



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:48 PM BST

PDB ID : 4V7A  
EMDB ID: : EMD-1724  
Title : E. coli 70S-fMetVal-tRNAVal post-translocation complex (post4)  
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 : 9.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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

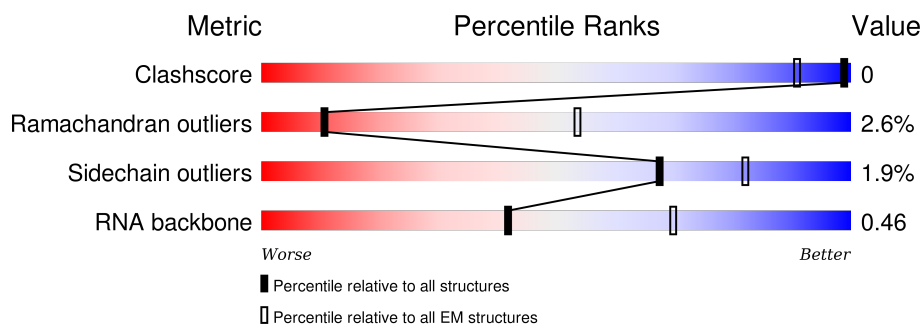
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.00 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.














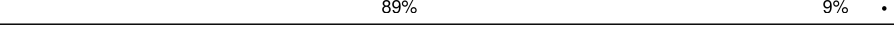
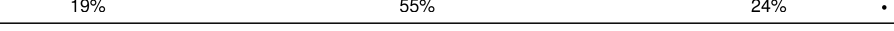
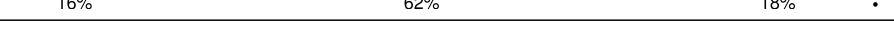
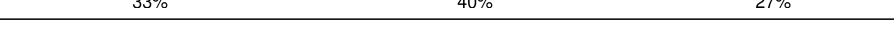




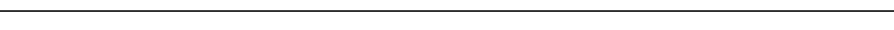

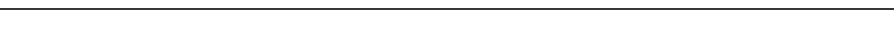
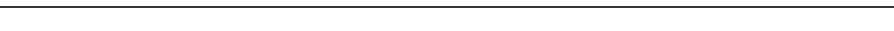


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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  $\geq 3$ , 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	87% 13%
3	AD	206	91% 8%
4	AE	152	91% 8% .
5	AF	101	90% 10%
6	AG	152	89% 11%
7	AH	130	95% . .
8	AI	128	86% 14%












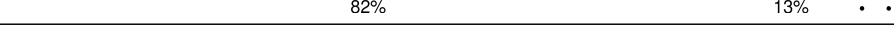







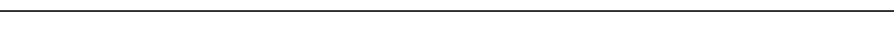

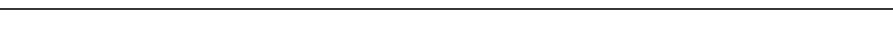
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Mol	Chain	Length	Quality of chain
9	AJ	100	 86% 13% .
10	AK	118	 92% 7% .
11	AL	124	 83% 16% .
12	AM	115	 87% 12% .
13	AN	101	 86% 11% ..
14	AO	89	 84% 15% .
15	AP	81	 91% 9%
16	AQ	82	 90% 9% .
17	AR	57	 89% 7% .
18	AS	81	 88% 11% .
19	AT	86	 90% 10%
20	AU	53	 89% 9% .
21	AA	1533	 19% 55% 24% .
22	A1	76	 16% 62% 18% .
23	A2	15	 33% 40% 27%
24	BC	273	 88% 12%
25	BD	209	 89% 11%
26	BE	201	 91% 8%
27	BF	179	 84% 15% ..
28	BG	177	 90% 8% ..
29	BH	149	 94% 6%
30	BI	142	 96% ..
31	BJ	142	 91% 8% .
32	BK	123	 85% 15% .
33	BL	144	 83% 15% ..

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Mol	Chain	Length	Quality of chain
34	BM	136	 89% 10% .
35	BN	121	 83% 16% .
36	BO	117	 91% 9% .
37	BP	115	 90% 9% ..
38	BQ	118	 87% 12% .
39	BR	103	 88% 12%
40	BS	110	 89% 11%
41	BT	94	 85% 15%
42	BU	104	 90% 8% ..
43	BV	94	 89% 11%
44	BW	80	 79% 20% .
45	BX	79	 82% 13% . .
46	BY	63	 90% 10%
47	BZ	59	 86% 8% . .
48	B0	57	 84% 14% .
49	B1	52	 87% 13%
50	B2	46	 78% 22%
51	B3	65	 85% 14% .
52	B4	38	 87% 11% .
53	BA	2903	 16% 55% 25% .
54	BB	118	 21% 53% 19% 5% .
55	B5	234	 89% 6% 5%

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 146011 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\*P\*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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	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 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	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 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	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 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	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 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	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 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	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 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	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 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	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 50 is a protein called 50S ribosomal protein L34.

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a RNA chain called 23S ribosomal RNA.

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

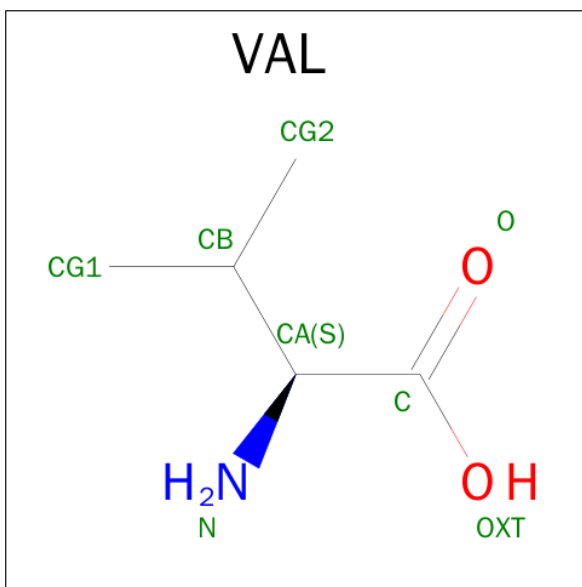
- Molecule 54 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 55 is a protein called 50S ribosomal protein L1.

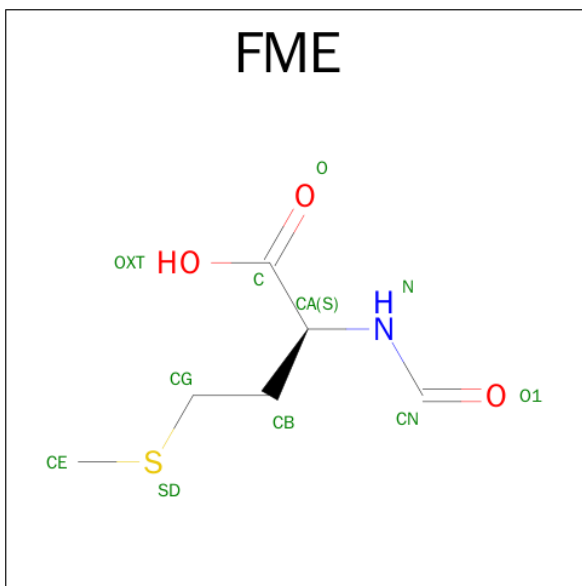
Mol	Chain	Residues	Atoms					AltConf	Trace
55	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 56 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



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

- Molecule 57 is N-FORMYLMETHIONINE (three-letter code: FME) (formula:  $C_6H_{11}NO_3S$ ).



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







- Molecule 7: 30S ribosomal protein S8

Chain AH: 95%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 86%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 86%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 92%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 83%



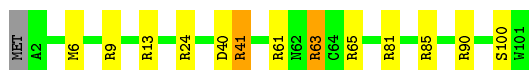
- Molecule 12: 30S ribosomal protein S13

Chain AM: 87%




- Molecule 13: 30S ribosomal protein S14

Chain AN: 86%



- Molecule 14: 30S ribosomal protein S15

Chain AO:  84% 15%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  91% 9%



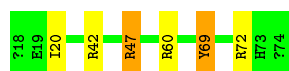
- Molecule 16: 30S ribosomal protein S17

Chain AQ:  90% 9%




- Molecule 17: 30S ribosomal protein S18

Chain AR:  89% 7%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  88% 11%



- Molecule 19: 30S ribosomal protein S20

Chain AT:  90% 10%



- Molecule 20: 30S ribosomal protein S21

Chain AU:  89% 9%



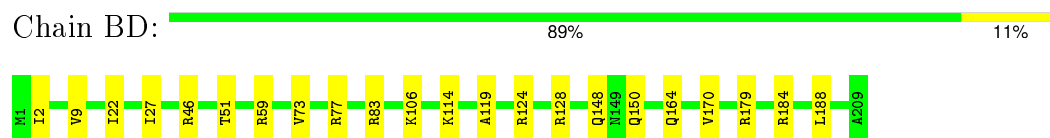
- Molecule 21: 16S ribosomal RNA

Chain AA:  19% 55% 24%

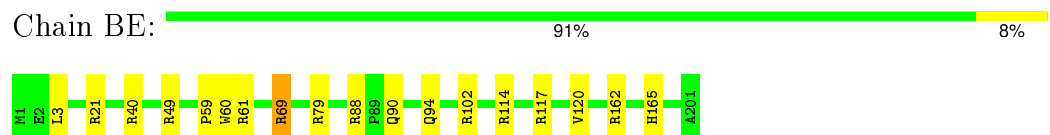
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G953	U956	U957	A958	A959	U960	G962	G963	A964	A965	U966	G966	G967	A968	A969	C970	C971	C972	G973	A974	A975	A976	G977	A978	C979	A980	A981	A982	A983	A984	C985	U986	G987	U988	U989	C990	U991	U992	G993	A994	C995	A996	U997	C998	U999	A1000	C1001	G1002	A1003	A1004	A1005	G1006	U1007	U1008	U1009	U1010	C1011	A1012	G1013		
A889	G890	U891	A892	C893	G894	G895	C896	G898	C899	A900	A901	G902	U903	U904	U905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	U916	G917	A918	A919	U920	U921	A922	A923	C924	G925	G926	U927	G928	U929	A930	C931	C932	G933	C934	A935	C936	A937	A938	C939	C940	U943	G944	G945	U946	G947	C948	A949			
G829	G830	A831	C832	U835	U836	U837	C838	C839	C840	C841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	C853	U854	U855	C856	C857	C858	C859	C860	C861	C862	U863	A864	A865	C866	U867	C868	C869	C870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888			
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U697	G698	C699	G700	U701	A702	G703	A704	U705	A706	U707	C708	G711	A712	G713	G714	A715	A716	U717	A718	C719	A720	A721	U722	U723	U726	G727	A728	A729	U732	G733	G734	C735	C736	C737	C738	C739	U740	G741	G742	C743	C744	G745	U746	A747	G748	A749	C750	U751	G752	A753	G754	G755	G756	U757	C758	A759				
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U697	G698	C699	G700	U701	A702	G703	A704	U705	A706	U707	C708	G711	A712	G713	G714	A715	A716	U717	A718	C719	A720	A721	U722	U723	U726	G727	A728	A729	U732	G733	G734	C735	C736	C737	C738	C739	U740	G741	G742	C743	C744	G745	U746	A747	G748	A749	C750	U751	G752	A753	G754	G755	G756	U757	C758	A759				
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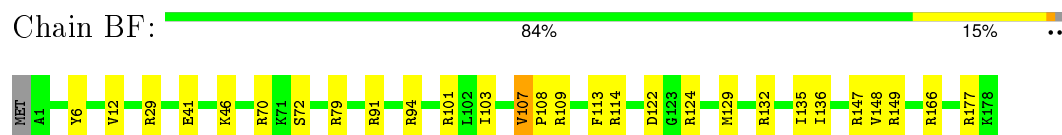
- Molecule 25: 50S ribosomal protein L3



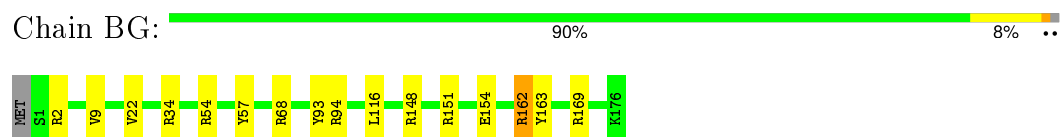
- Molecule 26: 50S ribosomal protein L4



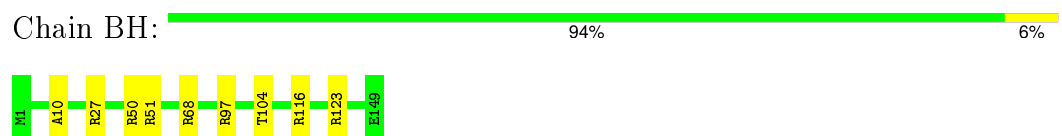
- Molecule 27: 50S ribosomal protein L5



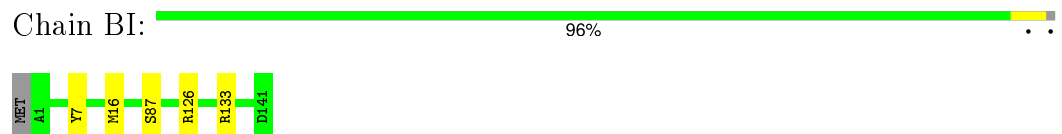
- Molecule 28: 50S ribosomal protein L6



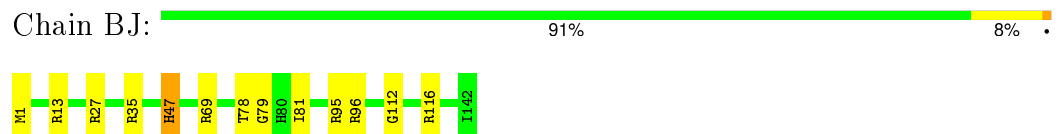
- Molecule 29: 50S ribosomal protein L9




- Molecule 30: 50S ribosomal protein L11



- Molecule 31: 50S ribosomal protein L13




- Molecule 32: 50S ribosomal protein L14

Chain BK:  85% 15% .



