	5.05	123.92	121.90
54	BA	664	G	O4'-C1'-N9	5.05	112.24	108.20
54	BA	677	A	O4'-C4'-C3'	5.05	110.14	106.10
54	BA	1025	G	N3-C2-N2	-5.05	116.37	119.90
54	BA	1196	C	N3-C2-O2	-5.05	118.37	121.90
54	BA	1685	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	1916	A	C6-C5-N7	5.05	135.83	132.30
54	BA	2451	A	C6-C5-N7	5.05	135.83	132.30
54	BA	2615	U	C5-C6-N1	-5.05	120.18	122.70
21	AA	128	G	N3-C4-C5	-5.04	126.08	128.60
21	AA	687	A	C4-C5-C6	-5.04	114.48	117.00
21	AA	725	G	C8-N9-C4	-5.04	104.38	106.40
21	AA	1406	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	172	A	C6-C5-N7	5.04	135.83	132.30
21	AA	421	U	N3-C2-O2	-5.04	118.67	122.20
21	AA	1038	C	N3-C2-O2	-5.04	118.37	121.90
21	AA	1182	G	N3-C4-C5	-5.04	126.08	128.60
21	AA	1259	C	C5'-C4'-O4'	5.04	115.15	109.10
54	BA	303	G	C5-C6-N1	5.04	114.02	111.50
54	BA	393	C	N3-C4-C5	5.04	123.92	121.90
54	BA	516	C	N3-C4-C5	5.04	123.92	121.90
54	BA	1487	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2244	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2744	G	N1-C6-O6	-5.04	116.87	119.90
55	BB	7	G	C8-N9-C4	-5.04	104.38	106.40
55	BB	98	G	C8-N9-C4	-5.04	104.38	106.40
21	AA	649	A	C4-C5-C6	-5.04	114.48	117.00
21	AA	687	A	C6-C5-N7	5.04	135.83	132.30
54	BA	281	C	N1-C2-O2	5.04	121.92	118.90
54	BA	430	A	C6-C5-N7	5.04	135.83	132.30
54	BA	555	G	C5-C6-N1	5.04	114.02	111.50
54	BA	555	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	710	U	N1-C2-N3	5.04	117.92	114.90
54	BA	1154	G	N3-C4-C5	-5.04	126.08	128.60
54	BA	1378	A	O4'-C4'-C3'	5.04	110.13	106.10
54	BA	1940	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	2415	G	N3-C2-N2	-5.04	116.37	119.90
54	BA	2670	A	C6-C5-N7	5.04	135.83	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	95	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	622	A	C6-C5-N7	5.04	135.83	132.30
21	AA	1149	C	N3-C2-O2	-5.04	118.37	121.90
54	BA	363	G	N3-C4-C5	-5.04	126.08	128.60
54	BA	2159	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	2597	G	N3-C4-C5	-5.04	126.08	128.60
54	BA	2752	C	C2-N3-C4	-5.04	117.38	119.90
21	AA	1248	A	C5'-C4'-O4'	5.04	115.14	109.10
24	A3	14	A	C4-C5-C6	-5.04	114.48	117.00
50	B1	43	ARG	NE-CZ-NH2	-5.04	117.78	120.30
54	BA	372	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	596	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	2132	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	2668	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	759	G	C8-N9-C4	-5.04	104.39	106.40
54	BA	939	G	C5-C6-N1	5.04	114.02	111.50
3	AD	187	ARG	NE-CZ-NH1	5.04	122.82	120.30
21	AA	343	U	C1'-O4'-C4'	-5.04	105.87	109.90
21	AA	847	G	N3-C4-C5	-5.04	126.08	128.60
21	AA	1113	C	N1-C2-O2	5.04	121.92	118.90
21	AA	1182	G	C6-N1-C2	-5.04	122.08	125.10
54	BA	71	A	C3'-C2'-C1'	5.04	105.53	101.50
54	BA	1122	G	N9-C4-C5	5.04	107.42	105.40
54	BA	1390	U	C4-C5-C6	5.04	122.72	119.70
54	BA	1399	C	N3-C2-O2	-5.04	118.37	121.90
54	BA	1779	U	N3-C2-O2	-5.04	118.68	122.20
54	BA	1927	A	C8-N9-C4	-5.04	103.79	105.80
21	AA	528	C	C2-N3-C4	-5.03	117.38	119.90
21	AA	1453	G	C8-N9-C4	-5.03	104.39	106.40
54	BA	250	G	O4'-C1'-N9	5.03	112.23	108.20
54	BA	529	A	C2-N3-C4	5.03	113.12	110.60
54	BA	1349	C	N1-C2-O2	5.03	121.92	118.90
54	BA	1597	A	P-O3'-C3'	5.03	125.74	119.70
54	BA	1996	C	N3-C4-N4	-5.03	114.48	118.00
54	BA	2272	U	C3'-C2'-C1'	5.03	105.53	101.50
54	BA	2899	A	O4'-C1'-N9	5.03	112.23	108.20
55	BB	75	G	C8-N9-C4	-5.03	104.39	106.40
21	AA	826	C	O4'-C1'-N1	5.03	112.23	108.20
21	AA	1001	C	N3-C2-O2	-5.03	118.38	121.90
22	A1	69	A	C4-C5-C6	-5.03	114.48	117.00
54	BA	435	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2388	A	C5-C6-N1	5.03	120.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AJ	45	ARG	NE-CZ-NH1	5.03	122.82	120.30
21	AA	120	A	O4'-C4'-C3'	5.03	110.12	106.10
21	AA	412	A	C5-C6-N6	5.03	127.72	123.70
21	AA	420	U	C1'-O4'-C4'	-5.03	105.88	109.90
54	BA	1770	G	C4'-C3'-C2'	-5.03	97.57	102.60
54	BA	1994	C	C6-N1-C2	-5.03	118.29	120.30
54	BA	2486	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	2571	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	2657	A	C5-C6-N1	5.03	120.22	117.70
55	BB	85	G	N3-C2-N2	-5.03	116.38	119.90
16	AQ	76	ARG	NE-CZ-NH1	5.03	122.81	120.30
21	AA	862	C	C6-N1-C2	-5.03	118.29	120.30
54	BA	54	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	1306	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	2836	U	O4'-C1'-N1	5.03	112.22	108.20
55	BB	96	G	C5-C6-N1	5.03	114.01	111.50
21	AA	365	U	O4'-C1'-N1	5.03	112.22	108.20
21	AA	523	A	P-O3'-C3'	5.03	125.73	119.70
21	AA	860	A	C6-C5-N7	5.03	135.82	132.30
46	BX	2	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
54	BA	107	G	C8-N9-C4	-5.03	104.39	106.40
54	BA	1301	A	O4'-C1'-N9	5.03	112.22	108.20
54	BA	1349	C	C2-N3-C4	-5.03	117.39	119.90
54	BA	1472	C	N3-C4-C5	5.03	123.91	121.90
54	BA	2155	U	C1'-O4'-C4'	-5.03	105.88	109.90
54	BA	2629	U	C3'-C2'-C1'	5.03	105.52	101.50
21	AA	1049	U	O4'-C4'-C3'	5.03	110.12	106.10
54	BA	188	G	O4'-C1'-N9	5.03	112.22	108.20
54	BA	809	G	N7-C8-N9	5.03	115.61	113.10
54	BA	1269	A	C5-C6-N1	5.03	120.21	117.70
54	BA	2029	G	N1-C6-O6	-5.03	116.88	119.90
55	BB	15	A	C1'-O4'-C4'	-5.03	105.88	109.90
21	AA	1104	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	1115	U	C4-C5-C6	5.02	122.72	119.70
38	BP	38	ARG	NH1-CZ-NH2	-5.02	113.87	119.40
54	BA	55	G	O4'-C1'-N9	5.02	112.22	108.20
54	BA	453	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	2024	G	C5-C6-N1	5.02	114.01	111.50
55	BB	37	C	C2-N3-C4	-5.02	117.39	119.90
21	AA	52	C	N1-C2-O2	5.02	121.91	118.90
21	AA	508	U	N3-C2-O2	-5.02	118.68	122.20
21	AA	551	U	N1-C2-N3	5.02	117.91	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	557	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	599	C	N1-C2-O2	5.02	121.91	118.90
54	BA	377	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	1718	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	2787	C	C4'-C3'-C2'	-5.02	97.58	102.60
54	BA	2830	C	N3-C2-O2	-5.02	118.38	121.90
54	BA	2858	C	C6-N1-C2	-5.02	118.29	120.30
21	AA	39	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	269	C	N1-C2-O2	5.02	121.91	118.90
21	AA	1048	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	1386	G	C5-C6-N1	5.02	114.01	111.50
52	B3	12	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
54	BA	1324	G	C5-C6-N1	5.02	114.01	111.50
54	BA	1494	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	1674	G	O4'-C1'-N9	5.02	112.22	108.20
54	BA	1896	G	C5-C6-N1	5.02	114.01	111.50
54	BA	2251	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	2486	C	N1-C2-O2	5.02	121.91	118.90
17	AR	42	ARG	NE-CZ-NH1	5.02	122.81	120.30
21	AA	521	G	C5-C6-N1	5.02	114.01	111.50
21	AA	736	C	O4'-C1'-N1	5.02	112.22	108.20
21	AA	1503	A	O4'-C1'-N9	5.02	112.22	108.20
54	BA	69	C	N3-C4-C5	5.02	123.91	121.90
54	BA	1191	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	1382	G	N9-C4-C5	5.02	107.41	105.40
54	BA	1743	G	C4'-C3'-C2'	-5.02	97.58	102.60
54	BA	1787	A	C3'-C2'-C1'	5.02	105.52	101.50
55	BB	48	U	O4'-C1'-N1	5.02	112.22	108.20
21	AA	20	U	C4-C5-C6	5.02	122.71	119.70
21	AA	307	C	N3-C4-C5	5.02	123.91	121.90
21	AA	733	G	C1'-O4'-C4'	-5.02	105.89	109.90
21	AA	792	A	C6-C5-N7	5.02	135.81	132.30
21	AA	942	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	1287	A	C6-C5-N7	5.02	135.81	132.30
54	BA	157	C	N3-C2-O2	-5.02	118.39	121.90
54	BA	1269	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	2500	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	2594	C	N3-C2-O2	-5.02	118.39	121.90
54	BA	2704	C	N3-C4-N4	-5.02	114.49	118.00
55	BB	75	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	552	U	N3-C2-O2	-5.02	118.69	122.20
21	AA	702	A	O4'-C1'-N9	5.02	112.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	867	G	C5-C6-N1	5.02	114.01	111.50
54	BA	591	U	O4'-C1'-N1	5.02	112.21	108.20
54	BA	839	U	C3'-C2'-C1'	5.02	105.51	101.50
54	BA	1605	C	N3-C2-O2	-5.02	118.39	121.90
54	BA	1969	A	C6-C5-N7	5.02	135.81	132.30
54	BA	2898	U	O4'-C1'-N1	5.02	112.21	108.20
21	AA	1043	G	C5-C6-N1	5.01	114.01	111.50
21	AA	1116	U	N1-C2-N3	5.01	117.91	114.90
21	AA	1349	A	C5-C6-N1	5.01	120.21	117.70
33	BK	105	ARG	NE-CZ-NH2	-5.01	117.79	120.30
54	BA	25	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	101	A	C5-C6-N1	5.01	120.21	117.70
54	BA	1711	A	C6-C5-N7	5.01	135.81	132.30
54	BA	1788	C	C2-N3-C4	-5.01	117.39	119.90
54	BA	2154	A	C5-C6-N1	5.01	120.21	117.70
21	AA	207	C	C6-N1-C2	-5.01	118.30	120.30
21	AA	405	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	915	A	C6-C5-N7	5.01	135.81	132.30
21	AA	1303	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1388	G	N7-C8-N9	5.01	115.61	113.10
54	BA	1477	A	C2-N3-C4	5.01	113.11	110.60
54	BA	1671	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	1893	C	N1-C2-O2	5.01	121.91	118.90
54	BA	2346	A	C6-C5-N7	5.01	135.81	132.30
54	BA	2755	C	O4'-C4'-C3'	5.01	110.11	106.10
54	BA	2897	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	107	G	C5-C6-N1	5.01	114.00	111.50
21	AA	1382	C	N3-C2-O2	-5.01	118.39	121.90
24	A3	9	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	1106	G	C5-C6-N1	5.01	114.00	111.50
54	BA	1174	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	1458	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	1647	U	C5-C6-N1	-5.01	120.20	122.70
54	BA	1033	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	2491	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	359	G	N3-C2-N2	-5.01	116.39	119.90
21	AA	470	C	N1-C2-O2	5.01	121.90	118.90
21	AA	508	U	C5-C6-N1	-5.01	120.20	122.70
21	AA	511	C	O4'-C1'-N1	5.01	112.20	108.20
21	AA	710	G	C5-C6-N1	5.01	114.00	111.50
21	AA	1445	U	N3-C2-O2	-5.01	118.70	122.20
34	BL	48	ARG	NE-CZ-NH1	5.01	122.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	810	U	C1'-O4'-C4'	-5.01	105.89	109.90
54	BA	1094	U	N1-C2-N3	5.01	117.90	114.90
54	BA	1426	G	N1-C6-O6	-5.01	116.90	119.90
54	BA	1449	G	O4'-C1'-N9	5.01	112.20	108.20
54	BA	1541	C	O4'-C1'-N1	5.01	112.20	108.20
54	BA	2140	G	N9-C4-C5	5.01	107.40	105.40
54	BA	2395	C	P-O3'-C3'	5.01	125.71	119.70
54	BA	2446	G	C4'-C3'-C2'	-5.01	97.59	102.60
55	BB	64	G	C8-N9-C4	-5.01	104.40	106.40
21	AA	45	G	C3'-C2'-C1'	5.00	105.50	101.50
54	BA	1946	U	N3-C2-O2	-5.00	118.70	122.20
54	BA	2398	U	C5-C6-N1	-5.00	120.20	122.70
54	BA	2683	C	C2-N3-C4	-5.00	117.40	119.90
55	BB	65	U	N1-C2-N3	5.00	117.90	114.90
21	AA	40	C	O4'-C1'-N1	5.00	112.20	108.20
21	AA	618	C	N3-C2-O2	-5.00	118.40	121.90
21	AA	843	U	N3-C2-O2	-5.00	118.70	122.20
21	AA	1471	U	N1-C2-N3	5.00	117.90	114.90
33	BK	70	ARG	NE-CZ-NH1	5.00	122.80	120.30
54	BA	669	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	752	A	C3'-C2'-C1'	-5.00	97.50	101.50
54	BA	2047	C	O4'-C1'-N1	5.00	112.20	108.20
54	BA	2692	G	N1-C6-O6	-5.00	116.90	119.90
21	AA	122	G	N3-C2-N2	-5.00	116.40	119.90
21	AA	543	U	O4'-C1'-N1	5.00	112.20	108.20
21	AA	642	A	C4-C5-C6	-5.00	114.50	117.00
21	AA	846	G	C8-N9-C4	-5.00	104.40	106.40
21	AA	985	C	N1-C2-O2	5.00	121.90	118.90
21	AA	1126	U	C5-C6-N1	-5.00	120.20	122.70
21	AA	1390	U	C3'-C2'-C1'	5.00	105.50	101.50
21	AA	1421	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	39	G	N9-C4-C5	5.00	107.40	105.40
54	BA	1625	C	N1-C2-O2	5.00	121.90	118.90
54	BA	1988	G	C5-C6-N1	5.00	114.00	111.50
54	BA	2780	G	N3-C4-C5	-5.00	126.10	128.60

There are no chirality outliers.

All (1094) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	23	A	Sidechain
22	A1	26	A	Sidechain

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Mol	Chain	Res	Type	Group
22	A1	31	C	Sidechain
22	A1	45	G	Sidechain
22	A1	49	G	Sidechain
22	A1	57	G	Sidechain
22	A1	59	U	Sidechain
22	A1	70	C	Sidechain
22	A1	72	C	Sidechain
22	A1	74	C	Sidechain
23	A2	81	U	Sidechain
24	A3	11	A	Sidechain
24	A3	24	C	Sidechain
24	A3	25	U	Sidechain
24	A3	27	G	Sidechain
24	A3	32	G	Sidechain
24	A3	34	U	Sidechain
24	A3	37	U	Sidechain
24	A3	47	G	Sidechain
24	A3	57	C	Sidechain
24	A3	71	G	Sidechain
24	A3	73	A	Sidechain
24	A3	76	C	Sidechain
24	A3	77	A	Sidechain
24	A3	9	G	Sidechain
21	AA	100	G	Sidechain
21	AA	1002	G	Sidechain
21	AA	1010	U	Sidechain
21	AA	1013	G	Sidechain
21	AA	1021	A	Sidechain
21	AA	1025	U	Sidechain
21	AA	1045	C	Sidechain
21	AA	1049	U	Sidechain
21	AA	1054	C	Sidechain
21	AA	1058	G	Sidechain
21	AA	1059	C	Sidechain
21	AA	1067	A	Sidechain
21	AA	107	G	Sidechain
21	AA	1077	G	Sidechain
21	AA	1085	U	Sidechain
21	AA	109	A	Sidechain
21	AA	1091	U	Sidechain
21	AA	1093	A	Sidechain
21	AA	110	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1103	C	Sidechain
21	AA	1106	G	Sidechain
21	AA	1107	C	Sidechain
21	AA	1108	G	Sidechain
21	AA	111	G	Sidechain
21	AA	1112	C	Sidechain
21	AA	1115	U	Sidechain
21	AA	1118	U	Sidechain
21	AA	1120	C	Sidechain
21	AA	1126	U	Sidechain
21	AA	1131	G	Sidechain
21	AA	1133	G	Sidechain
21	AA	1136	C	Sidechain
21	AA	114	U	Sidechain
21	AA	1142	G	Sidechain
21	AA	1146	A	Sidechain
21	AA	1159	U	Sidechain
21	AA	116	A	Sidechain
21	AA	1160	G	Sidechain
21	AA	1162	C	Sidechain
21	AA	1165	U	Sidechain
21	AA	1168	U	Sidechain
21	AA	117	G	Sidechain
21	AA	1170	A	Sidechain
21	AA	1178	G	Sidechain
21	AA	1189	U	Sidechain
21	AA	119	A	Sidechain
21	AA	1191	A	Sidechain
21	AA	1194	U	Sidechain
21	AA	1201	A	Sidechain
21	AA	1204	A	Sidechain
21	AA	1211	U	Sidechain
21	AA	1215	G	Sidechain
21	AA	122	G	Sidechain
21	AA	1221	G	Sidechain
21	AA	1223	C	Sidechain
21	AA	1224	U	Sidechain
21	AA	1227	A	Sidechain
21	AA	123	U	Sidechain
21	AA	1231	G	Sidechain
21	AA	1234	C	Sidechain
21	AA	1249	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	125	U	Sidechain
21	AA	1257	A	Sidechain
21	AA	1263	C	Sidechain
21	AA	1264	U	Sidechain
21	AA	1266	G	Sidechain
21	AA	1267	C	Sidechain
21	AA	1270	G	Sidechain
21	AA	1271	A	Sidechain
21	AA	1276	G	Sidechain
21	AA	1279	G	Sidechain
21	AA	1281	C	Sidechain
21	AA	1283	U	Sidechain
21	AA	1289	A	Sidechain
21	AA	1296	C	Sidechain
21	AA	130	A	Sidechain
21	AA	1300	G	Sidechain
21	AA	1303	C	Sidechain
21	AA	1305	G	Sidechain
21	AA	1307	U	Sidechain
21	AA	1308	U	Sidechain
21	AA	1309	G	Sidechain
21	AA	1311	A	Sidechain
21	AA	1312	G	Sidechain
21	AA	1316	G	Sidechain
21	AA	1319	A	Sidechain
21	AA	1336	C	Sidechain
21	AA	1339	A	Sidechain
21	AA	1342	C	Sidechain
21	AA	1343	G	Sidechain
21	AA	1345	U	Sidechain
21	AA	1347	G	Sidechain
21	AA	1351	U	Sidechain
21	AA	1356	G	Sidechain
21	AA	1358	U	Sidechain
21	AA	1360	A	Sidechain
21	AA	1361	G	Sidechain
21	AA	1363	A	Sidechain
21	AA	1370	G	Sidechain
21	AA	1377	A	Sidechain
21	AA	1378	C	Sidechain
21	AA	1380	U	Sidechain
21	AA	1387	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1388	C	Sidechain
21	AA	139	A	Sidechain
21	AA	1397	C	Sidechain
21	AA	1405	G	Sidechain
21	AA	1414	U	Sidechain
21	AA	1415	G	Sidechain
21	AA	1416	G	Sidechain
21	AA	1417	G	Sidechain
21	AA	1420	U	Sidechain
21	AA	1421	G	Sidechain
21	AA	1423	G	Sidechain
21	AA	1427	C	Sidechain
21	AA	1430	A	Sidechain
21	AA	1431	A	Sidechain
21	AA	1438	G	Sidechain
21	AA	1441	A	Sidechain
21	AA	1442	G	Sidechain
21	AA	1446	A	Sidechain
21	AA	1449	C	Sidechain
21	AA	1451	U	Sidechain
21	AA	1455	G	Sidechain
21	AA	1459	G	Sidechain
21	AA	1460	C	Sidechain
21	AA	1461	G	Sidechain
21	AA	1464	U	Sidechain
21	AA	1470	U	Sidechain
21	AA	1479	C	Sidechain
21	AA	148	G	Sidechain
21	AA	1485	U	Sidechain
21	AA	1496	C	Sidechain
21	AA	150	U	Sidechain
21	AA	1503	A	Sidechain
21	AA	151	A	Sidechain
21	AA	1516	G	Sidechain
21	AA	1519	A	Sidechain
21	AA	1525	G	Sidechain
21	AA	1526	G	Sidechain
21	AA	1529	G	Sidechain
21	AA	1530	G	Sidechain
21	AA	1532	U	Sidechain
21	AA	1534	A	Sidechain
21	AA	163	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	164	G	Sidechain
21	AA	165	G	Sidechain
21	AA	169	C	Sidechain
21	AA	173	U	Sidechain
21	AA	183	C	Sidechain
21	AA	187	G	Sidechain
21	AA	188	C	Sidechain
21	AA	195	A	Sidechain
21	AA	196	A	Sidechain
21	AA	20	U	Sidechain
21	AA	205	A	Sidechain
21	AA	210	C	Sidechain
21	AA	211	G	Sidechain
21	AA	215	C	Sidechain
21	AA	217	C	Sidechain
21	AA	218	U	Sidechain
21	AA	219	U	Sidechain
21	AA	232	G	Sidechain
21	AA	234	C	Sidechain
21	AA	235	C	Sidechain
21	AA	242	G	Sidechain
21	AA	245	U	Sidechain
21	AA	25	C	Sidechain
21	AA	256	U	Sidechain
21	AA	259	G	Sidechain
21	AA	261	U	Sidechain
21	AA	262	A	Sidechain
21	AA	263	A	Sidechain
21	AA	267	C	Sidechain
21	AA	27	G	Sidechain
21	AA	278	G	Sidechain
21	AA	280	C	Sidechain
21	AA	281	G	Sidechain
21	AA	29	U	Sidechain
21	AA	297	G	Sidechain
21	AA	309	A	Sidechain
21	AA	31	G	Sidechain
21	AA	313	A	Sidechain
21	AA	319	G	Sidechain
21	AA	321	A	Sidechain
21	AA	324	G	Sidechain
21	AA	326	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	328	C	Sidechain
21	AA	330	C	Sidechain
21	AA	331	G	Sidechain
21	AA	338	A	Sidechain
21	AA	340	U	Sidechain
21	AA	343	U	Sidechain
21	AA	346	G	Sidechain
21	AA	347	G	Sidechain
21	AA	349	A	Sidechain
21	AA	350	G	Sidechain
21	AA	353	A	Sidechain
21	AA	36	C	Sidechain
21	AA	362	G	Sidechain
21	AA	363	A	Sidechain
21	AA	37	U	Sidechain
21	AA	372	C	Sidechain
21	AA	375	U	Sidechain
21	AA	380	G	Sidechain
21	AA	389	A	Sidechain
21	AA	390	U	Sidechain
21	AA	397	A	Sidechain
21	AA	399	G	Sidechain
21	AA	400	C	Sidechain
21	AA	402	G	Sidechain
21	AA	408	A	Sidechain
21	AA	413	G	Sidechain
21	AA	429	U	Sidechain
21	AA	431	A	Sidechain
21	AA	432	A	Sidechain
21	AA	436	C	Sidechain
21	AA	439	U	Sidechain
21	AA	448	A	Sidechain
21	AA	449	G	Sidechain
21	AA	458	U	Sidechain
21	AA	461	A	Sidechain
21	AA	465	A	Sidechain
21	AA	466	A	Sidechain
21	AA	475	C	Sidechain
21	AA	479	U	Sidechain
21	AA	483	C	Sidechain
21	AA	484	G	Sidechain
21	AA	485	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	497	G	Sidechain
21	AA	499	A	Sidechain
21	AA	507	C	Sidechain
21	AA	511	C	Sidechain
21	AA	515	G	Sidechain
21	AA	517	G	Sidechain
21	AA	518	C	Sidechain
21	AA	519	C	Sidechain
21	AA	520	A	Sidechain
21	AA	527	G	Sidechain
21	AA	529	G	Sidechain
21	AA	530	G	Sidechain
21	AA	533	A	Sidechain
21	AA	54	C	Sidechain
21	AA	542	G	Sidechain
21	AA	549	C	Sidechain
21	AA	55	A	Sidechain
21	AA	555	U	Sidechain
21	AA	562	U	Sidechain
21	AA	563	A	Sidechain
21	AA	564	C	Sidechain
21	AA	566	G	Sidechain
21	AA	568	G	Sidechain
21	AA	586	C	Sidechain
21	AA	588	G	Sidechain
21	AA	591	U	Sidechain
21	AA	6	G	Sidechain
21	AA	60	A	Sidechain
21	AA	600	A	Sidechain
21	AA	61	G	Sidechain
21	AA	610	U	Sidechain
21	AA	615	G	Sidechain
21	AA	618	C	Sidechain
21	AA	621	A	Sidechain
21	AA	623	C	Sidechain
21	AA	634	C	Sidechain
21	AA	639	G	Sidechain
21	AA	650	G	Sidechain
21	AA	653	U	Sidechain
21	AA	654	G	Sidechain
21	AA	656	G	Sidechain
21	AA	660	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	664	G	Sidechain
21	AA	666	G	Sidechain
21	AA	669	G	Sidechain
21	AA	678	U	Sidechain
21	AA	68	G	Sidechain
21	AA	682	G	Sidechain
21	AA	683	G	Sidechain
21	AA	689	C	Sidechain
21	AA	69	G	Sidechain
21	AA	691	G	Sidechain
21	AA	695	A	Sidechain
21	AA	698	G	Sidechain
21	AA	700	G	Sidechain
21	AA	701	U	Sidechain
21	AA	702	A	Sidechain
21	AA	704	A	Sidechain
21	AA	705	G	Sidechain
21	AA	717	U	Sidechain
21	AA	725	G	Sidechain
21	AA	727	G	Sidechain
21	AA	730	G	Sidechain
21	AA	734	G	Sidechain
21	AA	743	A	Sidechain
21	AA	75	G	Sidechain
21	AA	752	G	Sidechain
21	AA	753	A	Sidechain
21	AA	76	G	Sidechain
21	AA	760	G	Sidechain
21	AA	761	G	Sidechain
21	AA	763	G	Sidechain
21	AA	764	C	Sidechain
21	AA	765	G	Sidechain
21	AA	772	U	Sidechain
21	AA	774	G	Sidechain
21	AA	778	G	Sidechain
21	AA	796	C	Sidechain
21	AA	81	A	Sidechain
21	AA	810	C	Sidechain
21	AA	811	C	Sidechain
21	AA	812	G	Sidechain
21	AA	818	G	Sidechain
21	AA	820	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	826	C	Sidechain
21	AA	827	U	Sidechain
21	AA	834	U	Sidechain
21	AA	836	G	Sidechain
21	AA	84	U	Sidechain
21	AA	841	C	Sidechain
21	AA	842	U	Sidechain
21	AA	849	G	Sidechain
21	AA	855	U	Sidechain
21	AA	858	G	Sidechain
21	AA	859	G	Sidechain
21	AA	863	U	Sidechain
21	AA	866	C	Sidechain
21	AA	869	G	Sidechain
21	AA	871	U	Sidechain
21	AA	88	U	Sidechain
21	AA	887	G	Sidechain
21	AA	888	G	Sidechain
21	AA	890	G	Sidechain
21	AA	891	U	Sidechain
21	AA	895	G	Sidechain
21	AA	898	G	Sidechain
21	AA	9	G	Sidechain
21	AA	903	G	Sidechain
21	AA	905	U	Sidechain
21	AA	91	U	Sidechain