- Molecule 33: 50S ribosomal protein L15

Chain BL:  83% 15% ..




- Molecule 34: 50S ribosomal protein L16

Chain BM:  89% 10% .



- Molecule 35: 50S ribosomal protein L17

Chain BN:  83% 16% .



- Molecule 36: 50S ribosomal protein L18

Chain BO:  91% 9% .




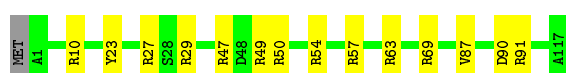
- Molecule 37: 50S ribosomal protein L19

Chain BP:  90% 9% ..



- Molecule 38: 50S ribosomal protein L20

Chain BQ:  87% 12% .



- Molecule 39: 50S ribosomal protein L21

Chain BR:  88% 12%



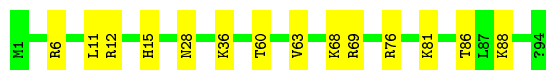
- Molecule 40: 50S ribosomal protein L22

Chain BS: 89% 11%



- Molecule 41: 50S ribosomal protein L23

Chain BT: 85% 15%



- Molecule 42: 50S ribosomal protein L24

Chain BU: 90% 8% ..



- Molecule 43: 50S ribosomal protein L25

Chain BV: 89% 11%



- Molecule 44: 50S ribosomal protein L27

Chain BW: 79% 20% .



- Molecule 45: 50S ribosomal protein L28

Chain BX: 82% 13% . .



- Molecule 46: 50S ribosomal protein L29

Chain BY: 90% 10%






- Molecule 47: 50S ribosomal protein L30

Chain BZ:  86% 8% . .




- Molecule 48: 50S ribosomal protein L32

Chain B0:  84% 14% .




- Molecule 49: 50S ribosomal protein L33

Chain B1:  87% 13%




- Molecule 50: 50S ribosomal protein L34

Chain B2:  78% 22%



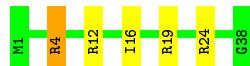
- Molecule 51: 50S ribosomal protein L35

Chain B3:  85% 14% .



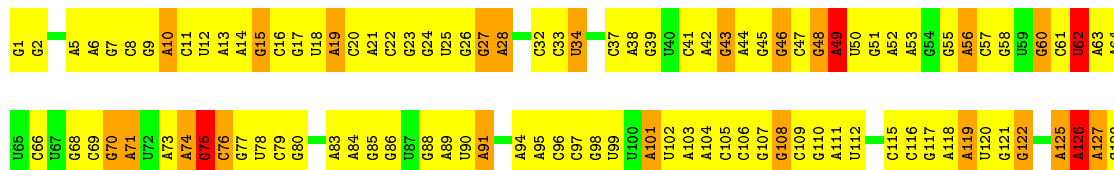
- Molecule 52: 50S ribosomal protein L36

Chain B4:  87% 11% .



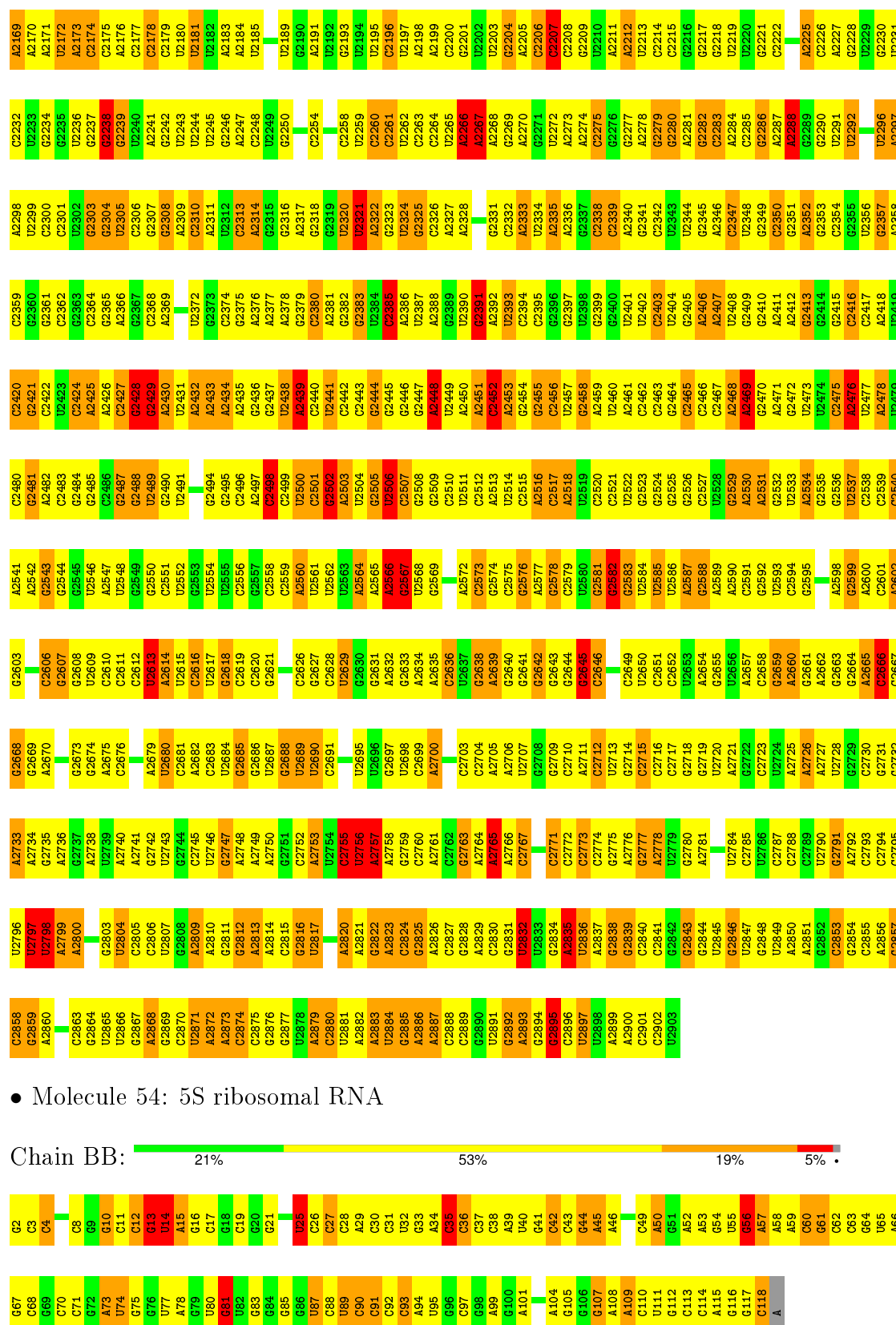
- Molecule 53: 23S ribosomal RNA

Chain BA:  16% 55% 25% .



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G1115	G1055	C992	G930	U870	U810	U744	G859	U499	G438	G377	G317	A254	A195	C130
G1116	G1056	C993	U931	U871	U811	U747	G860	G500	A439	G378	A319	A255	A196	A131
G1117	G1057	G994	U932	U872	G812	G748	G561	A501	A440	G379	G319	A256	A197	G132
G1118	U1058	C995	A933	G873	U813	A749	U562	A502	U441	G380	G320	G258	C198	U133
	A996		G934	G874	G814	A750	A563	A503	G442	G381	U321		A199	
G1121	U1060	G997	G935	G875	G815	A751	G564	A504	A443	A382	A322	G261	U200	U137
G1122	U1061	C998	A936	G876	G816	A752	U565	A505	C444	A383	A323	A262	C201	U138
G1123	U1062	U999	C937	A877	C817	A753	U566	G506	G445	A384	A324	G263	U202	U139
G1124	G1063	A1000	G938	A878	G818		U567	A507	G446	G385	G325	G264	A203	C140
G1125	C1064	A1001	G939	A879	A819		U568	A508	A447	G386	G326	A265	A204	G141
A1126	U1065	G1002	G940	G880	A820	G757	U569	C509	U448	U387	G327	G266	G205	A142
A1127	U1066	G1003	G941	G881	A821	G758	G570	C510	A449	G388	U328	G267	U206	C143
G1128	A1067	G1004	G942	G882	G822	G759	U571	U511	G450	G389	G329	C268	A207	A144
A1129	G1068	C1005	A943	G883	C823	G760	A572	G512	U451	U390	A330	C269	C208	C145
	U1069	C1006	G944	U884	U824	A761	U573	A513	A452	A391	A331	A270	C209	A146
U1132	A1070	C1007	A945	G885	A825	U762	A574	A514	A453	U392	A332	G271	C210	C147
A1133	A1071	A1008	G946	A886	U826	G763	A575	A515	A454	C393	G333	A272	C211	U148
A1134	C1072	A1009	A947	U887	U827	A764	U576	C516	A455	C394	C334	G273	G312	A149
G1135	A1073	A1010	A948	U888	U828	G765	G577	C517	A456	U395	C335	C274	A213	U150
G1136	G1074	U1011	G949	C889	U829	U766	U578	U519	U457	U397	G337	U276	G215	C151
G1137	C1075	C1012	G950	G890	G830	U767	U579	U520	U458	U398	G338	G277	A216	A152
G1138	C1076	C1013	G951	G891	U831		U580		U459	G399	U339	A278	A217	A155
A1139	U1077	A1014	A952	C892	U832	G772	G581	U521	A460	G400	A340	A279	A218	A156
C1140	U1078	U1015	C893	C893	A833	U773	A582	A522	C461	G401	A341	U280	A219	C157
U1141	C1079	G1016	U894	U894	G834	G774	G583	C523	C462	A401	G341	U281	G220	U158
A1142	A1080		C957	U895	G835		U584	G524	U463	U402	A342	C281	A221	A159
A1143	U1081	A1020	U958	G896	G836	G775	G585	U525	U464	U403	C343	A282	A222	A160
A1144	U1082	A1021	A959	C897	A837	G777	A586	A526	A471	A404	G344	G283	A223	A161
C1145	U1083	G1022	A960	C898	G838	G778	G587	C527	A472	U405	A345	U284	A224	U162
A1146	A1084	U1023	A961	A899	U839	U779	U588	A528	G473	G406	A346	G285	U224	G163
A1147	A1085	U1024	G962	A900	C840	U780	U589	A529	U469	G407	A347	U286	C225	C163
U1148	A1086	G1025	U963	C901	G841	A781	A590	G530	A470	G408	A348	G287	A226	C164
G1087	G1087	A1026	C964	C902	U842	A782	U591	C531	A471		U349	U288	A227	A165
C1150	A1088	A1027	G965	C903	G843	A783	A592	A532	A472	G411	G350	G289	C228	U166
A1151	A1089	A1028	G966	G904	A844	C719	U593	G533	G473	A412	C351	U290	C229	A167
C1152	A1090	A1029	U967	A905	A845	G785	U594	U534	G474	C413	A352	G230	G230	G168
C1153	G1091	C1030	C968	U906	U846	C786	C595	G535	C475	C414	C353	U293	A231	A172
C1092	C1092	G1031	G969	C907	U847	C787	U596	G536	A476	A415	A354	A294	G232	A173
G1154	G1093	A1032	U970	C908	C848	A788	G597	G537	G477	U416	U355	G295	A233	U174
A1156	U1094	U1033	G971	A909	A849	A789	U598	A538	A478	C417	G356	U296	U234	G175
G1157	A1095	G1034	A972	A910	U850	U790	A599	G539	A479	C418	C357	G297	U235	G176
A1096	U1096	U1035	A973	A911	C851	C791	G600	C540	A480	U419	U358	G298	C236	A176
U1097	U1097	G1036	G974	C912	U852	A792	G601	A541	G481	C420	G359	A299	C237	G177
A1098	A1098	G1037	A975	U913	C853	A793	A602	C542	A482	C421	U360	A300	C238	G178
G1099	G1099	G1038	G976	C914	G854	A794	A603	G543	A483	A422	G361	G301	C239	C179
C1100	C1100	A1039	G977	C915	G855	C795	A604	C544	C484	A423	A362	C302	C240	G180
U1101	U1101	A1040	G978	G916	G856	C796	U606	U545	C485	G424	G363	G303	A241	A181
C1102	C1102		A979	A917	G857	G797	U607	U546	C486	G425	C364	U304	G242	A182
A1103	A1103	C1043	A980	U918	G858	G798	A608	A547	C487	U426	U365	C305	U243	C183
C1104	U1104	C1044	A981	U919	G859	G799	A609	G548	G488	U427	C366	U306	A244	C184
U1105	U1105	C1045	C982	A920	U860	A800	C610	G549	G489	A428	G367	G307	G245	G185
G1168	G1168	A1046	A983	C921	A861	G801	C611	C550	C490	A429	A368	G308	C246	G186
A1169	G1107	G1047	A984	C922	G862	A802	G612	G551	G491	A430	U369	A309	G247	G187
C1170	U1108	A1048	C985	G923	A863	G803	A613	U552	A492	U431	G370	A310	G248	G188
G1171	C1109	C1049	C986	G924	G864	A804	A614	G553	G493	A432	A371	A311	C249	G189
G1172	G1110	A1050	C987	A925	C865	A804	U615	U554	G494	C433	G372	G312	G250	A190
A1173	A1111	G1051	G926	G926	A866	C740	U616	U555	G495	U434	U373	G313	A251	A191
U1174	G1112	C1052	G989	A927	C867	U741	A617	A556	G496	A435	A374	C314	G252	C192
A1175	U1113	C1053	A990	A928	U868	A743	G617	C557	A497	C436	G375	G315	C253	U193

C2104	U2041	A1978	C1914	A1854	C1793	G1733	U1671	A1608	G1546	U1484	A1420	G1358	C1298	G1236	U1176
A2108	A2042	A1979	U1915	U1855	A1794	G1734	A1672	A1609	C1547	U1487	G1421	A1359	G1299	A1237	G1177
U2109	C2043	G1980	A1916	U1856	C1795	A1735	G1673	A1610	A1548	U1488	G1422	A1360	G1300	U1240	C1178
G2110	C2044	A1981	U1917	G1857	U1796	U1736	G1674	A1611	A1549	C1488	G1423	G1361	A1301	U1241	U1180
G2111	G2045	U1982	A1918	A1858	G1797	G1737	A1675	A1612	C1550	C1489	G1424	A1362	A1302	U1242	U1181
G2112	G2046	G1983	A1919	U1859	U1798	G1738	A1676	G1613	A1551	C1490	G1425	C1363	A1303	U1243	G1182
G2113	C2047	G1984	C1920	G1860	G1799	A1739	A1677	A1614	A1552	G1491	G1426	G1364	A1304	G1244	U1183
A2114	G2048	G1985	G1921	G1861	C1800	A1740	A1678	A1615	A1553	G1492	A1427	A1365	C1305	A1245	U1184
G2115	A2049	G1986	G1922	G1862	A1801	C1741	A1679	A1616	G1554	C1493	G1428	A1366	C1306	G1246	G1185
G2116	C2050	A1987	U1923	G1863	A1802	G1742	U1680	C1617	G1555	A1494	G1429	A1367	A1307	A1247	G1186
A2117	G2051	G1988	A1924	A1864	A1803	G1743	G1681	A1618	C1556	A1495	A1431	A1308	A1308	U1248	G1187
G2118	A2052	G1989	G1925	U1865	A1804	A1744	G1682	A1619	C1557	A1496	A1432	G1370	G1309	U1249	U1188
G2119	C2053	C1990	U1926	A1866	A1805	A1745	U1683	G1620	C1558	U1497	G1433	A1309	G1310	U1250	A1189
A2120	A2054	A1927	A1927	G1867	C1806	A1746	G1684	U1624	U1559	C1498	A1433	U1372	G1311	C1251	U1190
C2121	C2055	G1992	A1928	C1868	G1807	U1747	C1685	U1625	G1560	U1499	A1434	U1373	G1312	G1252	G1191
G2122	G2056	U1993	G1929	A1869	A1808	G1748	C1686	G1626	C1561	C1500	G1435	A1374	U1313	A1253	G1192
A2123	A2057	C1994	A1929	C1870	A1809	A1749	U1687	A1627	U1562	G1501	U1439	U1375	C1314	A1254	U1193
G2124	G2058	U1995	A1932	A1871	A1810	U1750	G1688	G1628	C1563	A1502	U1440	G1376	C1315	U1255	A1194
G2125	A2059	C1996	G1933	A1872	G1811	U1751	U1689	U1629	C1564	A1503	G1441	G1377	U1316	G1256	U1195
G2126	A2060	C1997	G1934	G1873	U1812	C1752	A1690	U1630	C1565	A1504	U1442	A1378	G1317	C1257	G1196
C2127	C2061	A1998	U1935	C1874	G1813	G1753	A1691	A1631	G1567	U1506	U1443	U1379	U1318	U1258	G1197
U2130	A2062	C1999	A1936	G1875	A1814	A1754	G1692	A1632	C1568	C1507	G1444	C1320	C1320	A1260	U1198
U2131	C2063	C2000	A1937	A1876	A1815	A1755	U1693	A1633	A1569	A1508	G1445	A1321	A1322	A1261	U1199
U2132	C2064	C2001	A1938	A1877	C1816	G1756	G1695	A1634	A1570	A1509	G1446	A1383	A1322	A1262	C1200
G2133	C2065	G2002	U1939	G1878	G1817	U1757	G1696	A1635	A1571	G1510	C1447	A1384	C1323	U1263	U1201
A2134	C2066	A2003	U1940	C1879	U1818	U1758	G1697	A1636	A1572	G1511	G1448	A1385	G1324	A1264	G1202
G2135	U2004	G2004	C1941	U1880	A1819	A1759	A1698	A1637	C1573	G1512	C1451	A1386	U1325	A1265	U1203
G2136	C2069	A2005	C1942	C1881	U1820	C1760	G1699	A1638	C1574	U1513	C1452	A1387	U1326	G1266	A1204
U2137	A2070	C2006	U1943	U1882	A1821	C1761	A1700	G1638	C1575	G1514	A1453	A1388	A1327	U1267	A1205
G2138	A2071	U2007	U1944	U1883	C1822	A1762	A1701	C1639	C1576	U1515	A1454	A1389	A1328	U1268	G1206
U2139	C2072	C2008	G1945	G1884	G1823	G1763	G1702	A1640	U1576	U1515	C1455	A1390	U1329	A1269	C1207
G2140	C2073	A2009	U1946	A1885	G1824	C1764	G1703	A1641	C1577	U1518	C1456	U1391	C1330	A1270	U1208
G2141	U2081	U2013	C1947	U1886	U1825	U1765	C1704	G1642	U1578	G1455	G1456	A1392	G1331	G1271	U1209
A2142	A2082	A2014	U1951	C1887	G1826	G1766	A1705	A1643	A1579	U1520	C1457	A1393	G1332	A1272	G1210
C2143	C2078	A2015	A1952	G1888	U1827	G1767	C1706	G1644	A1580	G1521	U1458	A1395	G1333	U1273	G1211
G2144	G2079	C2016	A1953	A1889	G1828	G1768	G1707	G1645	G1581	G1522	G1459	U1396	G1334	A1274	G1212
C2145	A2080	U2016	G1954	A1890	A1829	U1769	C1708	C1646	C1582	U1523	U1460	U1397	C1335	A1275	A1213
G2146	C2080	U2017	G1955	C1892	G1831	C1770	U1709	U1647	A1583	G1524	C1461	C1398	A1336	A1276	A1214
U2147	U2081	A2019	U1956	C1893	C1832	C1771	A1711	G1648	U1584	A1525	C1462	C1399	G1337	G1277	G1215
G2148	A2020	C2021	C1957	C1894	C1833	A1772	U1712	A1650	C1585	A1526	C1463	C1338	G1338	G1278	G1216
U2149	C2083	U2022	C1958	C1895	U1834	C1773	A1713	G1651	U1586	G1527	U1466	G1401	U1339	U1279	U1217
C2150	C2084	U2023	G1959	G1896	G1835	U1774	U1714	A1652	U1590	A1528	U1467	U1402	U1340	G1280	G1218
G2151	U2085	G2024	A1960	C1897	C1836	G1775	G1715	A1653	A1591	G1529	U1467	A1403	G1341	G1281	U1219
U2152	U2086	C2025	C1961	U1898	C1837	U1776	U1716	A1654	C1592	U1530	U1468	C1404	A1342	U1282	G1220
C2153	G2087	U2026	U1962	A1899	G1838	U1777	G1717	A1655	C1593	U1531	A1469	U1405	G1343	C1291	G1228
A2154	A2088	U2027	G1963	C1899	G1839	U1778	A1718	C1656	U1594	A1532	A1470	U1406	U1344	A1284	C1221
U2155	C2089	U2028	U1964	G1899	G1840	U1779	G1719	U1657	C1595	G1471	G1471	U1345	A1285	G1223	U1222
G2156	A2090	U2029	C1965	A1901	A1841	A1780	U1720	C1658	A1596	U1534	C1472	G1407	G1346	A1286	G1224
G2157	C2091	A2030	A1966	G1902	G1842	U1781	A1722	G1659	A1597	U1535	G1473	U1408	G1347	A1287	G1225
A2158	U2092	C2031	C1967	G1903	C1843	U1782	G1723	G1660	A1598	C1536	U1474	U1409	C1348	G1288	A1226
G2159	G2093	A2032	G1968	G1904	C1844	A1783	G1724	G1661	U1599	G1537	G1475	U1411	C1349	G1227	G1227
C2160	A2094	G2033	U1969	C1905	C1844	U1784	U1725	U1662	C1600	U1538	U1476	U1412	C1350	G1228	G1228
G2161	A2095	A2033	G1970	G1906	G1845	A1785	C1726	A1664	G1601	U1539	A1477	A1413	C1351	C1290	G1229
C2162	C2096	U2034	A1970	G1907	G1846	U1786	C1727	A1665	U1602	U1540	G1478	C1414	U1352	G1230	U1230
A2163	A2097	G2035	A1971	A1847	A1847	A1787	C1728	A1666	U1603	C1541	G1479	U1415	U1353	G1293	U1231
G2164	U2098	C2036	G1972	G1908	G1848	C1788	U1729	A1667	C1604	U1542	C1480	G1416	A1354	U1294	G1232
C2165	A2037	G1973	G1973	G1910	G1849	A1789	U1730	A1668	C1605	U1543	U1481	G1417	G1355	G1295	G1233
U2166	G2038	U1911	U1911	A1912	U1852	C1790	G1731	A1669	C1606	A1544	G1482	G1418	G1356	U1234	U1234
U2167	C2039	A1912	U1912	A1913	U1853	G1792	C1732	C1670	C1607	A1545	G1483	A1419	C1357	C1297	G1235



Chain B5: 

89%

6%

5%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	26429	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	161000	Depositor
Image detector	4k CCD camera (TVIPS)	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, FME, ACE, 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	0.69	0/1736	1.15	8/2340 (0.3%)
10	AK	0.76	0/894	1.26	9/1207 (0.7%)
11	AL	0.77	0/969	1.37	17/1300 (1.3%)
12	AM	0.79	0/884	1.35	11/1181 (0.9%)
13	AN	0.82	0/817	1.41	11/1088 (1.0%)
14	AO	0.72	0/722	1.29	13/964 (1.3%)
15	AP	0.84	0/648	1.28	7/870 (0.8%)
16	AQ	0.73	0/658	1.19	5/883 (0.6%)
17	AR	0.80	0/463	1.21	5/623 (0.8%)
18	AS	0.76	0/653	1.27	4/879 (0.5%)
19	AT	0.71	0/672	1.12	5/890 (0.6%)
2	AC	0.77	0/1651	1.28	18/2225 (0.8%)
20	AU	0.85	0/431	1.31	6/572 (1.0%)
21	AA	1.75	365/36759 (1.0%)	2.28	2447/57346 (4.3%)
22	A1	1.75	20/1668 (1.2%)	2.26	110/2595 (4.2%)
23	A2	1.66	1/343 (0.3%)	2.18	17/531 (3.2%)
24	BC	0.81	0/2121	1.35	26/2852 (0.9%)
25	BD	0.71	0/1586	1.18	9/2134 (0.4%)
26	BE	0.72	0/1571	1.19	11/2113 (0.5%)
27	BF	0.77	0/1444	1.26	16/1937 (0.8%)
28	BG	0.71	0/1343	1.18	10/1816 (0.6%)
29	BH	0.68	0/1122	1.16	7/1515 (0.5%)
3	AD	0.80	0/1665	1.26	20/2227 (0.9%)
30	BI	0.68	0/1046	1.07	5/1410 (0.4%)
31	BJ	0.75	0/1152	1.23	9/1551 (0.6%)
32	BK	0.76	0/947	1.23	10/1268 (0.8%)
33	BL	0.79	0/1054	1.29	12/1403 (0.9%)
34	BM	0.80	0/1093	1.22	10/1460 (0.7%)
35	BN	0.83	0/973	1.44	18/1301 (1.4%)
36	BO	0.77	0/902	1.29	9/1209 (0.7%)
37	BP	0.78	0/929	1.25	9/1242 (0.7%)
38	BQ	0.81	0/960	1.36	14/1278 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BR	0.72	0/829	1.13	6/1107 (0.5%)
4	AE	0.72	0/1119	1.20	11/1506 (0.7%)
40	BS	0.70	0/864	1.28	10/1156 (0.9%)
41	BT	0.72	0/744	1.22	4/994 (0.4%)
42	BU	0.72	0/787	1.15	5/1051 (0.5%)
43	BV	0.74	0/766	1.27	8/1025 (0.8%)
44	BW	0.78	0/604	1.24	6/799 (0.8%)
45	BX	0.84	0/635	1.35	10/848 (1.2%)
46	BY	0.71	0/510	1.24	4/677 (0.6%)
47	BZ	0.73	0/453	1.31	6/605 (1.0%)
48	B0	0.80	0/450	1.26	8/599 (1.3%)
49	B1	0.73	0/417	1.14	3/556 (0.5%)
5	AF	0.76	0/835	1.23	7/1128 (0.6%)
50	B2	0.89	0/380	1.58	10/498 (2.0%)
51	B3	0.79	0/513	1.23	6/676 (0.9%)
52	B4	0.80	0/303	1.35	6/397 (1.5%)
53	BA	1.77	819/69796 (1.2%)	2.30	4869/108888 (4.5%)
54	BB	1.74	17/2800 (0.6%)	2.24	176/4367 (4.0%)
55	B5	0.69	0/1673	1.11	8/2255 (0.4%)
6	AG	0.76	0/1188	1.28	12/1593 (0.8%)
7	AH	0.71	0/989	1.11	5/1326 (0.4%)
8	AI	0.83	0/1035	1.37	14/1377 (1.0%)
9	AJ	0.78	0/797	1.33	11/1079 (1.0%)
All	All	1.54	1222/158363 (0.8%)	2.07	8093/236717 (3.4%)