21	AA	911	U	Sidechain
21	AA	916	U	Sidechain
21	AA	919	A	Sidechain
21	AA	921	U	Sidechain
21	AA	927	G	Sidechain
21	AA	931	C	Sidechain
21	AA	936	C	Sidechain
21	AA	937	A	Sidechain
21	AA	938	A	Sidechain
21	AA	941	G	Sidechain
21	AA	944	G	Sidechain
21	AA	951	G	Sidechain
21	AA	957	U	Sidechain
21	AA	960	U	Sidechain
21	AA	961	U	Sidechain
21	AA	962	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	968	A	Sidechain
21	AA	976	G	Sidechain
21	AA	977	A	Sidechain
21	AA	978	A	Sidechain
21	AA	982	U	Sidechain
21	AA	985	C	Sidechain
21	AA	989	U	Sidechain
21	AA	992	U	Sidechain
21	AA	995	C	Sidechain
21	AA	997	U	Sidechain
2	AC	168	ARG	Sidechain
2	AC	172	VAL	Peptide
8	AI	124	PRO	Peptide
10	AK	115	ILE	Peptide
54	BA	10	A	Sidechain
54	BA	100	U	Sidechain
54	BA	1000	A	Sidechain
54	BA	1006	C	Sidechain
54	BA	1009	A	Sidechain
54	BA	1020	A	Sidechain
54	BA	1025	G	Sidechain
54	BA	1026	G	Sidechain
54	BA	103	A	Sidechain
54	BA	1042	G	Sidechain
54	BA	1046	A	Sidechain
54	BA	1047	G	Sidechain
54	BA	1050	A	Sidechain
54	BA	1056	G	Sidechain
54	BA	106	C	Sidechain
54	BA	1066	U	Sidechain
54	BA	1069	A	Sidechain
54	BA	1074	G	Sidechain
54	BA	1079	C	Sidechain
54	BA	1086	A	Sidechain
54	BA	1088	A	Sidechain
54	BA	1095	A	Sidechain
54	BA	1098	A	Sidechain
54	BA	1101	U	Sidechain
54	BA	1106	G	Sidechain
54	BA	1127	A	Sidechain
54	BA	1130	U	Sidechain
54	BA	1131	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1132	U	Sidechain
54	BA	1133	A	Sidechain
54	BA	1135	C	Sidechain
54	BA	1138	G	Sidechain
54	BA	1139	G	Sidechain
54	BA	1140	C	Sidechain
54	BA	1160	G	Sidechain
54	BA	117	G	Sidechain
54	BA	1179	G	Sidechain
54	BA	1188	U	Sidechain
54	BA	119	A	Sidechain
54	BA	1191	G	Sidechain
54	BA	1193	G	Sidechain
54	BA	1199	U	Sidechain
54	BA	1200	C	Sidechain
54	BA	1203	U	Sidechain
54	BA	1209	U	Sidechain
54	BA	1210	G	Sidechain
54	BA	1212	G	Sidechain
54	BA	1215	G	Sidechain
54	BA	1224	U	Sidechain
54	BA	1225	G	Sidechain
54	BA	1226	A	Sidechain
54	BA	1232	G	Sidechain
54	BA	1233	C	Sidechain
54	BA	1235	G	Sidechain
54	BA	1236	G	Sidechain
54	BA	1237	A	Sidechain
54	BA	1244	A	Sidechain
54	BA	1248	G	Sidechain
54	BA	1251	C	Sidechain
54	BA	1253	A	Sidechain
54	BA	1256	G	Sidechain
54	BA	1259	G	Sidechain
54	BA	1266	G	Sidechain
54	BA	1268	A	Sidechain
54	BA	1270	C	Sidechain
54	BA	1272	A	Sidechain
54	BA	1276	A	Sidechain
54	BA	1283	G	Sidechain
54	BA	1287	A	Sidechain
54	BA	1288	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1291	C	Sidechain
54	BA	1292	G	Sidechain
54	BA	1293	C	Sidechain
54	BA	1297	C	Sidechain
54	BA	13	A	Sidechain
54	BA	1300	G	Sidechain
54	BA	1302	A	Sidechain
54	BA	1308	A	Sidechain
54	BA	1310	G	Sidechain
54	BA	1314	C	Sidechain
54	BA	1315	C	Sidechain
54	BA	1317	G	Sidechain
54	BA	1319	C	Sidechain
54	BA	1320	C	Sidechain
54	BA	1324	G	Sidechain
54	BA	1326	U	Sidechain
54	BA	1327	A	Sidechain
54	BA	1330	C	Sidechain
54	BA	1334	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1342	A	Sidechain
54	BA	1347	A	Sidechain
54	BA	1350	C	Sidechain
54	BA	1356	G	Sidechain
54	BA	1360	G	Sidechain
54	BA	1364	G	Sidechain
54	BA	1370	C	Sidechain
54	BA	1374	G	Sidechain
54	BA	1376	C	Sidechain
54	BA	1382	G	Sidechain
54	BA	1387	A	Sidechain
54	BA	1389	G	Sidechain
54	BA	1390	U	Sidechain
54	BA	1391	U	Sidechain
54	BA	1394	U	Sidechain
54	BA	1399	C	Sidechain
54	BA	1403	A	Sidechain
54	BA	1411	U	Sidechain
54	BA	1412	U	Sidechain
54	BA	1418	G	Sidechain
54	BA	1419	A	Sidechain
54	BA	1421	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1425	G	Sidechain
54	BA	1431	A	Sidechain
54	BA	1432	G	Sidechain
54	BA	1441	G	Sidechain
54	BA	1445	G	Sidechain
54	BA	1452	G	Sidechain
54	BA	1453	A	Sidechain
54	BA	1454	C	Sidechain
54	BA	1460	U	Sidechain
54	BA	1464	G	Sidechain
54	BA	147	C	Sidechain
54	BA	1470	A	Sidechain
54	BA	1483	G	Sidechain
54	BA	1484	U	Sidechain
54	BA	1492	G	Sidechain
54	BA	1498	C	Sidechain
54	BA	1505	A	Sidechain
54	BA	1510	G	Sidechain
54	BA	1519	G	Sidechain
54	BA	152	A	Sidechain
54	BA	1520	U	Sidechain
54	BA	1522	A	Sidechain
54	BA	1525	A	Sidechain
54	BA	1526	C	Sidechain
54	BA	1529	G	Sidechain
54	BA	153	U	Sidechain
54	BA	1536	C	Sidechain
54	BA	1537	G	Sidechain
54	BA	1539	U	Sidechain
54	BA	154	U	Sidechain
54	BA	1546	G	Sidechain
54	BA	1547	C	Sidechain
54	BA	1552	A	Sidechain
54	BA	1554	U	Sidechain
54	BA	1555	G	Sidechain
54	BA	156	A	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1562	U	Sidechain
54	BA	1567	G	Sidechain
54	BA	1581	G	Sidechain
54	BA	1585	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1595	C	Sidechain
54	BA	1600	C	Sidechain
54	BA	1601	G	Sidechain
54	BA	1602	U	Sidechain
54	BA	1618	A	Sidechain
54	BA	1621	U	Sidechain
54	BA	1632	A	Sidechain
54	BA	1633	G	Sidechain
54	BA	1636	U	Sidechain
54	BA	1641	A	Sidechain
54	BA	1642	G	Sidechain
54	BA	1651	G	Sidechain
54	BA	1653	G	Sidechain
54	BA	1655	A	Sidechain
54	BA	1656	C	Sidechain
54	BA	1657	U	Sidechain
54	BA	1664	A	Sidechain
54	BA	1665	A	Sidechain
54	BA	1667	G	Sidechain
54	BA	1672	A	Sidechain
54	BA	1682	G	Sidechain
54	BA	1688	U	Sidechain
54	BA	1705	A	Sidechain
54	BA	172	A	Sidechain
54	BA	1729	U	Sidechain
54	BA	1737	G	Sidechain
54	BA	1738	G	Sidechain
54	BA	1739	A	Sidechain
54	BA	1740	G	Sidechain
54	BA	1743	G	Sidechain
54	BA	1747	U	Sidechain
54	BA	1750	G	Sidechain
54	BA	1753	G	Sidechain
54	BA	1758	U	Sidechain
54	BA	1760	C	Sidechain
54	BA	1763	G	Sidechain
54	BA	1774	C	Sidechain
54	BA	1788	C	Sidechain
54	BA	1789	A	Sidechain
54	BA	1792	G	Sidechain
54	BA	1793	C	Sidechain
54	BA	1797	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1799	G	Sidechain
54	BA	1802	A	Sidechain
54	BA	1807	G	Sidechain
54	BA	181	A	Sidechain
54	BA	1814	G	Sidechain
54	BA	1817	G	Sidechain
54	BA	1821	A	Sidechain
54	BA	1825	U	Sidechain
54	BA	1827	U	Sidechain
54	BA	1831	G	Sidechain
54	BA	1833	C	Sidechain
54	BA	1835	G	Sidechain
54	BA	1838	C	Sidechain
54	BA	1839	G	Sidechain
54	BA	1843	C	Sidechain
54	BA	1849	G	Sidechain
54	BA	185	G	Sidechain
54	BA	1857	G	Sidechain
54	BA	1858	A	Sidechain
54	BA	1860	G	Sidechain
54	BA	1863	G	Sidechain
54	BA	1864	U	Sidechain
54	BA	1865	U	Sidechain
54	BA	1869	G	Sidechain
54	BA	1883	U	Sidechain
54	BA	1884	G	Sidechain
54	BA	1885	A	Sidechain
54	BA	1886	U	Sidechain
54	BA	1887	C	Sidechain
54	BA	1902	C	Sidechain
54	BA	1903	G	Sidechain
54	BA	1906	G	Sidechain
54	BA	1910	G	Sidechain
54	BA	1918	A	Sidechain
54	BA	1920	C	Sidechain
54	BA	1924	C	Sidechain
54	BA	1932	A	Sidechain
54	BA	1941	C	Sidechain
54	BA	1944	U	Sidechain
54	BA	1945	G	Sidechain
54	BA	1948	G	Sidechain
54	BA	1949	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1952	A	Sidechain
54	BA	1957	C	Sidechain
54	BA	196	A	Sidechain
54	BA	1960	A	Sidechain
54	BA	1962	C	Sidechain
54	BA	1966	A	Sidechain
54	BA	1969	A	Sidechain
54	BA	1976	U	Sidechain
54	BA	1978	A	Sidechain
54	BA	1983	G	Sidechain
54	BA	200	U	Sidechain
54	BA	2003	A	Sidechain
54	BA	2008	C	Sidechain
54	BA	2011	U	Sidechain
54	BA	2013	A	Sidechain
54	BA	2014	A	Sidechain
54	BA	2015	A	Sidechain
54	BA	2019	A	Sidechain
54	BA	202	U	Sidechain
54	BA	2028	U	Sidechain
54	BA	203	A	Sidechain
54	BA	2030	A	Sidechain
54	BA	2031	A	Sidechain
54	BA	2035	G	Sidechain
54	BA	2040	G	Sidechain
54	BA	2042	A	Sidechain
54	BA	2048	G	Sidechain
54	BA	206	U	Sidechain
54	BA	2065	C	Sidechain
54	BA	2066	C	Sidechain
54	BA	2069	G	Sidechain
54	BA	2074	U	Sidechain
54	BA	2075	U	Sidechain
54	BA	2077	A	Sidechain
54	BA	2079	U	Sidechain
54	BA	208	C	Sidechain
54	BA	2093	G	Sidechain
54	BA	2094	A	Sidechain
54	BA	2097	A	Sidechain
54	BA	2099	U	Sidechain
54	BA	2100	G	Sidechain
54	BA	2104	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2108	A	Sidechain
54	BA	2116	G	Sidechain
54	BA	2125	G	Sidechain
54	BA	2141	G	Sidechain
54	BA	2145	C	Sidechain
54	BA	2155	U	Sidechain
54	BA	2163	A	Sidechain
54	BA	2168	G	Sidechain
54	BA	2178	C	Sidechain
54	BA	2180	U	Sidechain
54	BA	2183	A	Sidechain
54	BA	2188	U	Sidechain
54	BA	2190	G	Sidechain
54	BA	2196	C	Sidechain
54	BA	2201	G	Sidechain
54	BA	2203	U	Sidechain
54	BA	2205	A	Sidechain
54	BA	2221	G	Sidechain
54	BA	2223	G	Sidechain
54	BA	2224	G	Sidechain
54	BA	2227	A	Sidechain
54	BA	2228	G	Sidechain
54	BA	2233	U	Sidechain
54	BA	2238	G	Sidechain
54	BA	2249	U	Sidechain
54	BA	2252	G	Sidechain
54	BA	2255	G	Sidechain
54	BA	2259	U	Sidechain
54	BA	226	A	Sidechain
54	BA	2260	C	Sidechain
54	BA	2262	U	Sidechain
54	BA	2269	G	Sidechain
54	BA	2272	U	Sidechain
54	BA	2273	A	Sidechain
54	BA	2278	A	Sidechain
54	BA	2279	G	Sidechain
54	BA	2280	G	Sidechain
54	BA	2282	G	Sidechain
54	BA	2295	C	Sidechain
54	BA	2299	U	Sidechain
54	BA	2301	C	Sidechain
54	BA	2304	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2309	A	Sidechain
54	BA	2312	U	Sidechain
54	BA	2325	G	Sidechain
54	BA	2327	A	Sidechain
54	BA	2332	C	Sidechain
54	BA	2345	G	Sidechain
54	BA	235	U	Sidechain
54	BA	2354	C	Sidechain
54	BA	2357	G	Sidechain
54	BA	2358	A	Sidechain
54	BA	2375	G	Sidechain
54	BA	238	C	Sidechain
54	BA	2383	G	Sidechain
54	BA	2384	U	Sidechain
54	BA	2385	C	Sidechain
54	BA	2388	A	Sidechain
54	BA	2389	G	Sidechain
54	BA	2391	G	Sidechain
54	BA	2396	G	Sidechain
54	BA	240	C	Sidechain
54	BA	2406	A	Sidechain
54	BA	2413	G	Sidechain
54	BA	2421	G	Sidechain
54	BA	2424	C	Sidechain
54	BA	2427	C	Sidechain
54	BA	2428	G	Sidechain
54	BA	2430	A	Sidechain
54	BA	2432	A	Sidechain
54	BA	2437	G	Sidechain
54	BA	2440	C	Sidechain
54	BA	2442	C	Sidechain
54	BA	2445	G	Sidechain
54	BA	2446	G	Sidechain
54	BA	2447	G	Sidechain
54	BA	2453	A	Sidechain
54	BA	2455	G	Sidechain
54	BA	2460	U	Sidechain
54	BA	2466	C	Sidechain
54	BA	2468	A	Sidechain
54	BA	2470	G	Sidechain
54	BA	2475	C	Sidechain
54	BA	2478	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2488	G	Sidechain
54	BA	2489	U	Sidechain
54	BA	249	C	Sidechain
54	BA	2491	U	Sidechain
54	BA	2494	G	Sidechain
54	BA	2498	C	Sidechain
54	BA	25	U	Sidechain
54	BA	250	G	Sidechain
54	BA	2502	G	Sidechain
54	BA	2506	U	Sidechain
54	BA	2510	C	Sidechain
54	BA	2516	A	Sidechain
54	BA	2517	C	Sidechain
54	BA	2520	C	Sidechain
54	BA	2523	G	Sidechain
54	BA	2530	A	Sidechain
54	BA	2534	A	Sidechain
54	BA	2540	C	Sidechain
54	BA	2543	G	Sidechain
54	BA	2544	G	Sidechain
54	BA	2545	G	Sidechain
54	BA	2553	G	Sidechain
54	BA	2554	U	Sidechain
54	BA	256	A	Sidechain
54	BA	2564	A	Sidechain
54	BA	2574	G	Sidechain
54	BA	2576	G	Sidechain
54	BA	2577	A	Sidechain
54	BA	2578	G	Sidechain
54	BA	2579	C	Sidechain
54	BA	2580	U	Sidechain
54	BA	2585	U	Sidechain
54	BA	2587	A	Sidechain
54	BA	2588	G	Sidechain
54	BA	2589	A	Sidechain
54	BA	2590	A	Sidechain
54	BA	2591	C	Sidechain
54	BA	2594	C	Sidechain
54	BA	2595	G	Sidechain
54	BA	2596	U	Sidechain
54	BA	2597	G	Sidechain
54	BA	2602	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2603	G	Sidechain
54	BA	2608	G	Sidechain
54	BA	2609	U	Sidechain
54	BA	261	G	Sidechain
54	BA	2614	A	Sidechain
54	BA	2615	U	Sidechain
54	BA	2621	G	Sidechain
54	BA	2625	G	Sidechain
54	BA	2627	G	Sidechain
54	BA	2629	U	Sidechain
54	BA	2635	A	Sidechain
54	BA	2636	C	Sidechain
54	BA	2637	U	Sidechain
54	BA	2639	A	Sidechain
54	BA	2644	G	Sidechain
54	BA	2645	G	Sidechain
54	BA	265	A	Sidechain
54	BA	2651	C	Sidechain
54	BA	2653	U	Sidechain
54	BA	2659	G	Sidechain
54	BA	2661	G	Sidechain
54	BA	2662	A	Sidechain
54	BA	2664	G	Sidechain
54	BA	2680	U	Sidechain
54	BA	2699	C	Sidechain
54	BA	2700	A	Sidechain
54	BA	2705	A	Sidechain
54	BA	2713	U	Sidechain
54	BA	272	A	Sidechain
54	BA	2721	A	Sidechain
54	BA	2722	G	Sidechain
54	BA	2725	A	Sidechain
54	BA	2730	C	Sidechain
54	BA	2731	G	Sidechain
54	BA	2739	U	Sidechain
54	BA	2743	U	Sidechain
54	BA	2751	G	Sidechain
54	BA	2753	A	Sidechain
54	BA	2759	G	Sidechain
54	BA	2765	A	Sidechain
54	BA	2780	G	Sidechain
54	BA	2782	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2783	U	Sidechain
54	BA	2786	U	Sidechain
54	BA	2790	U	Sidechain
54	BA	2794	C	Sidechain
54	BA	2796	U	Sidechain
54	BA	2799	A	Sidechain
54	BA	2801	G	Sidechain
54	BA	2805	C	Sidechain
54	BA	2808	G	Sidechain
54	BA	2816	G	Sidechain
54	BA	2819	G	Sidechain
54	BA	282	A	Sidechain
54	BA	2824	C	Sidechain
54	BA	2827	C	Sidechain
54	BA	2840	C	Sidechain
54	BA	2841	C	Sidechain
54	BA	2842	G	Sidechain
54	BA	2845	U	Sidechain
54	BA	2848	G	Sidechain
54	BA	2850	A	Sidechain
54	BA	2856	A	Sidechain
54	BA	2857	G	Sidechain
54	BA	2859	G	Sidechain
54	BA	2863	C	Sidechain
54	BA	2864	G	Sidechain
54	BA	2866	U	Sidechain
54	BA	2868	A	Sidechain
54	BA	2869	G	Sidechain
54	BA	2871	U	Sidechain
54	BA	2873	A	Sidechain
54	BA	2876	G	Sidechain
54	BA	2877	G	Sidechain
54	BA	2879	A	Sidechain
54	BA	2889	C	Sidechain
54	BA	2891	U	Sidechain
54	BA	2893	A	Sidechain
54	BA	2896	C	Sidechain
54	BA	298	G	Sidechain
54	BA	302	C	Sidechain
54	BA	303	G	Sidechain
54	BA	307	G	Sidechain
54	BA	313	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	315	G	Sidechain
54	BA	323	C	Sidechain
54	BA	325	G	Sidechain
54	BA	326	G	Sidechain
54	BA	327	G	Sidechain
54	BA	328	U	Sidechain
54	BA	333	G	Sidechain
54	BA	335	C	Sidechain
54	BA	339	U	Sidechain
54	BA	347	A	Sidechain
54	BA	354	A	Sidechain
54	BA	355	U	Sidechain
54	BA	357	C	Sidechain
54	BA	359	G	Sidechain
54	BA	361	G	Sidechain
54	BA	362	A	Sidechain
54	BA	384	A	Sidechain
54	BA	389	G	Sidechain
54	BA	39	G	Sidechain
54	BA	392	U	Sidechain
54	BA	395	U	Sidechain
54	BA	400	G	Sidechain
54	BA	401	A	Sidechain
54	BA	410	G	Sidechain
54	BA	412	A	Sidechain
54	BA	415	A	Sidechain
54	BA	416	U	Sidechain
54	BA	417	C	Sidechain
54	BA	418	C	Sidechain
54	BA	419	U	Sidechain
54	BA	420	C	Sidechain
54	BA	422	A	Sidechain
54	BA	426	C	Sidechain
54	BA	43	G	Sidechain
54	BA	432	A	Sidechain
54	BA	434	U	Sidechain
54	BA	442	G	Sidechain
54	BA	446	G	Sidechain
54	BA	449	A	Sidechain
54	BA	456	C	Sidechain
54	BA	458	G	Sidechain
54	BA	463	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	464	U	Sidechain
54	BA	470	A	Sidechain
54	BA	48	G	Sidechain
54	BA	489	G	Sidechain
54	BA	490	C	Sidechain
54	BA	491	G	Sidechain
54	BA	493	G	Sidechain
54	BA	494	G	Sidechain
54	BA	498	G	Sidechain
54	BA	500	G	Sidechain
54	BA	501	A	Sidechain
54	BA	503	A	Sidechain
54	BA	51	G	Sidechain
54	BA	511	U	Sidechain
54	BA	512	G	Sidechain
54	BA	514	A	Sidechain
54	BA	515	A	Sidechain
54	BA	528	A	Sidechain
54	BA	529	A	Sidechain
54	BA	533	G	Sidechain
54	BA	541	A	Sidechain
54	BA	544	C	Sidechain
54	BA	551	G	Sidechain
54	BA	556	A	Sidechain
54	BA	561	G	Sidechain
54	BA	562	U	Sidechain
54	BA	563	A	Sidechain
54	BA	569	U	Sidechain
54	BA	571	U	Sidechain
54	BA	572	A	Sidechain
54	BA	578	G	Sidechain
54	BA	579	G	Sidechain
54	BA	580	U	Sidechain
54	BA	581	C	Sidechain
54	BA	582	A	Sidechain
54	BA	587	C	Sidechain
54	BA	588	U	Sidechain
54	BA	589	U	Sidechain
54	BA	595	C	Sidechain
54	BA	608	A	Sidechain
54	BA	612	G	Sidechain
54	BA	617	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	624	C	Sidechain
54	BA	633	A	Sidechain
54	BA	636	G	Sidechain
54	BA	637	A	Sidechain
54	BA	644	A	Sidechain
54	BA	649	G	Sidechain
54	BA	653	U	Sidechain
54	BA	657	U	Sidechain
54	BA	659	G	Sidechain
54	BA	667	U	Sidechain
54	BA	669	G	Sidechain
54	BA	671	C	Sidechain
54	BA	680	C	Sidechain
54	BA	683	U	Sidechain
54	BA	686	U	Sidechain
54	BA	699	A	Sidechain
54	BA	703	U	Sidechain
54	BA	704	G	Sidechain
54	BA	707	G	Sidechain
54	BA	708	G	Sidechain
54	BA	711	G	Sidechain
54	BA	714	U	Sidechain
54	BA	715	A	Sidechain
54	BA	716	A	Sidechain
54	BA	718	A	Sidechain
54	BA	723	C	Sidechain
54	BA	724	U	Sidechain
54	BA	725	G	Sidechain
54	BA	726	G	Sidechain
54	BA	727	A	Sidechain
54	BA	728	G	Sidechain
54	BA	73	A	Sidechain
54	BA	739	A	Sidechain
54	BA	74	A	Sidechain
54	BA	743	A	Sidechain
54	BA	746	U	Sidechain
54	BA	754	U	Sidechain
54	BA	758	C	Sidechain
54	BA	759	G	Sidechain
54	BA	772	C	Sidechain
54	BA	774	G	Sidechain
54	BA	775	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	776	G	Sidechain
54	BA	782	A	Sidechain
54	BA	784	G	Sidechain
54	BA	785	G	Sidechain
54	BA	79	C	Sidechain
54	BA	801	G	Sidechain
54	BA	804	A	Sidechain
54	BA	810	U	Sidechain
54	BA	811	U	Sidechain
54	BA	816	C	Sidechain
54	BA	827	U	Sidechain
54	BA	828	U	Sidechain
54	BA	837	C	Sidechain
54	BA	84	A	Sidechain
54	BA	841	G	Sidechain
54	BA	851	C	Sidechain
54	BA	852	U	Sidechain
54	BA	856	G	Sidechain
54	BA	858	G	Sidechain
54	BA	859	G	Sidechain
54	BA	861	A	Sidechain
54	BA	864	G	Sidechain
54	BA	868	U	Sidechain
54	BA	882	G	Sidechain
54	BA	886	A	Sidechain
54	BA	891	G	Sidechain
54	BA	897	C	Sidechain
54	BA	9	G	Sidechain
54	BA	900	A	Sidechain
54	BA	904	G	Sidechain
54	BA	91	A	Sidechain
54	BA	910	A	Sidechain
54	BA	912	C	Sidechain
54	BA	917	A	Sidechain
54	BA	918	A	Sidechain
54	BA	92	U	Sidechain
54	BA	923	G	Sidechain
54	BA	932	U	Sidechain
54	BA	940	G	Sidechain
54	BA	950	G	Sidechain
54	BA	953	G	Sidechain
54	BA	955	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	957	C	Sidechain
54	BA	959	A	Sidechain
54	BA	966	G	Sidechain
54	BA	969	G	Sidechain
54	BA	975	A	Sidechain
54	BA	980	A	Sidechain
54	BA	983	A	Sidechain
54	BA	99	U	Sidechain
55	BB	10	G	Sidechain
55	BB	105	G	Sidechain
55	BB	106	G	Sidechain
55	BB	107	G	Sidechain
55	BB	117	G	Sidechain
55	BB	13	G	Sidechain
55	BB	14	U	Sidechain
55	BB	15	A	Sidechain
55	BB	2	G	Sidechain
55	BB	24	G	Sidechain
55	BB	25	U	Sidechain
55	BB	29	A	Sidechain
55	BB	33	G	Sidechain
55	BB	36	C	Sidechain
55	BB	40	U	Sidechain
55	BB	47	C	Sidechain
55	BB	48	U	Sidechain
55	BB	64	G	Sidechain
55	BB	66	A	Sidechain
55	BB	69	G	Sidechain
55	BB	7	G	Sidechain
55	BB	73	A	Sidechain
55	BB	75	G	Sidechain
55	BB	83	G	Sidechain
55	BB	85	G	Sidechain
55	BB	9	G	Sidechain
55	BB	91	C	Sidechain
55	BB	93	C	Sidechain
55	BB	94	A	Sidechain
55	BB	96	G	Sidechain
25	BC	142	ASN	Peptide
25	BC	62	ARG	Sidechain
33	BK	105	ARG	Sidechain
34	BL	123	ARG	Sidechain