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
18	AS	0	1
21	AA	0	328
22	A1	0	18
23	A2	0	2
53	BA	0	652
54	BB	0	27
All	All	0	1028

All (1222) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	2078	C	C4-N4	-7.15	1.27	1.33
21	AA	1521	C	C4-N4	-7.01	1.27	1.33
53	BA	897	C	C4-N4	-6.68	1.27	1.33
21	AA	1214	C	C4-N4	-6.67	1.27	1.33
21	AA	637	C	C4-N4	-6.64	1.27	1.33
53	BA	787	C	C4-N4	-6.62	1.27	1.33
53	BA	1059	G	C2-N2	-6.60	1.27	1.34
53	BA	2336	A	C6-N1	-6.59	1.30	1.35
53	BA	635	C	C4-N4	-6.59	1.28	1.33
53	BA	1410	G	C2-N2	-6.59	1.27	1.34
21	AA	1366	C	C4-N4	-6.57	1.28	1.33
21	AA	1293	C	C4-N4	-6.55	1.28	1.33
53	BA	2000	C	C4-N4	-6.54	1.28	1.33
53	BA	1507	C	C4-N4	-6.54	1.28	1.33
53	BA	2681	C	C4-N4	-6.53	1.28	1.33
21	AA	1266	G	C2-N2	-6.51	1.28	1.34
53	BA	2841	C	C4-N4	-6.50	1.28	1.33
21	AA	36	C	C4-N4	-6.49	1.28	1.33
53	BA	236	C	C4-N4	-6.48	1.28	1.33
53	BA	908	C	C4-N4	-6.47	1.28	1.33
53	BA	1158	C	C4-N4	-6.46	1.28	1.33
53	BA	1656	C	C4-N4	-6.45	1.28	1.33
53	BA	1659	G	C2-N2	-6.45	1.28	1.34
21	AA	207	C	C4-N4	-6.42	1.28	1.33
22	A1	11	C	C4-N4	-6.42	1.28	1.33
21	AA	569	C	C4-N4	-6.41	1.28	1.33
21	AA	1332	A	C6-N1	-6.41	1.31	1.35
53	BA	2646	C	C4-N4	-6.38	1.28	1.33
53	BA	786	C	C4-N4	-6.35	1.28	1.33
53	BA	1410	G	C6-N1	-6.35	1.35	1.39
53	BA	2496	C	C4-N4	-6.35	1.28	1.33
53	BA	835	C	C4-N4	-6.33	1.28	1.33
53	BA	1271	G	C2-N2	-6.33	1.28	1.34
21	AA	699	C	C4-N4	-6.33	1.28	1.33
21	AA	866	C	C4-N4	-6.33	1.28	1.33
53	BA	1298	C	C4-N4	-6.32	1.28	1.33
53	BA	452	G	C2-N2	-6.32	1.28	1.34
53	BA	1536	C	C4-N4	-6.31	1.28	1.33
53	BA	2463	C	C4-N4	-6.30	1.28	1.33
53	BA	817	C	C4-N4	-6.29	1.28	1.33
53	BA	2335	A	C6-N1	-6.28	1.31	1.35
53	BA	179	C	C4-N4	-6.27	1.28	1.33
53	BA	2525	G	C2-N2	-6.27	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	324	G	C2-N2	-6.27	1.28	1.34
21	AA	1331	G	C2-N2	-6.26	1.28	1.34
53	BA	2452	C	N3-C4	-6.25	1.29	1.33
21	AA	1197	A	C6-N1	-6.25	1.31	1.35
21	AA	1516	G	N1-C2	-6.25	1.32	1.37
53	BA	751	A	C6-N1	-6.24	1.31	1.35
53	BA	1814	G	C2-N2	-6.24	1.28	1.34
21	AA	1263	C	C4-N4	-6.24	1.28	1.33
53	BA	1104	C	C4-N4	-6.24	1.28	1.33
21	AA	898	G	C2-N2	-6.24	1.28	1.34
21	AA	912	C	C4-N4	-6.24	1.28	1.33
21	AA	86	G	C2-N2	-6.23	1.28	1.34
53	BA	2261	C	C4-N4	-6.23	1.28	1.33
21	AA	1309	G	C2-N2	-6.23	1.28	1.34
53	BA	1789	A	C6-N1	-6.22	1.31	1.35
21	AA	83	C	C4-N4	-6.22	1.28	1.33
53	BA	8	C	C4-N4	-6.22	1.28	1.33
53	BA	1153	C	C4-N4	-6.21	1.28	1.33
53	BA	2317	A	C6-N1	-6.21	1.31	1.35
53	BA	426	C	C4-N4	-6.21	1.28	1.33
53	BA	1293	C	C4-N4	-6.20	1.28	1.33
21	AA	1328	C	C4-N4	-6.20	1.28	1.33
53	BA	1644	C	C4-N4	-6.20	1.28	1.33
53	BA	1853	A	C6-N1	-6.20	1.31	1.35
53	BA	1215	G	C2-N2	-6.19	1.28	1.34
21	AA	896	C	C4-N4	-6.19	1.28	1.33
21	AA	856	C	C4-N4	-6.19	1.28	1.33
53	BA	201	C	C4-N4	-6.18	1.28	1.33
53	BA	1934	C	C4-N4	-6.18	1.28	1.33
53	BA	2391	G	C2-N2	-6.16	1.28	1.34
21	AA	849	G	C2-N2	-6.16	1.28	1.34
53	BA	742	A	C6-N1	-6.16	1.31	1.35
53	BA	1706	C	C4-N4	-6.16	1.28	1.33
53	BA	2278	A	C6-N1	-6.16	1.31	1.35
53	BA	560	C	C4-N4	-6.16	1.28	1.33
53	BA	2055	C	C4-N4	-6.15	1.28	1.33
53	BA	192	C	C4-N4	-6.15	1.28	1.33
53	BA	1894	C	C4-N4	-6.14	1.28	1.33
53	BA	2536	G	C2-N2	-6.14	1.28	1.34
53	BA	1233	C	C4-N4	-6.14	1.28	1.33
53	BA	111	A	C6-N1	-6.13	1.31	1.35
21	AA	1282	C	C4-N4	-6.12	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	543	G	C2-N2	-6.12	1.28	1.34
53	BA	2001	C	C4-N4	-6.12	1.28	1.33
21	AA	351	G	C2-N2	-6.12	1.28	1.34
53	BA	406	G	C2-N2	-6.11	1.28	1.34
53	BA	1021	A	C6-N1	-6.11	1.31	1.35
53	BA	1168	G	N1-C2	-6.11	1.32	1.37
21	AA	570	G	C2-N2	-6.10	1.28	1.34
53	BA	1052	C	C4-N4	-6.10	1.28	1.33
53	BA	2857	G	C2-N2	-6.10	1.28	1.34
53	BA	1236	G	C2-N2	-6.10	1.28	1.34
53	BA	1731	G	C2-N2	-6.10	1.28	1.34
53	BA	2575	C	N3-C4	-6.10	1.29	1.33
53	BA	2806	C	C4-N4	-6.10	1.28	1.33
53	BA	240	C	C4-N4	-6.10	1.28	1.33
21	AA	882	C	N3-C4	-6.09	1.29	1.33
53	BA	208	C	C4-N4	-6.09	1.28	1.33
21	AA	857	C	C4-N4	-6.09	1.28	1.33
53	BA	533	G	C2-N2	-6.09	1.28	1.34
53	BA	863	A	C6-N1	-6.09	1.31	1.35
53	BA	1235	G	C2-N2	-6.09	1.28	1.34
22	A1	30	C	C4-N4	-6.09	1.28	1.33
53	BA	1682	G	C2-N2	-6.08	1.28	1.34
53	BA	2003	A	C6-N1	-6.08	1.31	1.35
21	AA	1158	C	C4-N4	-6.08	1.28	1.33
53	BA	2763	G	C2-N2	-6.07	1.28	1.34
54	BB	30	C	C4-N4	-6.07	1.28	1.33
21	AA	99	C	C4-N4	-6.07	1.28	1.33
53	BA	1007	C	C4-N4	-6.07	1.28	1.33
53	BA	1924	C	C4-N4	-6.07	1.28	1.33
21	AA	328	C	C4-N4	-6.06	1.28	1.33
53	BA	1454	C	N3-C4	-6.06	1.29	1.33
53	BA	1721	G	C2-N2	-6.06	1.28	1.34
53	BA	1480	C	C4-N4	-6.06	1.28	1.33
53	BA	1799	G	C2-N2	-6.06	1.28	1.34
53	BA	421	C	C4-N4	-6.05	1.28	1.33
53	BA	512	G	C2-N2	-6.05	1.28	1.34
53	BA	109	C	C4-N4	-6.04	1.28	1.33
54	BB	88	C	C4-N4	-6.04	1.28	1.33
53	BA	2405	G	N1-C2	-6.04	1.32	1.37
53	BA	2848	G	C2-N2	-6.04	1.28	1.34
21	AA	265	G	C2-N2	-6.04	1.28	1.34
53	BA	916	G	C2-N2	-6.04	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	2487	G	C2-N2	-6.04	1.28	1.34
53	BA	1843	C	C4-N4	-6.03	1.28	1.33
21	AA	286	C	C4-N4	-6.03	1.28	1.33
21	AA	1028	C	N3-C4	-6.02	1.29	1.33
53	BA	1296	G	C2-N2	-6.02	1.28	1.34
53	BA	1838	C	C4-N4	-6.02	1.28	1.33
53	BA	2538	C	C4-N4	-6.02	1.28	1.33
53	BA	1079	C	C4-N4	-6.01	1.28	1.33
21	AA	1271	A	C6-N1	-6.01	1.31	1.35
53	BA	2146	C	C4-N4	-6.01	1.28	1.33
53	BA	2250	G	C2-N2	-6.01	1.28	1.34
22	A1	16	C	N3-C4	-6.01	1.29	1.33
53	BA	971	G	N1-C2	-6.01	1.32	1.37
53	BA	469	G	C2-N2	-6.00	1.28	1.34
53	BA	634	C	C4-N4	-6.00	1.28	1.33
53	BA	436	C	C4-N4	-6.00	1.28	1.33
22	A1	24	G	C2-N2	-6.00	1.28	1.34
53	BA	2811	G	C2-N2	-6.00	1.28	1.34
53	BA	298	G	C6-N1	-5.99	1.35	1.39
53	BA	2839	G	C2-N2	-5.99	1.28	1.34
21	AA	1400	C	C4-N4	-5.99	1.28	1.33
53	BA	1903	G	C2-N2	-5.98	1.28	1.34
21	AA	556	C	C4-N4	-5.98	1.28	1.33
21	AA	1352	C	C4-N4	-5.98	1.28	1.33
53	BA	540	C	C4-N4	-5.98	1.28	1.33
53	BA	2787	C	C4-N4	-5.98	1.28	1.33
21	AA	388	G	C2-N2	-5.97	1.28	1.34
53	BA	2521	C	N3-C4	-5.97	1.29	1.33
53	BA	1521	G	C2-N2	-5.97	1.28	1.34
53	BA	1006	C	N3-C4	-5.97	1.29	1.33
21	AA	383	A	C6-N1	-5.96	1.31	1.35
53	BA	1540	G	C2-N2	-5.96	1.28	1.34
21	AA	940	C	C4-N4	-5.96	1.28	1.33
21	AA	643	C	C4-N4	-5.96	1.28	1.33
53	BA	778	G	C6-N1	-5.96	1.35	1.39
53	BA	1323	C	C4-N4	-5.95	1.28	1.33
53	BA	1575	C	C4-N4	-5.95	1.28	1.33
53	BA	812	C	C4-N4	-5.95	1.28	1.33
53	BA	298	G	C2-N2	-5.95	1.28	1.34
53	BA	869	G	C6-N1	-5.95	1.35	1.39
53	BA	2517	C	C4-N4	-5.94	1.28	1.33
53	BA	723	C	C4-N4	-5.94	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	212	G	C2-N2	-5.94	1.28	1.34
53	BA	965	C	N3-C4	-5.94	1.29	1.33
53	BA	2153	C	C4-N4	-5.94	1.28	1.33
53	BA	1022	G	C2-N2	-5.94	1.28	1.34
21	AA	67	C	C4-N4	-5.94	1.28	1.33
53	BA	1889	A	C6-N1	-5.94	1.31	1.35
54	BB	35	C	C4-N4	-5.94	1.28	1.33
21	AA	322	C	C4-N4	-5.93	1.28	1.33
53	BA	156	A	C6-N1	-5.93	1.31	1.35
21	AA	640	A	C6-N1	-5.93	1.31	1.35
21	AA	1343	G	C2-N2	-5.93	1.28	1.34
53	BA	898	C	C4-N4	-5.93	1.28	1.33
53	BA	1893	C	N3-C4	-5.93	1.29	1.33
21	AA	702	A	C6-N1	-5.93	1.31	1.35
53	BA	957	C	C4-N4	-5.92	1.28	1.33
21	AA	1327	C	C4-N4	-5.92	1.28	1.33
53	BA	269	C	C4-N4	-5.92	1.28	1.33
53	BA	2567	G	C2-N2	-5.92	1.28	1.34
53	BA	2304	G	C2-N2	-5.92	1.28	1.34
21	AA	549	C	N3-C4	-5.92	1.29	1.33
53	BA	1161	C	N3-C4	-5.92	1.29	1.33
21	AA	601	G	C6-N1	-5.92	1.35	1.39