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	AB	1708	0	1736	2	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	1	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	1	0
19	AT	668	0	718	2	0
20	AU	429	0	453	0	0
21	AA	32828	0	15886	9	0
22	A1	1627	0	798	0	0
23	A2	309	0	156	0	0
24	A3	1642	0	801	1	0
25	BC	2083	0	2157	2	0
26	BD	1565	0	1616	3	0
27	BE	1552	0	1619	1	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	2	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	1	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	0
49	B0	444	0	461	0	0
50	B1	413	0	444	1	0
51	B2	377	0	418	1	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	30186	21	0
55	BB	2504	0	1181	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	97702	45	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 (45) 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)
19:AT:40:ALA:HB1	19:AT:41:GLY:HA2	1.81	0.62
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.76	0.51
26:BD:154:LYS:HE3	26:BD:156:PHE:CE1	2.46	0.51
54:BA:931:U:C5	54:BA:1167:C:H1'	2.46	0.50
21:AA:5:U:H4'	21:AA:6:G:C6	2.46	0.50
54:BA:1021:A:N6	54:BA:1142:A:H62	2.11	0.49
54:BA:1025:G:C4	54:BA:1135:C:H1'	2.48	0.48
54:BA:1451:C:H4'	54:BA:1452:G:C4	2.50	0.46
26:BD:58:ASN:H	26:BD:59:ARG:HB2	1.79	0.46
54:BA:36:G:H4'	54:BA:451:U:C4	2.50	0.46
54:BA:561:G:H2'	54:BA:562:U:H5"	1.98	0.45
45:BW:11:ASN:ND2	54:BA:2264:C:H41	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AA:1533:C:H3'	21:AA:1534:A:H5''	1.98	0.44
24:A3:76:C:H1'	54:BA:2252:G:N2	2.33	0.44
54:BA:2144:G:H2'	54:BA:2146:C:C5	2.52	0.44
21:AA:87:C:H2'	21:AA:88:U:C6	2.52	0.44
33:BK:103:VAL:HG12	33:BK:104:THR:H	1.82	0.44
54:BA:2557:G:H2'	54:BA:2558:C:C6	2.53	0.44
33:BK:103:VAL:HG12	33:BK:104:THR:N	2.34	0.43
54:BA:783:A:C4	54:BA:785:G:H1'	2.54	0.43
27:BE:165:HIS:HA	54:BA:1205:A:C5	2.54	0.43
54:BA:1826:G:H2'	54:BA:1827:U:C6	2.54	0.43
19:AT:40:ALA:HB1	19:AT:41:GLY:CA	2.47	0.42
54:BA:532:A:C8	54:BA:2021:C:C4	3.07	0.42
51:B2:37:LYS:HE3	54:BA:458:G:N7	2.34	0.42
50:B1:20:TYR:CE1	50:B1:37:LYS:HE3	2.55	0.42
21:AA:5:U:H4'	21:AA:6:G:C5	2.54	0.42
1:AB:162:VAL:HG22	1:AB:164:ASP:H	1.85	0.42
9:AJ:71:LEU:HD23	9:AJ:72:ARG:N	2.35	0.42
54:BA:2440:C:C5	54:BA:2441:U:H1'	2.55	0.41
25:BC:222:THR:HG22	54:BA:1826:G:H5''	2.03	0.41
54:BA:61:C:H3'	54:BA:62:U:H5''	2.03	0.41
54:BA:1729:U:C5	54:BA:1730:C:H1'	2.55	0.41
26:BD:106:LYS:HE3	26:BD:206:ALA:O	2.20	0.41
1:AB:30:ILE:HG22	1:AB:32:GLY:H	1.86	0.41
54:BA:1631:G:C2	54:BA:1633:G:H5''	2.56	0.41
21:AA:6:G:N3	21:AA:6:G:H2'	2.36	0.41
18:AS:5:LYS:HE2	21:AA:1312:G:H5'	2.02	0.41
21:AA:765:G:C8	21:AA:813:U:C4	3.08	0.41
21:AA:35:G:H1'	21:AA:36:C:C6	2.56	0.41
37:BO:40:ILE:N	37:BO:40:ILE:HD12	2.36	0.41
21:AA:410:G:H2'	21:AA:429:U:C4	2.56	0.40
54:BA:1712:U:H3'	54:BA:1713:A:H3'	2.03	0.40
25:BC:75:ALA:HB2	25:BC:95:TYR:CD2	2.57	0.40
34:BL:70:LYS:HE2	34:BL:107:PHE:CZ	2.56	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	
1	AB	218/220 (99%)	195 (89%)	22 (10%)	1 (0%)	34	77
2	AC	205/208 (99%)	191 (93%)	12 (6%)	2 (1%)	19	65
3	AD	203/206 (98%)	185 (91%)	15 (7%)	3 (2%)	13	57
4	AE	150/152 (99%)	134 (89%)	9 (6%)	7 (5%)	3	32
5	AF	99/101 (98%)	86 (87%)	6 (6%)	7 (7%)	1	22
6	AG	150/152 (99%)	143 (95%)	7 (5%)	0	100	100
7	AH	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
8	AI	126/128 (98%)	110 (87%)	12 (10%)	4 (3%)	5	41
9	AJ	98/100 (98%)	88 (90%)	5 (5%)	5 (5%)	2	30
10	AK	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	21	67
11	AL	121/124 (98%)	111 (92%)	10 (8%)	0	100	100
12	AM	112/115 (97%)	98 (88%)	12 (11%)	2 (2%)	11	53
13	AN	98/101 (97%)	90 (92%)	7 (7%)	1 (1%)	19	65
14	AO	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	16	61
15	AP	79/81 (98%)	68 (86%)	7 (9%)	4 (5%)	2	30
16	AQ	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	7	46
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	11	53
18	AS	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
19	AT	84/86 (98%)	74 (88%)	8 (10%)	2 (2%)	7	47
20	AU	51/53 (96%)	27 (53%)	14 (28%)	10 (20%)	0	3
25	BC	270/273 (99%)	238 (88%)	21 (8%)	11 (4%)	3	35
26	BD	207/209 (99%)	178 (86%)	18 (9%)	11 (5%)	2	29
27	BE	199/201 (99%)	177 (89%)	17 (8%)	5 (2%)	7	46
28	BF	176/179 (98%)	151 (86%)	21 (12%)	4 (2%)	8	48
29	BG	174/177 (98%)	152 (87%)	13 (8%)	9 (5%)	2	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BH	147/149 (99%)	132 (90%)	13 (9%)	2 (1%)	14	58
31	BI	139/142 (98%)	125 (90%)	10 (7%)	4 (3%)	6	43
32	BJ	140/142 (99%)	125 (89%)	8 (6%)	7 (5%)	3	31
33	BK	121/123 (98%)	106 (88%)	12 (10%)	3 (2%)	7	46
34	BL	141/144 (98%)	117 (83%)	12 (8%)	12 (8%)	1	18
35	BM	134/136 (98%)	117 (87%)	12 (9%)	5 (4%)	4	38
36	BN	119/121 (98%)	107 (90%)	10 (8%)	2 (2%)	11	55
37	BO	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
38	BP	112/115 (97%)	91 (81%)	15 (13%)	6 (5%)	2	29
39	BQ	115/118 (98%)	100 (87%)	15 (13%)	0	100	100
40	BR	101/103 (98%)	94 (93%)	3 (3%)	4 (4%)	4	35
41	BS	108/110 (98%)	100 (93%)	6 (6%)	2 (2%)	10	52
42	BT	92/94 (98%)	78 (85%)	11 (12%)	3 (3%)	5	40
43	BU	101/104 (97%)	85 (84%)	12 (12%)	4 (4%)	4	35
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	65 (83%)	6 (8%)	7 (9%)	1	17
46	BX	75/79 (95%)	70 (93%)	3 (4%)	2 (3%)	6	45
47	BY	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	12	56
48	BZ	56/59 (95%)	50 (89%)	4 (7%)	2 (4%)	4	38
49	B0	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	10	52
50	B1	50/52 (96%)	43 (86%)	3 (6%)	4 (8%)	1	19
51	B2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
52	B3	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	5	41
53	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
56	B5	221/234 (94%)	210 (95%)	8 (4%)	3 (1%)	14	58
All	All	5876/6008 (98%)	5249 (89%)	458 (8%)	169 (3%)	9	43

All (169) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	149	PRO
8	AI	44	ARG
16	AQ	80	LYS

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Mol	Chain	Res	Type
20	AU	6	ARG
20	AU	9	GLU
20	AU	13	VAL
25	BC	141	HIS
26	BD	80	TRP
27	BE	31	VAL
33	BK	71	ARG
33	BK	103	VAL
34	BL	55	MET
34	BL	66	PHE
35	BM	21	ALA
35	BM	110	GLU
43	BU	70	ALA
49	B0	39	ARG
2	AC	195	ILE
3	AD	47	LEU
4	AE	54	GLU
4	AE	104	ILE
4	AE	105	ILE
5	AF	10	VAL
5	AF	59	TYR
8	AI	119	LYS
12	AM	22	TYR
12	AM	42	VAL
15	AP	17	TYR
19	AT	42	ASP
20	AU	22	CYS
20	AU	48	LYS
25	BC	161	VAL
25	BC	185	ALA
26	BD	51	THR
26	BD	60	VAL
26	BD	75	ALA
27	BE	96	VAL
28	BF	103	ILE
29	BG	46	ASP
29	BG	167	VAL
29	BG	174	LYS
31	BI	10	LEU
31	BI	119	ALA
32	BJ	15	TRP
33	BK	25	LEU

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Mol	Chain	Res	Type
34	BL	82	LEU
34	BL	83	ALA
34	BL	101	ILE
36	BN	47	VAL
38	BP	69	VAL
40	BR	29	THR
40	BR	53	PHE
45	BW	10	ARG
45	BW	14	ASP
45	BW	23	LYS
46	BX	27	ARG
50	B1	36	LYS
52	B3	46	LYS
4	AE	43	GLY
5	AF	6	ILE
5	AF	86	ARG
8	AI	120	ALA
9	AJ	41	PRO
9	AJ	57	VAL
9	AJ	75	ASP
10	AK	16	SER
20	AU	20	ARG
20	AU	34	ARG
25	BC	13	ARG
25	BC	36	ASN
26	BD	34	VAL
26	BD	86	GLU
26	BD	136	ASN
28	BF	77	LYS
29	BG	39	ALA
29	BG	59	ASP
30	BH	10	ALA
32	BJ	81	ILE
34	BL	15	ALA
34	BL	44	GLY
38	BP	26	GLU
38	BP	50	ARG
38	BP	64	SER
40	BR	30	GLY
42	BT	11	LEU
43	BU	5	ARG
45	BW	41	GLY

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Mol	Chain	Res	Type
45	BW	74	LYS
50	B1	45	HIS
56	B5	109	MET
1	AB	18	GLN
5	AF	90	MET
8	AI	122	ARG
15	AP	9	HIS
15	AP	79	ASN
16	AQ	17	GLU
19	AT	65	LEU
20	AU	21	SER
25	BC	189	ALA
25	BC	196	ASN
26	BD	95	SER
26	BD	114	LYS
27	BE	94	GLN
27	BE	97	ASN
27	BE	123	LYS
28	BF	136	ILE
29	BG	22	VAL
29	BG	151	ARG
30	BH	88	GLY
31	BI	135	MET
32	BJ	44	TYR
32	BJ	45	THR
34	BL	5	THR
34	BL	29	LYS
34	BL	30	THR
35	BM	36	VAL
35	BM	58	LYS
38	BP	32	VAL
42	BT	78	SER
45	BW	11	ASN
47	BY	61	ALA
48	BZ	3	THR
50	B1	24	LYS
52	B3	25	HIS
3	AD	26	ALA
3	AD	84	ASN
4	AE	106	ALA
5	AF	92	THR
5	AF	98	GLU

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Mol	Chain	Res	Type
9	AJ	42	LEU
9	AJ	92	LEU
15	AP	13	LYS
20	AU	28	LEU
25	BC	153	LEU
26	BD	15	PHE
28	BF	107	VAL
31	BI	64	ARG
32	BJ	53	TYR
34	BL	17	LYS
34	BL	69	ARG
36	BN	10	LEU
41	BS	90	LYS
43	BU	12	VAL
45	BW	44	PHE
46	BX	53	LYS
4	AE	158	LYS
13	AN	70	PRO
20	AU	23	GLU
25	BC	169	ALA
25	BC	235	GLU
26	BD	119	ALA
32	BJ	42	ALA
35	BM	80	VAL
42	BT	9	LYS
50	B1	4	ILE
32	BJ	112	GLY
56	B5	91	GLY
56	B5	107	GLY
38	BP	31	VAL
2	AC	14	VAL
25	BC	9	SER
29	BG	112	VAL
48	BZ	31	ILE
14	AO	40	GLY
17	AR	20	ILE
40	BR	27	ILE
41	BS	29	VAL
43	BU	19	GLY
29	BG	97	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	
1	AB	180/180 (100%)	177 (98%)	3 (2%)	68	87
2	AC	170/171 (99%)	167 (98%)	3 (2%)	66	87
3	AD	172/173 (99%)	168 (98%)	4 (2%)	58	83
4	AE	113/113 (100%)	110 (97%)	3 (3%)	52	79
5	AF	87/87 (100%)	86 (99%)	1 (1%)	80	91
6	AG	123/123 (100%)	123 (100%)	0	100	100
7	AH	104/105 (99%)	102 (98%)	2 (2%)	65	86
8	AI	105/105 (100%)	105 (100%)	0	100	100
9	AJ	86/86 (100%)	82 (95%)	4 (5%)	32	68
10	AK	90/90 (100%)	88 (98%)	2 (2%)	60	83
11	AL	103/104 (99%)	102 (99%)	1 (1%)	82	92
12	AM	91/92 (99%)	88 (97%)	3 (3%)	45	76
13	AN	83/84 (99%)	81 (98%)	2 (2%)	57	82
14	AO	76/77 (99%)	76 (100%)	0	100	100
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	74 (100%)	0	100	100
17	AR	48/48 (100%)	47 (98%)	1 (2%)	61	84
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	62 (95%)	3 (5%)	33	68
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	210 (97%)	6 (3%)	51	78
26	BD	164/164 (100%)	161 (98%)	3 (2%)	66	87
27	BE	165/165 (100%)	163 (99%)	2 (1%)	78	90
28	BF	149/150 (99%)	148 (99%)	1 (1%)	88	94
29	BG	137/138 (99%)	134 (98%)	3 (2%)	60	83
30	BH	114/114 (100%)	113 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	BI	109/110 (99%)	106 (97%)	3 (3%)	51	78
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	68	87
33	BK	103/103 (100%)	99 (96%)	4 (4%)	39	72
34	BL	102/103 (99%)	101 (99%)	1 (1%)	82	92
35	BM	109/109 (100%)	106 (97%)	3 (3%)	51	78
36	BN	100/100 (100%)	99 (99%)	1 (1%)	82	92
37	BO	86/87 (99%)	85 (99%)	1 (1%)	78	90
38	BP	99/100 (99%)	95 (96%)	4 (4%)	38	71
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	80	91
40	BR	84/84 (100%)	83 (99%)	1 (1%)	78	90
41	BS	93/93 (100%)	90 (97%)	3 (3%)	46	76
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	83 (100%)	0	100	100
44	BV	78/78 (100%)	76 (97%)	2 (3%)	54	80
45	BW	59/59 (100%)	55 (93%)	4 (7%)	20	57
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	45 (96%)	2 (4%)	35	70
50	B1	45/45 (100%)	45 (100%)	0	100	100
51	B2	38/38 (100%)	37 (97%)	1 (3%)	54	80
52	B3	51/52 (98%)	50 (98%)	1 (2%)	63	85
53	B4	34/34 (100%)	33 (97%)	1 (3%)	50	78
56	B5	173/181 (96%)	170 (98%)	3 (2%)	68	87
All	All	4842/4870 (99%)	4756 (98%)	86 (2%)	69	87

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	22	TRP
1	AB	88	GLN
1	AB	164	ASP
2	AC	35	ASP
2	AC	128	MET

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Mol	Chain	Res	Type
2	AC	175	HIS
3	AD	39	GLN
3	AD	40	HIS
3	AD	169	TRP
3	AD	197	HIS
4	AE	30	PHE
4	AE	47	PHE
4	AE	151	MET
5	AF	52	ASN
7	AH	76	ARG
7	AH	104	SER
9	AJ	42	LEU
9	AJ	48	ARG
9	AJ	49	PHE
9	AJ	59	LYS
10	AK	52	ARG
10	AK	121	ARG
11	AL	4	ASN
12	AM	3	ILE
12	AM	18	LEU
12	AM	54	THR
13	AN	62	ASN
13	AN	71	HIS
17	AR	34	GLU
19	AT	22	SER
19	AT	35	TYR
19	AT	67	HIS
25	BC	80	LEU
25	BC	173	LEU
25	BC	188	ARG
25	BC	190	THR
25	BC	200	MET
25	BC	235	GLU
26	BD	33	ARG
26	BD	67	HIS
26	BD	124	ARG
27	BE	78	TRP
27	BE	116	ASP
28	BF	162	ASP
29	BG	59	ASP
29	BG	66	THR
29	BG	162	ARG

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Mol	Chain	Res	Type
30	BH	137	GLU
31	BI	22	PRO
31	BI	34	ILE
31	BI	87	SER
32	BJ	1	MET
32	BJ	135	GLN
33	BK	32	TYR
33	BK	65	THR
33	BK	84	CYS
33	BK	105	ARG
34	BL	46	VAL
35	BM	57	VAL
35	BM	97	GLN
35	BM	131	VAL
36	BN	4	ARG
37	BO	9	ARG
38	BP	32	VAL
38	BP	64	SER
38	BP	67	GLU
38	BP	98	TYR
39	BQ	32	ARG
40	BR	32	THR
41	BS	1	MET
41	BS	3	THR
41	BS	15	GLN
44	BV	24	ASN
44	BV	51	GLN
45	BW	31	LEU
45	BW	38	ARG
45	BW	39	GLN
45	BW	40	ARG
49	B0	26	SER
49	B0	45	ASP
51	B2	16	HIS
52	B3	25	HIS
53	B4	19	ARG
56	B5	109	MET
56	B5	129	GLN
56	B5	180	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	145	ASN
13	AN	62	ASN
18	AS	51	HIS
18	AS	56	HIS
26	BD	134	HIS
32	BJ	77	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	250 (16%)	72 (4%)
22	A1	73/76 (96%)	8 (10%)	6 (8%)
23	A2	14/15 (93%)	3 (21%)	1 (7%)
24	A3	76/77 (98%)	9 (11%)	6 (7%)
54	BA	2902/2903 (99%)	460 (15%)	132 (4%)
55	BB	116/118 (98%)	17 (14%)	3 (2%)
All	All	4710/4722 (99%)	747 (15%)	220 (4%)

All (747) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	16	A
21	AA	27	G
21	AA	31	G
21	AA	32	A
21	AA	34	C
21	AA	35	G
21	AA	39	G
21	AA	46	G
21	AA	48	C
21	AA	51	A
21	AA	65	A
21	AA	66	A
21	AA	69	G
21	AA	71	A
21	AA	72	A
21	AA	83	C

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Mol	Chain	Res	Type
21	AA	84	U
21	AA	85	U
21	AA	86	G
21	AA	87	C
21	AA	95	C
21	AA	110	C
21	AA	121	U
21	AA	130	A
21	AA	132	C
21	AA	133	U
21	AA	144	G
21	AA	159	G
21	AA	160	A
21	AA	163	C
21	AA	165	G
21	AA	182	A
21	AA	183	C
21	AA	195	A
21	AA	197	A
21	AA	198	G
21	AA	211	G
21	AA	212	G
21	AA	239	U
21	AA	240	G
21	AA	243	A
21	AA	244	U
21	AA	246	A
21	AA	249	U
21	AA	250	A
21	AA	251	G
21	AA	252	U
21	AA	272	C
21	AA	275	G
21	AA	282	A
21	AA	285	C
21	AA	289	G
21	AA	293	G
21	AA	306	A
21	AA	309	A
21	AA	310	G
21	AA	316	C
21	AA	317	U

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Mol	Chain	Res	Type
21	AA	328	C
21	AA	329	A
21	AA	330	C
21	AA	340	U
21	AA	341	C
21	AA	347	G
21	AA	348	G
21	AA	352	C
21	AA	354	G
21	AA	355	C
21	AA	367	U
21	AA	381	C
21	AA	382	A
21	AA	383	A
21	AA	397	A
21	AA	398	U
21	AA	412	A
21	AA	413	G
21	AA	415	A
21	AA	421	U
21	AA	422	C
21	AA	424	G
21	AA	428	G
21	AA	429	U
21	AA	452	A
21	AA	456	A
21	AA	461	A
21	AA	467	U
21	AA	468	A
21	AA	470	C
21	AA	484	G
21	AA	485	U
21	AA	493	A
21	AA	496	A
21	AA	497	G
21	AA	504	C
21	AA	505	G
21	AA	506	G
21	AA	509	A
21	AA	510	A
21	AA	511	C
21	AA	523	A

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Mol	Chain	Res	Type
21	AA	527	G
21	AA	532	A
21	AA	533	A
21	AA	534	U
21	AA	547	A
21	AA	550	G
21	AA	562	U
21	AA	564	C
21	AA	572	A
21	AA	573	A
21	AA	575	G
21	AA	576	C
21	AA	577	G
21	AA	610	U
21	AA	618	C
21	AA	619	U
21	AA	642	A
21	AA	649	A
21	AA	653	U
21	AA	660	C
21	AA	675	A
21	AA	700	G
21	AA	722	G
21	AA	723	U
21	AA	724	G
21	AA	731	G
21	AA	734	G
21	AA	735	C
21	AA	755	G
21	AA	767	A
21	AA	777	A
21	AA	794	A
21	AA	808	C
21	AA	811	C
21	AA	812	G
21	AA	819	A
21	AA	841	C
21	AA	842	U
21	AA	843	U
21	AA	846	G
21	AA	867	G
21	AA	872	A