53	BA	822	G	C6-N1	-5.92	1.35	1.39
53	BA	783	A	C6-N1	-5.91	1.31	1.35
53	BA	2895	G	C2-N2	-5.91	1.28	1.34
21	AA	739	C	C4-N4	-5.91	1.28	1.33
53	BA	1574	C	C4-N4	-5.91	1.28	1.33
53	BA	989	G	C2-N2	-5.91	1.28	1.34
21	AA	611	C	C4-N4	-5.89	1.28	1.33
53	BA	1994	C	C4-N4	-5.89	1.28	1.33
22	A1	74	C	C4-N4	-5.89	1.28	1.33
21	AA	862	C	C4-N4	-5.89	1.28	1.33
53	BA	406	G	C6-N1	-5.89	1.35	1.39
21	AA	339	C	C4-N4	-5.89	1.28	1.33
53	BA	2043	C	C4-N4	-5.89	1.28	1.33
21	AA	597	G	C2-N2	-5.89	1.28	1.34
53	BA	439	A	C6-N1	-5.89	1.31	1.35
53	BA	2501	C	C4-N4	-5.88	1.28	1.33
53	BA	2072	C	C4-N4	-5.88	1.28	1.33
21	AA	1046	A	C6-N1	-5.88	1.31	1.35
21	AA	1037	C	N3-C4	-5.87	1.29	1.33
21	AA	601	G	C2-N2	-5.87	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	264	C	C4-N4	-5.87	1.28	1.33
21	AA	60	A	C6-N1	-5.86	1.31	1.35
21	AA	206	C	C4-N4	-5.86	1.28	1.33
53	BA	370	G	C2-N2	-5.86	1.28	1.34
53	BA	822	G	C2-N2	-5.86	1.28	1.34
53	BA	1761	C	C4-N4	-5.86	1.28	1.33
53	BA	2502	G	C2-N2	-5.86	1.28	1.34
54	BB	54	G	C2-N2	-5.86	1.28	1.34
53	BA	2594	C	C4-N4	-5.85	1.28	1.33
53	BA	823	C	C4-N4	-5.85	1.28	1.33
21	AA	182	A	C6-N1	-5.85	1.31	1.35
53	BA	2864	G	C2-N2	-5.85	1.28	1.34
21	AA	885	G	C2-N2	-5.85	1.28	1.34
21	AA	646	G	C2-N2	-5.84	1.28	1.34
21	AA	1369	C	N3-C4	-5.84	1.29	1.33
21	AA	69	G	C2-N2	-5.84	1.28	1.34
21	AA	169	C	C4-N4	-5.84	1.28	1.33
21	AA	1012	A	C6-N1	-5.84	1.31	1.35
53	BA	1116	G	C2-N2	-5.84	1.28	1.34
53	BA	379	G	C2-N2	-5.84	1.28	1.34
53	BA	981	A	C6-N1	-5.84	1.31	1.35
21	AA	770	C	N3-C4	-5.83	1.29	1.33
21	AA	27	G	C2-N2	-5.83	1.28	1.34
53	BA	758	C	N3-C4	-5.83	1.29	1.33
53	BA	1055	G	C2-N2	-5.82	1.28	1.34
21	AA	1344	C	N3-C4	-5.82	1.29	1.33
21	AA	1524	C	N3-C4	-5.82	1.29	1.33
53	BA	2525	G	C6-N1	-5.82	1.35	1.39
53	BA	1031	G	C2-N2	-5.82	1.28	1.34
53	BA	97	C	N3-C4	-5.82	1.29	1.33
21	AA	1251	A	C6-N1	-5.82	1.31	1.35
53	BA	1691	C	C4-N4	-5.82	1.28	1.33
53	BA	1086	A	C6-N1	-5.81	1.31	1.35
21	AA	667	G	C2-N2	-5.81	1.28	1.34
21	AA	948	C	C4-N4	-5.81	1.28	1.33
53	BA	1115	G	C2-N2	-5.81	1.28	1.34
53	BA	1314	C	N3-C4	-5.81	1.29	1.33
21	AA	1200	C	C4-N4	-5.80	1.28	1.33
53	BA	553	G	C2-N2	-5.80	1.28	1.34
53	BA	795	C	C4-N4	-5.80	1.28	1.33
21	AA	1336	C	C4-N4	-5.80	1.28	1.33
53	BA	2467	C	N3-C4	-5.80	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	548	G	C2-N2	-5.79	1.28	1.34
53	BA	1196	C	N3-C4	-5.79	1.29	1.33
21	AA	75	G	C2-N2	-5.79	1.28	1.34
53	BA	1666	G	C2-N2	-5.79	1.28	1.34
53	BA	2726	A	C6-N1	-5.79	1.31	1.35
21	AA	381	C	C4-N4	-5.79	1.28	1.33
21	AA	345	C	C4-N4	-5.78	1.28	1.33
53	BA	66	C	C4-N4	-5.78	1.28	1.33
53	BA	168	G	C2-N2	-5.78	1.28	1.34
53	BA	650	C	C4-N4	-5.78	1.28	1.33
53	BA	706	A	C6-N6	-5.78	1.29	1.33
21	AA	1501	C	C4-N4	-5.77	1.28	1.33
21	AA	1021	A	C6-N1	-5.77	1.31	1.35
21	AA	1059	C	C4-N4	-5.77	1.28	1.33
53	BA	342	A	C6-N1	-5.77	1.31	1.35
53	BA	1659	G	C6-N1	-5.77	1.35	1.39
53	BA	1190	G	C2-N2	-5.77	1.28	1.34
53	BA	1592	C	C4-N4	-5.77	1.28	1.33
21	AA	885	G	C6-N1	-5.76	1.35	1.39
21	AA	829	G	C2-N2	-5.76	1.28	1.34
53	BA	1854	A	C6-N1	-5.76	1.31	1.35
53	BA	2839	G	C6-N1	-5.76	1.35	1.39
53	BA	1292	G	N1-C2	-5.76	1.33	1.37
53	BA	2771	C	C4-N4	-5.76	1.28	1.33
53	BA	2461	A	C6-N1	-5.75	1.31	1.35
53	BA	960	A	C6-N1	-5.75	1.31	1.35
53	BA	1962	C	C4-N4	-5.75	1.28	1.33
53	BA	1277	G	C2-N2	-5.75	1.28	1.34
21	AA	864	A	C6-N1	-5.75	1.31	1.35
22	A1	24	G	C6-N1	-5.75	1.35	1.39
53	BA	2212	A	C6-N1	-5.74	1.31	1.35
21	AA	1031	C	C4-N4	-5.74	1.28	1.33
53	BA	1152	C	N3-C4	-5.74	1.29	1.33
21	AA	1272	G	C2-N2	-5.74	1.28	1.34
53	BA	1660	G	C2-N2	-5.74	1.28	1.34
21	AA	87	C	N3-C4	-5.74	1.29	1.33
21	AA	95	C	C4-N4	-5.74	1.28	1.33
53	BA	2089	C	C4-N4	-5.74	1.28	1.33
21	AA	881	G	C2-N2	-5.73	1.28	1.34
53	BA	2543	G	C2-N2	-5.73	1.28	1.34
21	AA	198	G	C2-N2	-5.73	1.28	1.34
53	BA	2876	G	C2-N2	-5.73	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	1069	A	C6-N1	-5.73	1.31	1.35
21	AA	82	G	N1-C2	-5.73	1.33	1.37
21	AA	836	G	C2-N2	-5.72	1.28	1.34
53	BA	1202	G	C2-N2	-5.72	1.28	1.34
53	BA	2652	C	C4-N4	-5.72	1.28	1.33
53	BA	367	G	C2-N2	-5.72	1.28	1.34
53	BA	708	G	C2-N2	-5.72	1.28	1.34
21	AA	1514	G	C2-N2	-5.72	1.28	1.34
53	BA	1107	G	C2-N2	-5.72	1.28	1.34
53	BA	1638	C	N3-C4	-5.72	1.29	1.33
53	BA	2456	C	N3-C4	-5.72	1.29	1.33
53	BA	2526	G	C2-N2	-5.72	1.28	1.34
22	A1	40	G	C2-N2	-5.72	1.28	1.34
53	BA	2424	C	C4-N4	-5.72	1.28	1.33
53	BA	628	G	C2-N2	-5.71	1.28	1.34
53	BA	2298	A	C6-N1	-5.71	1.31	1.35
53	BA	2859	G	C2-N2	-5.71	1.28	1.34
21	AA	194	C	C4-N4	-5.71	1.28	1.33
53	BA	948	C	C4-N4	-5.71	1.28	1.33
53	BA	687	C	C4-N4	-5.71	1.28	1.33
53	BA	2263	C	C4-N4	-5.71	1.28	1.33
21	AA	1288	A	C6-N1	-5.71	1.31	1.35
53	BA	2579	C	C4-N4	-5.70	1.28	1.33
21	AA	210	C	N3-C4	-5.70	1.29	1.33
53	BA	484	C	C4-N4	-5.70	1.28	1.33
53	BA	2442	C	C4-N4	-5.70	1.28	1.33
53	BA	2599	G	C2-N2	-5.70	1.28	1.34
21	AA	595	A	C6-N1	-5.70	1.31	1.35
21	AA	1368	A	C6-N1	-5.70	1.31	1.35
21	AA	886	G	C2-N2	-5.70	1.28	1.34
21	AA	1006	G	C2-N2	-5.69	1.28	1.34
21	AA	984	C	C4-N4	-5.69	1.28	1.33
21	AA	1356	G	C2-N2	-5.69	1.28	1.34
53	BA	510	C	C4-N4	-5.69	1.28	1.33
21	AA	1245	C	C4-N4	-5.69	1.28	1.33
53	BA	336	C	C4-N4	-5.69	1.28	1.33
53	BA	2287	A	C6-N1	-5.69	1.31	1.35
53	BA	21	A	C6-N1	-5.69	1.31	1.35
53	BA	800	A	C6-N1	-5.69	1.31	1.35
53	BA	901	C	N3-C4	-5.69	1.29	1.33
53	BA	1633	G	C2-N2	-5.69	1.28	1.34
53	BA	2551	C	N3-C4	-5.69	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	934	C	C4-N4	-5.68	1.28	1.33
21	AA	212	G	C6-N1	-5.68	1.35	1.39
53	BA	935	C	C4-N4	-5.68	1.28	1.33
53	BA	2515	C	N3-C4	-5.68	1.29	1.33
53	BA	2144	G	C2-N2	-5.67	1.28	1.34
53	BA	522	A	C6-N1	-5.67	1.31	1.35
53	BA	640	C	C4-N4	-5.67	1.28	1.33
53	BA	1932	A	C6-N1	-5.67	1.31	1.35
53	BA	2668	G	C2-N2	-5.67	1.28	1.34
54	BB	31	C	N3-C4	-5.67	1.29	1.33
53	BA	1311	G	C2-N2	-5.67	1.28	1.34
53	BA	629	G	C6-N1	-5.67	1.35	1.39
53	BA	2674	G	C2-N2	-5.67	1.28	1.34
53	BA	533	G	C6-N1	-5.67	1.35	1.39
53	BA	778	G	C2-N2	-5.66	1.28	1.34
53	BA	2066	C	C4-N4	-5.66	1.28	1.33
53	BA	2560	A	C6-N1	-5.66	1.31	1.35
21	AA	998	C	N3-C4	-5.66	1.29	1.33
53	BA	1642	G	C2-N2	-5.66	1.28	1.34
53	BA	2853	C	C4-N4	-5.66	1.28	1.33
21	AA	599	C	C4-N4	-5.66	1.28	1.33
53	BA	440	C	N3-C4	-5.66	1.29	1.33
53	BA	777	G	C2-N2	-5.66	1.28	1.34
53	BA	2342	C	C4-N4	-5.66	1.28	1.33
53	BA	2412	A	C6-N1	-5.65	1.31	1.35
53	BA	865	C	C4-N4	-5.65	1.28	1.33
53	BA	912	C	N3-C4	-5.65	1.29	1.33
53	BA	1014	A	C6-N1	-5.65	1.31	1.35
53	BA	994	C	C4-N4	-5.65	1.28	1.33
53	BA	2164	C	C4-N4	-5.65	1.28	1.33
21	AA	688	G	C2-N2	-5.65	1.28	1.34
53	BA	1482	G	C2-N2	-5.65	1.28	1.34
53	BA	902	C	C4-N4	-5.65	1.28	1.33
21	AA	615	G	C2-N2	-5.64	1.28	1.34
21	AA	883	C	C4-N4	-5.64	1.28	1.33
53	BA	1500	G	C2-N2	-5.64	1.28	1.34
53	BA	1685	C	C4-N4	-5.64	1.28	1.33
53	BA	2481	G	C2-N2	-5.64	1.28	1.34
53	BA	1076	C	C4-N4	-5.64	1.28	1.33
53	BA	2876	G	C6-N1	-5.64	1.35	1.39
53	BA	880	G	C2-N2	-5.64	1.28	1.34
21	AA	187	G	C2-N2	-5.64	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1310	G	C2-N2	-5.64	1.28	1.34
53	BA	1791	A	C6-N1	-5.64	1.31	1.35
22	A1	25	C	C4-N4	-5.64	1.28	1.33
21	AA	1357	A	C6-N1	-5.63	1.31	1.35
53	BA	46	G	C2-N2	-5.63	1.28	1.34
53	BA	854	C	C4-N4	-5.63	1.28	1.33
53	BA	1905	C	C4-N4	-5.63	1.28	1.33
53	BA	2444	G	C2-N2	-5.63	1.28	1.34