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Mol	Chain	Res	Type
21	AA	885	G
21	AA	891	U
21	AA	892	A
21	AA	893	C
21	AA	914	A
21	AA	926	G
21	AA	927	G
21	AA	929	G
21	AA	934	C
21	AA	939	G
21	AA	960	U
21	AA	961	U
21	AA	968	A
21	AA	969	A
21	AA	974	A
21	AA	976	G
21	AA	978	A
21	AA	980	C
21	AA	981	U
21	AA	983	A
21	AA	992	U
21	AA	993	G
21	AA	994	A
21	AA	1004	A
21	AA	1030	U
21	AA	1031	C
21	AA	1033	G
21	AA	1053	G
21	AA	1054	C
21	AA	1055	A
21	AA	1056	U
21	AA	1065	U
21	AA	1068	G
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1124	G
21	AA	1125	U
21	AA	1137	C
21	AA	1139	G
21	AA	1152	A

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Mol	Chain	Res	Type
21	AA	1157	A
21	AA	1159	U
21	AA	1160	G
21	AA	1161	C
21	AA	1167	A
21	AA	1183	U
21	AA	1189	U
21	AA	1190	G
21	AA	1191	A
21	AA	1196	A
21	AA	1201	A
21	AA	1202	U
21	AA	1204	A
21	AA	1213	A
21	AA	1217	C
21	AA	1222	G
21	AA	1225	A
21	AA	1227	A
21	AA	1228	C
21	AA	1241	G
21	AA	1256	A
21	AA	1257	A
21	AA	1258	G
21	AA	1266	G
21	AA	1280	A
21	AA	1281	C
21	AA	1286	U
21	AA	1301	U
21	AA	1302	C
21	AA	1304	G
21	AA	1305	G
21	AA	1312	G
21	AA	1317	C
21	AA	1318	A
21	AA	1322	C
21	AA	1329	A
21	AA	1336	C
21	AA	1337	G
21	AA	1338	G
21	AA	1345	U
21	AA	1346	A
21	AA	1360	A

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Mol	Chain	Res	Type
21	AA	1363	A
21	AA	1381	U
21	AA	1397	C
21	AA	1398	A
21	AA	1419	G
21	AA	1432	G
21	AA	1446	A
21	AA	1447	A
21	AA	1448	C
21	AA	1470	U
21	AA	1493	A
21	AA	1494	G
21	AA	1497	G
21	AA	1503	A
21	AA	1506	U
21	AA	1529	G
21	AA	1530	G
21	AA	1533	C
21	AA	1534	A
22	A1	10	G
22	A1	11	C
22	A1	17	U
22	A1	48	C
22	A1	57	G
22	A1	60	C
22	A1	61	C
22	A1	75	C
23	A2	89	U
23	A2	90	U
23	A2	91	A
24	A3	9	G
24	A3	16	C
24	A3	17	C
24	A3	18	U
24	A3	48	U
24	A3	49	C
24	A3	62	C
24	A3	63	C
24	A3	73	A
54	BA	10	A
54	BA	11	C
54	BA	34	U

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Mol	Chain	Res	Type
54	BA	48	G
54	BA	52	A
54	BA	61	C
54	BA	62	U
54	BA	71	A
54	BA	72	U
54	BA	73	A
54	BA	75	G
54	BA	84	A
54	BA	100	U
54	BA	101	A
54	BA	102	U
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	122	G
54	BA	142	A
54	BA	143	C
54	BA	149	A
54	BA	162	U
54	BA	181	A
54	BA	196	A
54	BA	199	A
54	BA	205	G
54	BA	216	A
54	BA	222	A
54	BA	225	C
54	BA	233	A
54	BA	248	G
54	BA	249	C
54	BA	250	G
54	BA	263	G
54	BA	271	G
54	BA	272	A
54	BA	273	G
54	BA	279	A
54	BA	280	U
54	BA	295	G
54	BA	317	G
54	BA	323	C
54	BA	324	A
54	BA	326	G

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Mol	Chain	Res	Type
54	BA	327	G
54	BA	329	G
54	BA	330	A
54	BA	331	C
54	BA	332	A
54	BA	345	A
54	BA	346	A
54	BA	370	G
54	BA	372	G
54	BA	386	G
54	BA	404	A
54	BA	405	U
54	BA	406	G
54	BA	412	A
54	BA	428	A
54	BA	430	A
54	BA	443	A
54	BA	449	A
54	BA	451	U
54	BA	452	G
54	BA	453	A
54	BA	454	A
54	BA	456	C
54	BA	457	A
54	BA	458	G
54	BA	473	G
54	BA	478	A
54	BA	479	A
54	BA	480	A
54	BA	481	G
54	BA	484	C
54	BA	491	G
54	BA	504	A
54	BA	505	A
54	BA	520	G
54	BA	526	A
54	BA	527	C
54	BA	529	A
54	BA	531	C
54	BA	532	A
54	BA	533	G
54	BA	544	C

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Mol	Chain	Res	Type
54	BA	546	U
54	BA	547	A
54	BA	548	G
54	BA	573	U
54	BA	575	A
54	BA	586	A
54	BA	587	C
54	BA	603	A
54	BA	607	U
54	BA	612	G
54	BA	613	A
54	BA	614	A
54	BA	615	U
54	BA	620	G
54	BA	627	A
54	BA	631	A
54	BA	632	A
54	BA	637	A
54	BA	646	U
54	BA	653	U
54	BA	654	A
54	BA	671	C
54	BA	672	C
54	BA	685	A
54	BA	686	U
54	BA	715	A
54	BA	716	A
54	BA	719	C
54	BA	727	A
54	BA	730	A
54	BA	747	U
54	BA	751	A
54	BA	758	C
54	BA	759	G
54	BA	763	G
54	BA	775	G
54	BA	781	A
54	BA	782	A
54	BA	783	A
54	BA	784	G
54	BA	785	G
54	BA	791	C

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Mol	Chain	Res	Type
54	BA	792	A
54	BA	794	A
54	BA	805	G
54	BA	809	G
54	BA	812	C
54	BA	847	U
54	BA	848	C
54	BA	858	G
54	BA	866	A
54	BA	889	C
54	BA	890	C
54	BA	891	G
54	BA	896	A
54	BA	897	C
54	BA	907	G
54	BA	910	A
54	BA	914	G
54	BA	915	C
54	BA	931	U
54	BA	941	A
54	BA	946	C
54	BA	955	U
54	BA	959	A
54	BA	961	C
54	BA	972	A
54	BA	974	G
54	BA	975	A
54	BA	980	A
54	BA	982	C
54	BA	983	A
54	BA	985	C
54	BA	990	A
54	BA	995	C
54	BA	996	A
54	BA	1012	U
54	BA	1013	C
54	BA	1021	A
54	BA	1022	G
54	BA	1024	G
54	BA	1025	G
54	BA	1033	U
54	BA	1044	C

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Mol	Chain	Res	Type
54	BA	1048	A
54	BA	1060	U
54	BA	1062	G
54	BA	1063	G
54	BA	1067	A
54	BA	1068	G
54	BA	1070	A
54	BA	1071	G
54	BA	1073	A
54	BA	1076	C
54	BA	1078	U
54	BA	1079	C
54	BA	1088	A
54	BA	1089	A
54	BA	1090	A
54	BA	1094	U
54	BA	1096	A
54	BA	1112	G
54	BA	1126	A
54	BA	1128	G
54	BA	1129	A
54	BA	1132	U
54	BA	1134	A
54	BA	1135	C
54	BA	1143	A
54	BA	1155	A
54	BA	1175	A
54	BA	1176	U
54	BA	1186	G
54	BA	1210	G
54	BA	1211	C
54	BA	1225	G
54	BA	1242	U
54	BA	1247	A
54	BA	1251	C
54	BA	1253	A
54	BA	1255	U
54	BA	1256	G
54	BA	1265	A
54	BA	1266	G
54	BA	1267	U
54	BA	1272	A

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Mol	Chain	Res	Type
54	BA	1273	U
54	BA	1275	A
54	BA	1276	A
54	BA	1287	A
54	BA	1291	C
54	BA	1300	G
54	BA	1301	A
54	BA	1314	C
54	BA	1319	C
54	BA	1320	C
54	BA	1326	U
54	BA	1328	A
54	BA	1332	G
54	BA	1341	G
54	BA	1365	A
54	BA	1374	G
54	BA	1379	U
54	BA	1383	A
54	BA	1385	A
54	BA	1386	C
54	BA	1390	U
54	BA	1394	U
54	BA	1396	U
54	BA	1397	U
54	BA	1416	G
54	BA	1420	A
54	BA	1421	G
54	BA	1427	A
54	BA	1428	C
54	BA	1440	U
54	BA	1452	G
54	BA	1453	A
54	BA	1454	C
54	BA	1458	U
54	BA	1459	G
54	BA	1461	C
54	BA	1466	U
54	BA	1482	G
54	BA	1490	A
54	BA	1493	C
54	BA	1524	G
54	BA	1535	A

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Mol	Chain	Res	Type
54	BA	1536	C
54	BA	1537	G
54	BA	1538	G
54	BA	1539	U
54	BA	1540	G
54	BA	1550	C
54	BA	1560	G
54	BA	1569	A
54	BA	1584	U
54	BA	1598	A
54	BA	1599	U
54	BA	1607	C
54	BA	1608	A
54	BA	1618	A
54	BA	1625	C
54	BA	1626	A
54	BA	1629	U
54	BA	1633	G
54	BA	1634	A
54	BA	1635	A
54	BA	1648	U
54	BA	1652	A
54	BA	1656	C
54	BA	1674	G
54	BA	1675	C
54	BA	1707	G
54	BA	1712	U
54	BA	1714	U
54	BA	1730	C
54	BA	1758	U
54	BA	1764	C
54	BA	1773	A
54	BA	1800	C
54	BA	1808	A
54	BA	1816	C
54	BA	1821	A
54	BA	1827	U
54	BA	1833	C
54	BA	1847	A
54	BA	1873	G
54	BA	1888	G
54	BA	1900	A

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Mol	Chain	Res	Type
54	BA	1901	A
54	BA	1906	G
54	BA	1913	A
54	BA	1914	C
54	BA	1929	G
54	BA	1930	G
54	BA	1937	A
54	BA	1938	A
54	BA	1939	U
54	BA	1940	U
54	BA	1941	C
54	BA	1943	U
54	BA	1944	U
54	BA	1946	U
54	BA	1955	U
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1981	A
54	BA	1993	U
54	BA	1997	C
54	BA	2002	G
54	BA	2003	A
54	BA	2018	G
54	BA	2020	A
54	BA	2030	A
54	BA	2031	A
54	BA	2032	G
54	BA	2043	C
54	BA	2055	C
54	BA	2058	A
54	BA	2061	G
54	BA	2069	G
54	BA	2076	U
54	BA	2093	G
54	BA	2112	G
54	BA	2113	U
54	BA	2115	G
54	BA	2117	A
54	BA	2119	A
54	BA	2126	A
54	BA	2127	G

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Mol	Chain	Res	Type
54	BA	2133	G
54	BA	2135	A
54	BA	2137	U
54	BA	2138	G
54	BA	2155	U
54	BA	2157	G
54	BA	2159	G
54	BA	2160	C
54	BA	2169	A
54	BA	2172	U
54	BA	2173	A
54	BA	2181	U
54	BA	2198	A
54	BA	2203	U
54	BA	2211	A
54	BA	2212	A
54	BA	2213	U
54	BA	2216	G
54	BA	2226	C
54	BA	2238	G
54	BA	2250	G
54	BA	2251	G
54	BA	2267	A
54	BA	2276	G
54	BA	2283	C
54	BA	2296	U
54	BA	2297	A
54	BA	2305	U
54	BA	2307	G
54	BA	2308	G
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2324	U
54	BA	2325	G
54	BA	2333	A
54	BA	2334	U
54	BA	2335	A
54	BA	2339	C
54	BA	2347	C
54	BA	2350	C
54	BA	2352	A

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Mol	Chain	Res	Type
54	BA	2353	G
54	BA	2383	G
54	BA	2385	C
54	BA	2389	G
54	BA	2391	G
54	BA	2392	A
54	BA	2396	G
54	BA	2402	U
54	BA	2406	A
54	BA	2407	A
54	BA	2409	G
54	BA	2419	U
54	BA	2425	A
54	BA	2429	G
54	BA	2430	A
54	BA	2431	U
54	BA	2432	A
54	BA	2433	A
54	BA	2441	U
54	BA	2447	G
54	BA	2448	A
54	BA	2476	A
54	BA	2491	U
54	BA	2495	G
54	BA	2498	C
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2505	G
54	BA	2514	U
54	BA	2518	A
54	BA	2529	G
54	BA	2531	A
54	BA	2540	C
54	BA	2544	G
54	BA	2554	U
54	BA	2566	A
54	BA	2573	C
54	BA	2576	G
54	BA	2578	G
54	BA	2581	G
54	BA	2609	U

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Mol	Chain	Res	Type
54	BA	2613	U
54	BA	2614	A
54	BA	2628	C
54	BA	2629	U
54	BA	2630	G
54	BA	2631	G
54	BA	2645	G
54	BA	2646	C
54	BA	2647	U
54	BA	2655	G
54	BA	2660	A
54	BA	2683	C
54	BA	2689	U
54	BA	2690	U
54	BA	2691	C
54	BA	2721	A
54	BA	2726	A
54	BA	2744	G
54	BA	2751	G
54	BA	2757	A
54	BA	2765	A
54	BA	2778	A
54	BA	2779	U
54	BA	2791	G
54	BA	2797	U
54	BA	2798	U
54	BA	2821	A
54	BA	2823	A
54	BA	2824	C
54	BA	2833	U
54	BA	2846	G
54	BA	2858	C
54	BA	2859	G
54	BA	2867	G
54	BA	2868	A
54	BA	2880	C
54	BA	2884	U
55	BB	9	G
55	BB	13	G
55	BB	16	G
55	BB	37	C
55	BB	41	G

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Mol	Chain	Res	Type
55	BB	44	G
55	BB	45	A
55	BB	52	A
55	BB	56	G
55	BB	57	A
55	BB	58	A
55	BB	67	G
55	BB	70	C
55	BB	74	U
55	BB	87	U
55	BB	90	C
55	BB	109	A

All (220) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	13	U
21	AA	34	C
21	AA	46	G
21	AA	65	A
21	AA	85	U
21	AA	109	A
21	AA	132	C
21	AA	173	U
21	AA	194	C
21	AA	211	G
21	AA	243	A
21	AA	251	G
21	AA	281	G
21	AA	309	A
21	AA	316	C
21	AA	328	C
21	AA	340	U
21	AA	350	G
21	AA	354	G
21	AA	366	A
21	AA	382	A
21	AA	383	A
21	AA	414	A
21	AA	451	A
21	AA	496	A
21	AA	504	C

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Mol	Chain	Res	Type
21	AA	509	A
21	AA	527	G
21	AA	532	A
21	AA	535	A
21	AA	575	G
21	AA	641	U
21	AA	653	U
21	AA	675	A
21	AA	733	G
21	AA	734	G
21	AA	792	A
21	AA	811	C
21	AA	840	C
21	AA	891	U
21	AA	892	A
21	AA	925	G
21	AA	965	U
21	AA	983	A
21	AA	1029	U
21	AA	1030	U
21	AA	1049	U
21	AA	1101	A
21	AA	1124	G
21	AA	1139	G
21	AA	1151	A
21	AA	1166	G
21	AA	1190	G
21	AA	1196	A
21	AA	1201	A
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1231	G
21	AA	1233	G
21	AA	1257	A
21	AA	1298	U
21	AA	1300	G
21	AA	1304	G
21	AA	1305	G
21	AA	1336	C
21	AA	1345	U
21	AA	1381	U

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Mol	Chain	Res	Type
21	AA	1429	A
21	AA	1431	A
21	AA	1447	A
21	AA	1469	C
22	A1	10	G
22	A1	46	7MG
22	A1	47	U
22	A1	59	U
22	A1	60	C
22	A1	74	C
23	A2	90	U
24	A3	9	G
24	A3	16	C
24	A3	17	C
24	A3	19	G
24	A3	48	U
24	A3	62	C
54	BA	10	A
54	BA	60	G
54	BA	71	A
54	BA	72	U
54	BA	74	A
54	BA	101	A
54	BA	149	A
54	BA	196	A
54	BA	249	C
54	BA	279	A
54	BA	322	A
54	BA	323	C
54	BA	329	G
54	BA	345	A
54	BA	384	A
54	BA	387	U
54	BA	388	G
54	BA	405	U
54	BA	411	G
54	BA	428	A
54	BA	442	G
54	BA	455	C
54	BA	456	C
54	BA	457	A
54	BA	506	G

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Mol	Chain	Res	Type
54	BA	547	A
54	BA	548	G
54	BA	613	A
54	BA	627	A
54	BA	631	A
54	BA	651	G
54	BA	654	A
54	BA	656	G
54	BA	670	A
54	BA	675	A
54	BA	685	A
54	BA	715	A
54	BA	762	U
54	BA	764	A
54	BA	782	A
54	BA	790	U
54	BA	846	U
54	BA	847	U
54	BA	866	A
54	BA	931	U
54	BA	973	A
54	BA	989	G
54	BA	1008	A
54	BA	1021	A
54	BA	1089	A
54	BA	1128	G
54	BA	1132	U
54	BA	1134	A
54	BA	1142	A
54	BA	1224	U
54	BA	1254	A
54	BA	1266	G
54	BA	1288	G
54	BA	1300	G
54	BA	1320	C
54	BA	1325	U
54	BA	1332	G
54	BA	1378	A
54	BA	1385	A
54	BA	1396	U
54	BA	1397	U
54	BA	1420	A

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Mol	Chain	Res	Type
54	BA	1427	A
54	BA	1453	A
54	BA	1465	G
54	BA	1490	A
54	BA	1535	A
54	BA	1539	U
54	BA	1607	C
54	BA	1625	C
54	BA	1634	A
54	BA	1651	G
54	BA	1674	G
54	BA	1706	C
54	BA	1711	A
54	BA	1713	A
54	BA	1769	U
54	BA	1783	A
54	BA	1787	A
54	BA	1826	G
54	BA	1913	A
54	BA	1936	A
54	BA	1938	A
54	BA	1940	U
54	BA	1943	U
54	BA	1945	G
54	BA	1955	U
54	BA	1971	U
54	BA	1980	G
54	BA	2002	G
54	BA	2030	A
54	BA	2031	A
54	BA	2060	A
54	BA	2126	A
54	BA	2150	C
54	BA	2172	U
54	BA	2197	U
54	BA	2212	A
54	BA	2225	A
54	BA	2249	U
54	BA	2286	G
54	BA	2296	U
54	BA	2324	U
54	BA	2343	U

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Mol	Chain	Res	Type
54	BA	2389	G
54	BA	2391	G
54	BA	2429	G
54	BA	2447	G
54	BA	2453	A
54	BA	2494	G
54	BA	2497	A
54	BA	2503	A
54	BA	2513	A
54	BA	2529	G
54	BA	2572	A
54	BA	2576	G
54	BA	2609	U
54	BA	2628	C
54	BA	2630	G
54	BA	2720	U
54	BA	2721	A
54	BA	2726	A
54	BA	2751	G
54	BA	2756	U
54	BA	2788	C
54	BA	2790	U
54	BA	2823	A
55	BB	12	C
55	BB	56	G
55	BB	57	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	CM0	A1	34	22,23	15,26,27	2.11	4 (26%)	18,37,40	3.24	4 (22%)
22	6MZ	A1	37	22	17,25,26	0.87	0	15,36,39	1.30	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	7MG	A1	46	22	20,26,27	2.23	3 (15%)	23,39,42	2.22	2 (8%)
22	5MU	A1	54	22	13,22,23	0.98	1 (7%)	16,32,35	4.08	2 (12%)
22	PSU	A1	55	22	15,21,22	1.28	2 (13%)	16,30,33	3.45	5 (31%)
22	4SU	A1	7	22	12,21,22	1.12	1 (8%)	15,30,33	2.33	3 (20%)
24	H2U	A3	21	24	17,21,22	1.41	2 (11%)	23,30,33	1.25	4 (17%)
24	OMC	A3	33	24	15,22,23	1.22	1 (6%)	20,31,34	0.83	0
24	5MU	A3	55	24	13,22,23	1.30	2 (15%)	16,32,35	4.22	3 (18%)
24	PSU	A3	56	24	15,21,22	1.20	2 (13%)	16,30,33	3.41	5 (31%)
24	4SU	A3	8	24	12,21,22	1.45	3 (25%)	15,30,33	2.14	1 (6%)

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
22	CM0	A1	34	22,23	-	0/6/30/31	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	7MG	A1	46	22	-	0/7/37/38	0/3/3/3
22	5MU	A1	54	22	-	0/3/25/26	0/2/2/2
22	PSU	A1	55	22	-	0/7/25/26	0/2/2/2
22	4SU	A1	7	22	-	0/3/25/26	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
24	OMC	A3	33	24	-	0/5/27/28	0/2/2/2
24	5MU	A3	55	24	-	0/3/25/26	0/2/2/2
24	PSU	A3	56	24	-	0/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/3/25/26	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.43	1.33	1.45
22	A1	34	CM0	O5-C5	-6.31	1.24	1.37
24	A3	21	H2U	C2-N3	-3.44	1.31	1.38
24	A3	21	H2U	C4-N3	-3.28	1.32	1.37
22	A1	46	7MG	C8-N7	-2.87	1.30	1.43
22	A1	55	PSU	O4'-C1'	-2.79	1.40	1.44
22	A1	34	CM0	C6-C5	-2.62	1.33	1.37
22	A1	7	4SU	C2'-C1'	-2.55	1.49	1.53
24	A3	55	5MU	C6-C5	-2.46	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	33	OMC	C4-N3	-2.42	1.31	1.35
24	A3	8	4SU	O4'-C4'	-2.30	1.39	1.45
24	A3	56	PSU	C6-C5	-2.23	1.35	1.38
24	A3	8	4SU	C5-C4	-2.17	1.35	1.38
24	A3	56	PSU	C5-C1'	-2.09	1.50	1.52
22	A1	54	5MU	C6-C5	-2.05	1.34	1.40
22	A1	34	CM0	C4-N3	2.01	1.36	1.33
22	A1	55	PSU	C4-N3	2.06	1.36	1.33
24	A3	55	5MU	C4-N3	2.17	1.36	1.33
24	A3	8	4SU	C6-N1	2.19	1.38	1.35
22	A1	46	7MG	C6-N1	2.26	1.37	1.33
22	A1	34	CM0	C4-C5	2.70	1.47	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C5-C4-N3	-11.73	115.51	125.35
24	A3	55	5MU	C5-C4-N3	-11.46	115.73	125.35
24	A3	8	4SU	C5-C4-N3	-7.56	115.55	123.56
22	A1	7	4SU	C5-C4-N3	-7.52	115.58	123.56
22	A1	46	7MG	C5-C6-N1	-6.87	113.16	123.39
24	A3	56	PSU	C4'-O4'-C1'	-3.68	105.75	109.54
24	A3	56	PSU	C5-C6-N1	-3.53	119.45	124.38
22	A1	55	PSU	C5-C6-N1	-3.45	119.57	124.38
22	A1	55	PSU	C4'-O4'-C1'	-2.70	106.76	109.54
22	A1	55	PSU	C5-C1'-C2'	-2.57	111.07	115.44
24	A3	56	PSU	C5-C1'-C2'	-2.47	111.24	115.44
22	A1	7	4SU	C4'-O4'-C1'	-2.21	107.30	109.64
24	A3	21	H2U	O2-C2-N3	-2.05	117.42	121.44
24	A3	55	5MU	C5M-C5-C4	2.10	122.29	119.97
24	A3	21	H2U	C5-C4-N3	2.41	119.17	116.62
24	A3	21	H2U	C5-C6-N1	2.57	113.58	110.76
22	A1	34	CM0	C7-O5-C5	2.68	122.76	117.83
22	A1	34	CM0	O5-C7-C8	2.89	113.98	108.01
22	A1	7	4SU	O4'-C1'-N1	3.07	113.93	108.10
24	A3	21	H2U	N3-C2-N1	3.14	119.55	116.64
22	A1	55	PSU	O4'-C1'-C2'	3.36	108.32	104.69
22	A1	37	6MZ	C2-N1-C6	3.75	119.17	116.47
24	A3	56	PSU	O4'-C1'-C2'	3.96	108.97	104.69
22	A1	34	CM0	O5-C5-C4	4.95	121.91	115.20
22	A1	46	7MG	C6-N1-C2	7.04	124.13	115.88
22	A1	54	5MU	C4-N3-C2	10.98	124.32	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	56	PSU	C4-N3-C2	11.30	124.59	115.16
24	A3	55	5MU	C4-N3-C2	11.67	124.90	115.16
22	A1	34	CM0	C4-N3-C2	11.82	125.02	115.16
22	A1	55	PSU	C4-N3-C2	12.03	125.20	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
57	VAL	A1	101	58,22	5,6,7	0.62	0	5,7,9	1.66	2 (40%)
58	FME	BA	3001	57	8,9,10	0.81	0	5,9,11	1.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	VAL	A1	101	58,22	-	0/4/6/8	0/0/0/0
58	FME	BA	3001	57	-	1/6/9/11	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
57	A1	101	VAL	O-C-CA	-2.85	117.91	125.69
57	A1	101	VAL	C-CA-N	2.37	115.19	109.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3001	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.