53	BA	2509	G	C2-N2	-5.63	1.28	1.34
53	BA	2840	C	C4-N4	-5.63	1.28	1.33
53	BA	1243	C	C4-N4	-5.63	1.28	1.33
53	BA	1817	G	C2-N2	-5.63	1.28	1.34
21	AA	769	G	C2-N2	-5.63	1.28	1.34
53	BA	1337	G	C2-N2	-5.63	1.28	1.34
53	BA	1780	A	C6-N1	-5.63	1.31	1.35
53	BA	2004	G	C2-N2	-5.63	1.28	1.34
21	AA	311	C	C4-N4	-5.62	1.28	1.33
53	BA	869	G	C2-N2	-5.62	1.28	1.34
54	BB	28	C	C4-N4	-5.62	1.28	1.33
53	BA	327	G	C2-N2	-5.62	1.28	1.34
53	BA	2844	G	C2-N2	-5.62	1.28	1.34
53	BA	452	G	C6-N1	-5.62	1.35	1.39
21	AA	1096	C	C4-N4	-5.62	1.28	1.33
53	BA	1059	G	C6-N1	-5.62	1.35	1.39
53	BA	1315	C	C4-N4	-5.62	1.28	1.33
53	BA	1489	C	C4-N4	-5.62	1.28	1.33
53	BA	257	C	N3-C4	-5.62	1.30	1.33
53	BA	792	A	C6-N1	-5.62	1.31	1.35
53	BA	943	A	C6-N1	-5.62	1.31	1.35
21	AA	1350	A	C6-N1	-5.62	1.31	1.35
53	BA	2683	C	C4-N4	-5.62	1.28	1.33
53	BA	985	C	C4-N4	-5.61	1.28	1.33
53	BA	1117	C	N3-C4	-5.61	1.30	1.33
21	AA	195	A	C5-C4	-5.61	1.34	1.38
21	AA	1136	C	C4-N4	-5.61	1.28	1.33
53	BA	1336	A	C6-N1	-5.61	1.31	1.35
53	BA	2857	G	C6-N1	-5.61	1.35	1.39
53	BA	213	A	C6-N1	-5.61	1.31	1.35
21	AA	350	G	C2-N2	-5.61	1.28	1.34
53	BA	876	C	C4-N4	-5.61	1.28	1.33
53	BA	1897	G	C6-N1	-5.61	1.35	1.39
21	AA	97	G	C2-N2	-5.60	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	1531	C	C4-N4	-5.60	1.28	1.33
21	AA	859	G	C2-N2	-5.60	1.28	1.34
53	BA	867	C	C4-N4	-5.60	1.28	1.33
53	BA	1633	G	C6-N1	-5.60	1.35	1.39
53	BA	2411	A	C6-N1	-5.60	1.31	1.35
53	BA	463	G	C2-N2	-5.59	1.28	1.34
53	BA	2268	A	C6-N1	-5.59	1.31	1.35
21	AA	836	G	C6-N1	-5.59	1.35	1.39
21	AA	646	G	C6-N1	-5.59	1.35	1.39
53	BA	1909	C	C4-N4	-5.59	1.28	1.33
21	AA	149	A	C6-N1	-5.59	1.31	1.35
21	AA	612	C	C4-N4	-5.59	1.28	1.33
53	BA	80	G	N1-C2	-5.59	1.33	1.37
53	BA	2290	G	C2-N2	-5.59	1.28	1.34
21	AA	1395	C	N3-C4	-5.59	1.30	1.33
53	BA	689	A	C6-N1	-5.59	1.31	1.35
21	AA	102	G	C2-N2	-5.58	1.28	1.34
21	AA	647	C	N3-C4	-5.58	1.30	1.33
21	AA	903	G	C2-N2	-5.58	1.28	1.34
21	AA	1281	C	C4-N4	-5.58	1.28	1.33
53	BA	353	C	C4-N4	-5.58	1.28	1.33
53	BA	2242	G	C2-N2	-5.58	1.28	1.34
53	BA	2662	A	C6-N1	-5.58	1.31	1.35
21	AA	549	C	C4-N4	-5.58	1.28	1.33
53	BA	858	G	C2-N2	-5.58	1.28	1.34
21	AA	756	C	C4-N4	-5.58	1.28	1.33
21	AA	865	A	C5-C4	-5.58	1.34	1.38
53	BA	266	G	C2-N2	-5.58	1.28	1.34
53	BA	1311	G	C6-N1	-5.58	1.35	1.39
21	AA	1244	G	C2-N2	-5.57	1.28	1.34
53	BA	2004	G	C6-N1	-5.57	1.35	1.39
21	AA	867	G	C2-N2	-5.57	1.28	1.34
53	BA	1321	A	C6-N1	-5.57	1.31	1.35
53	BA	2279	G	C2-N2	-5.57	1.28	1.34
21	AA	332	G	C2-N2	-5.57	1.28	1.34
53	BA	1068	G	C2-N2	-5.57	1.28	1.34
53	BA	2273	A	C6-N1	-5.57	1.31	1.35
21	AA	240	G	C2-N2	-5.56	1.28	1.34
21	AA	715	A	C6-N1	-5.56	1.31	1.35
21	AA	1523	G	C2-N2	-5.56	1.28	1.34
53	BA	261	G	C2-N2	-5.56	1.28	1.34
53	BA	173	A	C6-N1	-5.56	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	923	G	C2-N2	-5.56	1.28	1.34
53	BA	456	C	C4-N4	-5.55	1.28	1.33
53	BA	1490	A	C6-N1	-5.55	1.31	1.35
53	BA	2440	C	C4-N4	-5.55	1.28	1.33
53	BA	1524	G	C2-N2	-5.55	1.28	1.34
22	A1	10	G	C6-N1	-5.55	1.35	1.39
53	BA	1927	A	C6-N1	-5.55	1.31	1.35
53	BA	903	C	C4-N4	-5.55	1.28	1.33
53	BA	2316	G	C2-N2	-5.55	1.29	1.34
21	AA	752	G	C2-N2	-5.54	1.29	1.34
53	BA	2527	C	C4-N4	-5.54	1.28	1.33
53	BA	2902	C	C4-N4	-5.54	1.28	1.33
21	AA	73	C	C4-N4	-5.54	1.28	1.33
21	AA	76	G	C2-N2	-5.54	1.29	1.34
21	AA	568	G	N1-C2	-5.54	1.33	1.37
53	BA	1123	C	C4-N4	-5.54	1.28	1.33
21	AA	282	A	C6-N6	-5.54	1.29	1.33
21	AA	174	A	C6-N6	-5.54	1.29	1.33
53	BA	1125	G	C2-N2	-5.54	1.29	1.34
53	BA	1135	C	C4-N4	-5.54	1.28	1.33
53	BA	1210	G	C2-N2	-5.54	1.29	1.34
53	BA	2104	C	N3-C4	-5.54	1.30	1.33
53	BA	2506	U	C4'-C3'	-5.54	1.47	1.52
53	BA	848	C	N3-C4	-5.54	1.30	1.33
53	BA	1136	G	C2-N2	-5.54	1.29	1.34
53	BA	1837	C	C4-N4	-5.54	1.28	1.33
53	BA	2614	A	C6-N1	-5.54	1.31	1.35
21	AA	1043	G	N1-C2	-5.54	1.33	1.37
53	BA	364	C	C4-N4	-5.54	1.28	1.33
53	BA	1151	A	C6-N1	-5.54	1.31	1.35
53	BA	1423	G	C2-N2	-5.53	1.29	1.34
53	BA	2512	C	C4-N4	-5.53	1.28	1.33
53	BA	1179	G	C2-N2	-5.53	1.29	1.34
53	BA	157	C	N3-C4	-5.53	1.30	1.33
53	BA	402	A	C6-N6	-5.53	1.29	1.33
53	BA	374	A	C6-N1	-5.53	1.31	1.35
53	BA	1050	A	C6-N1	-5.53	1.31	1.35
53	BA	1847	A	C6-N1	-5.53	1.31	1.35
53	BA	43	G	C2-N2	-5.53	1.29	1.34
53	BA	79	C	N3-C4	-5.53	1.30	1.33
53	BA	1164	C	C4-N4	-5.53	1.28	1.33
53	BA	122	G	C2-N2	-5.52	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	476	G	C2-N2	-5.52	1.29	1.34
53	BA	2260	C	N3-C4	-5.52	1.30	1.33
53	BA	1965	C	N3-C4	-5.52	1.30	1.33
53	BA	1288	G	C2-N2	-5.52	1.29	1.34
53	BA	1717	A	C6-N1	-5.52	1.31	1.35
53	BA	1715	G	C2-N2	-5.52	1.29	1.34
53	BA	2455	G	C2-N2	-5.52	1.29	1.34
53	BA	1006	C	C4-N4	-5.51	1.28	1.33
53	BA	1771	C	C4-N4	-5.51	1.28	1.33
53	BA	2171	A	C6-N1	-5.51	1.31	1.35
21	AA	326	G	C2-N2	-5.51	1.29	1.34
21	AA	572	A	C6-N1	-5.51	1.31	1.35
21	AA	1038	C	C4-N4	-5.51	1.28	1.33
53	BA	935	C	N3-C4	-5.51	1.30	1.33
21	AA	573	A	C6-N1	-5.51	1.31	1.35
21	AA	1504	G	C2-N2	-5.51	1.29	1.34
22	A1	15	G	C2-N2	-5.51	1.29	1.34
53	BA	524	G	N1-C2	-5.51	1.33	1.37
53	BA	1190	G	C6-N1	-5.51	1.35	1.39
53	BA	1805	A	C6-N1	-5.51	1.31	1.35
21	AA	45	G	C2-N2	-5.51	1.29	1.34
21	AA	808	C	C4-N4	-5.51	1.28	1.33
53	BA	1823	G	C2-N2	-5.51	1.29	1.34
21	AA	879	C	C4-N4	-5.50	1.28	1.33
21	AA	1196	A	C5-C4	-5.50	1.34	1.38
53	BA	1998	A	C6-N1	-5.50	1.31	1.35
53	BA	225	C	C4-N4	-5.50	1.28	1.33
53	BA	915	C	C4-N4	-5.50	1.28	1.33
53	BA	2896	C	N3-C4	-5.50	1.30	1.33
53	BA	2087	G	N1-C2	-5.50	1.33	1.37
53	BA	221	A	C5-C4	-5.50	1.34	1.38
53	BA	796	C	C4-N4	-5.50	1.28	1.33
53	BA	2882	A	C6-N1	-5.50	1.31	1.35
53	BA	2531	A	C6-N1	-5.50	1.31	1.35
53	BA	2642	G	C2-N2	-5.50	1.29	1.34
53	BA	2448	A	C6-N1	-5.50	1.31	1.35
53	BA	2815	C	N3-C4	-5.50	1.30	1.33
21	AA	195	A	C6-N6	-5.49	1.29	1.33
21	AA	967	C	C4-N4	-5.49	1.29	1.33
21	AA	1037	C	C4-N4	-5.49	1.29	1.33
21	AA	1297	G	N1-C2	-5.49	1.33	1.37
53	BA	256	A	C6-N1	-5.49	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	230	G	C2-N2	-5.49	1.29	1.34
53	BA	237	C	C4-N4	-5.49	1.29	1.33
53	BA	488	G	C2-N2	-5.49	1.29	1.34
21	AA	823	C	N3-C4	-5.49	1.30	1.33
53	BA	433	C	N3-C4	-5.49	1.30	1.33
53	BA	1844	C	C4-N4	-5.49	1.29	1.33
53	BA	2834	G	N1-C2	-5.49	1.33	1.37
21	AA	1255	G	C2-N2	-5.49	1.29	1.34
53	BA	76	C	C4-N4	-5.49	1.29	1.33
53	BA	110	G	C2-N2	-5.49	1.29	1.34
53	BA	1008	A	C6-N1	-5.49	1.31	1.35
53	BA	46	G	C6-N1	-5.49	1.35	1.39
53	BA	1521	G	C6-N1	-5.48	1.35	1.39
53	BA	1062	G	C2-N2	-5.48	1.29	1.34
53	BA	2529	G	C2-N2	-5.48	1.29	1.34
53	BA	2651	C	C4-N4	-5.48	1.29	1.33
21	AA	1292	G	C2-N2	-5.48	1.29	1.34
53	BA	194	G	C2-N2	-5.48	1.29	1.34
53	BA	916	G	C6-N1	-5.48	1.35	1.39
53	BA	1118	C	C4-N4	-5.48	1.29	1.33
53	BA	1967	C	N3-C4	-5.48	1.30	1.33
53	BA	791	C	N3-C4	-5.48	1.30	1.33
53	BA	2274	A	C6-N6	-5.48	1.29	1.33
21	AA	1063	C	N3-C4	-5.47	1.30	1.33
21	AA	1067	A	C5-C4	-5.47	1.34	1.38
53	BA	2466	C	N3-C4	-5.47	1.30	1.33
21	AA	860	A	C6-N1	-5.47	1.31	1.35
53	BA	959	A	C6-N1	-5.47	1.31	1.35
53	BA	1319	C	N3-C4	-5.47	1.30	1.33
53	BA	2844	G	C6-N1	-5.47	1.35	1.39
53	BA	995	C	C4-N4	-5.46	1.29	1.33
53	BA	1005	C	N3-C4	-5.46	1.30	1.33
53	BA	1908	C	N3-C4	-5.46	1.30	1.33
21	AA	831	A	C5-C4	-5.46	1.34	1.38
53	BA	716	A	C6-N1	-5.46	1.31	1.35
53	BA	2300	C	C4-N4	-5.46	1.29	1.33
53	BA	2581	G	C2-N2	-5.46	1.29	1.34
53	BA	420	C	C4-N4	-5.46	1.29	1.33
53	BA	1331	G	C2-N2	-5.46	1.29	1.34
53	BA	1541	C	N3-C4	-5.46	1.30	1.33
53	BA	1002	G	C2-N2	-5.46	1.29	1.34
53	BA	1473	G	C2-N2	-5.46	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	690	G	N1-C2	-5.45	1.33	1.37
53	BA	1469	A	C5-C4	-5.45	1.34	1.38
53	BA	523	C	N3-C4	-5.45	1.30	1.33
53	BA	914	G	C2-N2	-5.45	1.29	1.34
53	BA	1745	A	C6-N6	-5.45	1.29	1.33
53	BA	446	G	C2-N2	-5.45	1.29	1.34
53	BA	1064	C	C4-N4	-5.45	1.29	1.33
53	BA	2772	C	C4-N4	-5.45	1.29	1.33
54	BB	29	A	C6-N6	-5.45	1.29	1.33
53	BA	1728	C	C4-N4	-5.45	1.29	1.33
53	BA	253	C	C4-N4	-5.45	1.29	1.33
21	AA	313	A	C6-N1	-5.44	1.31	1.35
21	AA	1252	A	C5-C4	-5.44	1.34	1.38
53	BA	2088	A	C6-N6	-5.44	1.29	1.33
53	BA	2462	C	C4-N4	-5.44	1.29	1.33
21	AA	399	G	C2-N2	-5.44	1.29	1.34
53	BA	2277	G	C2-N2	-5.44	1.29	1.34
53	BA	268	C	C4-N4	-5.44	1.29	1.33
53	BA	986	C	C4-N4	-5.44	1.29	1.33
53	BA	2436	G	C2-N2	-5.44	1.29	1.34
22	A1	48	C	C4-N4	-5.43	1.29	1.33
53	BA	338	G	C2-N2	-5.43	1.29	1.34
53	BA	732	C	N3-C4	-5.43	1.30	1.33
53	BA	922	C	N3-C4	-5.43	1.30	1.33
53	BA	1160	G	C2-N2	-5.43	1.29	1.34
53	BA	1274	A	C6-N1	-5.43	1.31	1.35
53	BA	1300	G	C2-N2	-5.43	1.29	1.34
22	A1	31	C	C4-N4	-5.43	1.29	1.33
53	BA	61	C	N3-C4	-5.43	1.30	1.33
54	BB	61	G	C2-N2	-5.43	1.29	1.34
21	AA	1051	C	N3-C4	-5.43	1.30	1.33
53	BA	335	C	C4-N4	-5.43	1.29	1.33
53	BA	340	A	C6-N6	-5.43	1.29	1.33
53	BA	672	C	N3-C4	-5.43	1.30	1.33
21	AA	316	C	C4-N4	-5.42	1.29	1.33
21	AA	334	C	C4-N4	-5.42	1.29	1.33
53	BA	1795	C	C4-N4	-5.42	1.29	1.33
53	BA	1417	C	C4-N4	-5.42	1.29	1.33
53	BA	2532	G	C2-N2	-5.42	1.29	1.34
21	AA	814	A	C6-N1	-5.42	1.31	1.35
21	AA	894	G	C2-N2	-5.42	1.29	1.34
21	AA	791	G	C2-N2	-5.42	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	1879	C	C4-N4	-5.42	1.29	1.33
53	BA	2065	C	C4-N4	-5.42	1.29	1.33
53	BA	2416	C	N3-C4	-5.42	1.30	1.33
21	AA	266	G	C2-N2	-5.42	1.29	1.34
53	BA	517	C	N3-C4	-5.42	1.30	1.33
53	BA	679	C	C4-N4	-5.42	1.29	1.33
53	BA	2008	C	N3-C4	-5.42	1.30	1.33
21	AA	750	C	C4-N4	-5.41	1.29	1.33
53	BA	1178	C	C4-N4	-5.41	1.29	1.33
53	BA	1459	G	C2-N2	-5.41	1.29	1.34
21	AA	689	C	N3-C4	-5.41	1.30	1.33
53	BA	1307	A	C6-N1	-5.41	1.31	1.35
21	AA	1497	G	C2-N2	-5.41	1.29	1.34
53	BA	108	G	N1-C2	-5.41	1.33	1.37
53	BA	550	C	C4-N4	-5.41	1.29	1.33
53	BA	1322	A	C5-C4	-5.41	1.34	1.38
53	BA	438	G	C2-N2	-5.41	1.29	1.34
53	BA	1518	C	C4-N4	-5.41	1.29	1.33
21	AA	1531	A	C6-N1	-5.40	1.31	1.35
53	BA	704	G	C2-N2	-5.40	1.29	1.34
53	BA	2230	G	C2-N2	-5.40	1.29	1.34
22	A1	45	G	C2-N2	-5.40	1.29	1.34
53	BA	1100	C	C4-N4	-5.40	1.29	1.33
53	BA	1247	A	C6-N1	-5.40	1.31	1.35
53	BA	1305	C	C4-N4	-5.40	1.29	1.33
53	BA	2437	G	C2-N2	-5.40	1.29	1.34
53	BA	879	G	C2-N2	-5.40	1.29	1.34
53	BA	2033	A	C5-C4	-5.40	1.34	1.38
53	BA	2313	C	C4-N4	-5.40	1.29	1.33
21	AA	1160	G	C2-N2	-5.40	1.29	1.34
22	A1	28	C	N3-C4	-5.39	1.30	1.33
21	AA	576	C	C4-N4	-5.39	1.29	1.33
53	BA	783	A	O3 <sup>1</sup> -P	-5.39	1.54	1.61
53	BA	706	A	C5-C4	-5.39	1.34	1.38
53	BA	725	G	C2-N2	-5.39	1.29	1.34
53	BA	997	G	C2-N2	-5.39	1.29	1.34
53	BA	1091	G	C2-N2	-5.39	1.29	1.34
21	AA	100	G	N1-C2	-5.39	1.33	1.37
21	AA	1309	G	C6-N1	-5.39	1.35	1.39
53	BA	969	G	C2-N2	-5.39	1.29	1.34
53	BA	1469	A	C6-N6	-5.39	1.29	1.33
53	BA	1639	C	N3-C4	-5.39	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	1424	G	C2-N2	-5.39	1.29	1.34
53	BA	2676	C	C4-N4	-5.39	1.29	1.33
53	BA	2816	G	C2-N2	-5.39	1.29	1.34
53	BA	1600	C	C4-N4	-5.38	1.29	1.33
53	BA	2227	A	C6-N1	-5.38	1.31	1.35
53	BA	2530	A	C6-N1	-5.38	1.31	1.35
53	BA	677	A	C6-N1	-5.38	1.31	1.35
53	BA	1498	C	C4-N4	-5.38	1.29	1.33
53	BA	1835	G	C2-N2	-5.38	1.29	1.34
53	BA	859	G	N1-C2	-5.38	1.33	1.37
53	BA	1025	G	C2-N2	-5.38	1.29	1.34
21	AA	792	A	C6-N1	-5.37	1.31	1.35
21	AA	1192	C	C4-N4	-5.37	1.29	1.33
21	AA	1356	G	C6-N1	-5.37	1.35	1.39
53	BA	1581	G	C2-N2	-5.37	1.29	1.34
54	BB	26	C	C4-N4	-5.37	1.29	1.33
53	BA	209	C	C4-N4	-5.37	1.29	1.33
53	BA	2855	C	C4-N4	-5.37	1.29	1.33
21	AA	714	G	C2-N2	-5.37	1.29	1.34
53	BA	1846	G	C2-N2	-5.37	1.29	1.34
21	AA	1493	A	C6-N6	-5.37	1.29	1.33
53	BA	1668	A	C5-C4	-5.37	1.34	1.38
53	BA	2628	C	C4-N4	-5.37	1.29	1.33
21	AA	624	C	C4-N4	-5.37	1.29	1.33
21	AA	1252	A	C6-N6	-5.37	1.29	1.33
21	AA	738	C	C4-N4	-5.36	1.29	1.33
21	AA	824	G	N1-C2	-5.36	1.33	1.37
21	AA	796	C	N3-C4	-5.36	1.30	1.33
53	BA	1694	C	N3-C4	-5.36	1.30	1.33
54	BB	41	G	N1-C2	-5.36	1.33	1.37
21	AA	509	A	C6-N1	-5.36	1.31	1.35
53	BA	1522	A	C5-C4	-5.36	1.34	1.38
21	AA	1020	G	C2-N2	-5.36	1.29	1.34
21	AA	1373	G	C6-N1	-5.36	1.35	1.39
53	BA	638	G	C2-N2	-5.36	1.29	1.34
53	BA	1722	A	C6-N1	-5.36	1.31	1.35
53	BA	2616	C	N3-C4	-5.36	1.30	1.33
53	BA	1907	G	C2-N2	-5.35	1.29	1.34
53	BA	2260	C	C4-N4	-5.35	1.29	1.33
21	AA	1246	A	C6-N6	-5.35	1.29	1.33
53	BA	465	G	C2-N2	-5.35	1.29	1.34
53	BA	2116	G	C2-N2	-5.35	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	2467	C	C4-N4	-5.35	1.29	1.33
53	BA	1170	C	C4-N4	-5.35	1.29	1.33
53	BA	2685	G	C2-N2	-5.35	1.29	1.34
53	BA	1625	C	N3-C4	-5.35	1.30	1.33
21	AA	693	G	C2-N2	-5.35	1.29	1.34
21	AA	698	G	N1-C2	-5.35	1.33	1.37
53	BA	261	G	C6-N1	-5.35	1.35	1.39
22	A1	36	C	N3-C4	-5.34	1.30	1.33
53	BA	128	C	C4-N4	-5.34	1.29	1.33
53	BA	2892	G	C2-N2	-5.34	1.29	1.34
21	AA	1487	G	C2-N2	-5.34	1.29	1.34
53	BA	544	C	N3-C4	-5.34	1.30	1.33
53	BA	782	A	C6-N1	-5.34	1.31	1.35
53	BA	2080	A	C6-N1	-5.34	1.31	1.35
21	AA	1022	A	C5-C4	-5.34	1.35	1.38
53	BA	2147	A	C5-C4	-5.34	1.35	1.38
53	BA	2318	G	N1-C2	-5.34	1.33	1.37
53	BA	2539	C	C4-N4	-5.34	1.29	1.33
21	AA	1262	C	C4-N4	-5.34	1.29	1.33
21	AA	631	C	C4-N4	-5.34	1.29	1.33
53	BA	1897	G	C2-N2	-5.34	1.29	1.34
53	BA	1957	C	N3-C4	-5.34	1.30	1.33
21	AA	900	A	C6-N1	-5.33	1.31	1.35
53	BA	1652	A	C6-N1	-5.33	1.31	1.35
21	AA	1016	A	C6-N1	-5.33	1.31	1.35
53	BA	1296	G	C6-N1	-5.33	1.35	1.39
53	BA	1739	A	C5-C4	-5.33	1.35	1.38
54	BB	29	A	C5-C4	-5.33	1.35	1.38
21	AA	574	A	C5-C4	-5.33	1.35	1.38
53	BA	2445	G	C2-N2	-5.33	1.29	1.34
53	BA	1511	G	C2-N2	-5.33	1.29	1.34
21	AA	1128	C	O3'-P	-5.33	1.54	1.61
53	BA	266	G	C6-N1	-5.33	1.35	1.39
53	BA	2483	C	C4-N4	-5.33	1.29	1.33
53	BA	356	G	C6-N1	-5.32	1.35	1.39
53	BA	918	A	C6-N1	-5.32	1.31	1.35
21	AA	1520	C	C4-N4	-5.32	1.29	1.33
53	BA	923	G	C6-N1	-5.32	1.35	1.39
53	BA	324	A	C6-N6	-5.32	1.29	1.33
53	BA	2641	G	C2-N2	-5.32	1.29	1.34
21	AA	267	C	C4-N4	-5.31	1.29	1.33
21	AA	1058	G	C2-N2	-5.31	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1325	C	N3-C4	-5.31	1.30	1.33
53	BA	273	G	C2-N2	-5.31	1.29	1.34
53	BA	414	C	N3-C4	-5.31	1.30	1.33
53	BA	2232	C	C4-N4	-5.31	1.29	1.33
53	BA	2270	A	N9-C4	-5.31	1.34	1.37
53	BA	2325	G	C2-N2	-5.31	1.29	1.34
53	BA	1328	A	C5-C4	-5.31	1.35	1.38
21	AA	694	A	C5-C4	-5.30	1.35	1.38
21	AA	1306	A	C6-N1	-5.30	1.31	1.35
21	AA	1404	C	C4-N4	-5.30	1.29	1.33
53	BA	1399	C	N3-C4	-5.30	1.30	1.33
53	BA	1512	C	C4-N4	-5.30	1.29	1.33
53	BA	1642	G	C6-N1	-5.30	1.35	1.39
53	BA	2447	G	C2-N2	-5.30	1.29	1.34
53	BA	1106	G	C2-N2	-5.30	1.29	1.34
21	AA	1191	A	C6-N1	-5.30	1.31	1.35
21	AA	1249	C	N3-C4	-5.30	1.30	1.33
21	AA	1446	A	C6-N1	-5.30	1.31	1.35
53	BA	444	C	C4-N4	-5.30	1.29	1.33
53	BA	2084	C	C4-N4	-5.30	1.29	1.33
53	BA	2775	G	C2-N2	-5.30	1.29	1.34
53	BA	254	G	C2-N2	-5.29	1.29	1.34
53	BA	1914	C	C4-N4	-5.29	1.29	1.33
53	BA	2429	G	C2-N2	-5.29	1.29	1.34
21	AA	858	G	C2-N2	-5.29	1.29	1.34
53	BA	2226	C	C4-N4	-5.29	1.29	1.33
53	BA	2527	C	N3-C4	-5.29	1.30	1.33
53	BA	1928	A	C6-N1	-5.29	1.31	1.35
21	AA	582	C	C4-N4	-5.29	1.29	1.33
53	BA	343	C	N3-C4	-5.29	1.30	1.33
53	BA	1404	C	N3-C4	-5.29	1.30	1.33
21	AA	34	C	N3-C4	-5.29	1.30	1.33
21	AA	1033	G	N1-C2	-5.29	1.33	1.37
21	AA	211	G	N1-C2	-5.29	1.33	1.37
21	AA	342	C	N3-C4	-5.29	1.30	1.33
21	AA	829	G	C6-N1	-5.29	1.35	1.39
53	BA	966	G	N1-C2	-5.29	1.33	1.37
53	BA	1424	G	C6-N1	-5.29	1.35	1.39
53	BA	2516	A	C6-N1	-5.28	1.31	1.35
21	AA	679	C	N3-C4	-5.28	1.30	1.33
21	AA	946	A	C6-N1	-5.28	1.31	1.35
21	AA	38	G	C2-N2	-5.28	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	98	G	C2-N2	-5.28	1.29	1.34
53	BA	1848	A	C6-N1	-5.28	1.31	1.35
53	BA	2165	C	C4-N4	-5.28	1.29	1.33
21	AA	1403	C	C4-N4	-5.28	1.29	1.33
53	BA	1990	C	C4-N4	-5.28	1.29	1.33
53	BA	2682	A	C6-N6	-5.28	1.29	1.33
53	BA	823	C	N3-C4	-5.28	1.30	1.33
53	BA	2874	C	C4-N4	-5.27	1.29	1.33
21	AA	282	A	C5-C4	-5.27	1.35	1.38
21	AA	1083	U	O3'-P	-5.27	1.54	1.61
53	BA	1921	G	C2-N2	-5.27	1.29	1.34
53	BA	864	G	N1-C2	-5.27	1.33	1.37
53	BA	2507	C	C4-N4	-5.27	1.29	1.33
21	AA	744	C	C4-N4	-5.27	1.29	1.33
21	AA	536	C	C4-N4	-5.27	1.29	1.33
21	AA	553	A	C6-N1	-5.27	1.31	1.35
53	BA	1483	G	C2-N2	-5.27	1.29	1.34
21	AA	117	G	C2-N2	-5.26	1.29	1.34
21	AA	1237	C	C4-N4	-5.26	1.29	1.33
53	BA	267	C	N3-C4	-5.26	1.30	1.33
53	BA	1185	G	C2-N2	-5.26	1.29	1.34
53	BA	1903	G	C6-N1	-5.26	1.35	1.39
53	BA	713	G	C2-N2	-5.26	1.29	1.34
53	BA	1842	G	C2-N2	-5.26	1.29	1.34
53	BA	2767	C	C4-N4	-5.26	1.29	1.33
21	AA	314	C	N3-C4	-5.26	1.30	1.33
21	AA	647	C	C4-N4	-5.26	1.29	1.33
53	BA	663	G	C2-N2	-5.26	1.29	1.34
53	BA	2788	C	C4-N4	-5.26	1.29	1.33
21	AA	1260	G	C2-N2	-5.26	1.29	1.34
21	AA	1432	G	C2-N2	-5.26	1.29	1.34
53	BA	838	C	C4-N4	-5.26	1.29	1.33
53	BA	1596	A	C6-N1	-5.26	1.31	1.35
53	BA	2506	U	O3'-P	-5.26	1.54	1.61
21	AA	1041	G	C2-N2	-5.25	1.29	1.34
53	BA	71	A	C6-N1	-5.25	1.31	1.35
21	AA	596	A	C6-N1	-5.25	1.31	1.35
53	BA	844	A	C6-N6	-5.25	1.29	1.33
53	BA	326	G	C2-N2	-5.25	1.29	1.34
21	AA	1244	G	C6-N1	-5.25	1.35	1.39
21	AA	72	A	C5-C4	-5.25	1.35	1.38
21	AA	1233	G	C2-N2	-5.25	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	1054	A	C6-N1	-5.25	1.31	1.35
53	BA	1062	G	C6-N1	-5.25	1.35	1.39
53	BA	1389	G	N1-C2	-5.25	1.33	1.37
53	BA	2510	C	N3-C4	-5.25	1.30	1.33
21	AA	1013	G	N1-C2	-5.25	1.33	1.37
53	BA	1322	A	C6-N6	-5.25	1.29	1.33
53	BA	2158	A	C5-C4	-5.25	1.35	1.38
53	BA	2830	C	C4-N4	-5.25	1.29	1.33
53	BA	372	G	C2-N2	-5.25	1.29	1.34
53	BA	1346	G	C2-N2	-5.25	1.29	1.34
53	BA	1896	G	C2-N2	-5.25	1.29	1.34
53	BA	2582	G	C2-N2	-5.25	1.29	1.34
53	BA	1140	C	N3-C4	-5.24	1.30	1.33
53	BA	245	G	C2-N2	-5.24	1.29	1.34
53	BA	2542	A	C6-N1	-5.24	1.31	1.35
53	BA	232	G	N1-C2	-5.24	1.33	1.37
53	BA	874	G	C2-N2	-5.24	1.29	1.34
53	BA	1738	G	N1-C2	-5.24	1.33	1.37
53	BA	1999	C	C4-N4	-5.24	1.29	1.33
53	BA	2145	C	N3-C4	-5.24	1.30	1.33
21	AA	48	C	C4-N4	-5.24	1.29	1.33
21	AA	832	G	N1-C2	-5.24	1.33	1.37
53	BA	881	G	C2-N2	-5.24	1.29	1.34
53	BA	2073	C	C4-N4	-5.24	1.29	1.33
21	AA	338	A	C5-C4	-5.23	1.35	1.38
21	AA	1418	A	O3'-P	-5.23	1.54	1.61
53	BA	2239	G	N1-C2	-5.23	1.33	1.37
53	BA	2070	A	C6-N1	-5.23	1.31	1.35
53	BA	2510	C	C4-N4	-5.23	1.29	1.33
21	AA	86	G	C6-N1	-5.23	1.35	1.39
53	BA	1744	A	C6-N1	-5.23	1.31	1.35
53	BA	1964	G	C2-N2	-5.23	1.29	1.34
53	BA	2870	C	N3-C4	-5.23	1.30	1.33
53	BA	1	G	C2-N2	-5.23	1.29	1.34
21	AA	570	G	C6-N1	-5.23	1.35	1.39
53	BA	85	G	N1-C2	-5.23	1.33	1.37
53	BA	1139	G	C2-N2	-5.23	1.29	1.34
53	BA	1920	C	N3-C4	-5.23	1.30	1.33
53	BA	685	A	C6-N6	-5.23	1.29	1.33
53	BA	2303	G	C2-N2	-5.23	1.29	1.34
53	BA	1752	C	C4-N4	-5.22	1.29	1.33
53	BA	2052	A	C5-C4	-5.22	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	2606	C	C4-N4	-5.22	1.29	1.33
21	AA	1399	C	C4-N4	-5.22	1.29	1.33
53	BA	402	A	C5-C4	-5.22	1.35	1.38
53	BA	1279	G	N1-C2	-5.22	1.33	1.37
53	BA	1969	A	C6-N1	-5.22	1.31	1.35
53	BA	2535	G	C2-N2	-5.22	1.29	1.34
53	BA	1002	G	C6-N1	-5.22	1.35	1.39
53	BA	183	C	C4-N4	-5.22	1.29	1.33
53	BA	891	G	N1-C2	-5.22	1.33	1.37
53	BA	2397	G	C2-N2	-5.22	1.29	1.34
21	AA	830	G	C2-N2	-5.21	1.29	1.34
21	AA	1407	C	N3-C4	-5.21	1.30	1.33
53	BA	1509	A	C6-N1	-5.21	1.31	1.35
53	BA	1625	C	C4-N4	-5.21	1.29	1.33
53	BA	394	C	C4-N4	-5.21	1.29	1.33
22	A1	35	A	C6-N1	-5.21	1.31	1.35
53	BA	495	G	C2-N2	-5.21	1.29	1.34
21	AA	81	A	C6-N1	-5.21	1.31	1.35
21	AA	232	G	C2-N2	-5.21	1.29	1.34
21	AA	75	G	C6-N1	-5.21	1.35	1.39
21	AA	242	G	N1-C2	-5.21	1.33	1.37
21	AA	766	A	C6-N1	-5.21	1.31	1.35
23	A2	82	A	C5-C4	-5.21	1.35	1.38
53	BA	2727	A	C5-C4	-5.21	1.35	1.38
21	AA	47	C	C4-N4	-5.21	1.29	1.33
53	BA	380	G	C2-N2	-5.21	1.29	1.34
21	AA	382	A	C6-N1	-5.21	1.31	1.35
53	BA	430	A	C6-N1	-5.21	1.31	1.35
53	BA	1737	G	C2-N2	-5.21	1.29	1.34
53	BA	2612	C	C4-N4	-5.21	1.29	1.33
54	BB	37	C	N3-C4	-5.21	1.30	1.33
53	BA	1297	C	C4-N4	-5.20	1.29	1.33
21	AA	944	G	C2-N2	-5.20	1.29	1.34
53	BA	1210	G	C6-N1	-5.20	1.35	1.39
53	BA	262	A	C6-N1	-5.20	1.31	1.35
53	BA	1300	G	C6-N1	-5.20	1.35	1.39
53	BA	1639	C	C4-N4	-5.20	1.29	1.33
21	AA	958	A	C5-C4	-5.20	1.35	1.38
53	BA	1288	G	C6-N1	-5.20	1.35	1.39
53	BA	1727	C	N3-C4	-5.20	1.30	1.33
21	AA	1365	G	N1-C2	-5.20	1.33	1.37
53	BA	471	A	C6-N1	-5.20	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	1271	G	C6-N1	-5.20	1.35	1.39
53	BA	2879	A	C5-C4	-5.20	1.35	1.38
21	AA	33	A	C6-N1	-5.19	1.31	1.35
53	BA	2046	G	C2-N2	-5.19	1.29	1.34
53	BA	1537	G	C2-N2	-5.19	1.29	1.34
53	BA	1707	G	C2-N2	-5.19	1.29	1.34
21	AA	847	G	C2-N2	-5.19	1.29	1.34
21	AA	962	C	C4-N4	-5.19	1.29	1.33
53	BA	2082	A	C6-N1	-5.19	1.31	1.35
53	BA	1748	C	N3-C4	-5.19	1.30	1.33
53	BA	1906	G	C2-N2	-5.19	1.29	1.34
21	AA	732	C	C4-N4	-5.18	1.29	1.33
53	BA	57	C	C4-N4	-5.18	1.29	1.33
53	BA	623	C	C4-N4	-5.18	1.29	1.33
21	AA	974	A	C5-C4	-5.18	1.35	1.38
53	BA	629	G	C2-N2	-5.18	1.29	1.34
53	BA	950	G	C2-N2	-5.18	1.29	1.34
21	AA	887	G	N1-C2	-5.18	1.33	1.37
21	AA	1006	G	C6-N1	-5.18	1.35	1.39
53	BA	997	G	C6-N1	-5.18	1.35	1.39
21	AA	260	G	C2-N2	-5.18	1.29	1.34
21	AA	767	A	C5-C4	-5.18	1.35	1.38
53	BA	2626	C	N3-C4	-5.18	1.30	1.33
21	AA	888	G	C2-N2	-5.18	1.29	1.34
53	BA	250	G	C2-N2	-5.18	1.29	1.34
53	BA	1628	G	N1-C2	-5.18	1.33	1.37
21	AA	1311	A	C5-C4	-5.18	1.35	1.38
53	BA	417	C	C4-N4	-5.18	1.29	1.33
53	BA	1616	A	C6-N1	-5.18	1.31	1.35
53	BA	2140	G	C2-N2	-5.18	1.29	1.34
53	BA	2469	A	C5-C4	-5.18	1.35	1.38
53	BA	572	A	C6-N1	-5.17	1.31	1.35
53	BA	1526	C	C4-N4	-5.17	1.29	1.33
53	BA	1824	G	C2-N2	-5.17	1.29	1.34
53	BA	2069	G	C2-N2	-5.17	1.29	1.34
53	BA	2417	C	C4-N4	-5.17	1.29	1.33
21	AA	999	C	C4-N4	-5.17	1.29	1.33
53	BA	164	C	N3-C4	-5.17	1.30	1.33
53	BA	2036	C	N3-C4	-5.17	1.30	1.33
53	BA	2201	G	O3'-P	-5.17	1.54	1.61
53	BA	2550	G	C2-N2	-5.17	1.29	1.34
21	AA	64	G	C2-N2	-5.17	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	628	G	C2-N2	-5.17	1.29	1.34
21	AA	1515	G	C2-N2	-5.17	1.29	1.34
53	BA	643	A	C6-N1	-5.16	1.31	1.35
53	BA	1669	A	C5-C4	-5.16	1.35	1.38
53	BA	1760	C	C4-N4	-5.16	1.29	1.33
21	AA	172	A	C6-N1	-5.16	1.31	1.35
21	AA	550	G	N1-C2	-5.16	1.33	1.37
21	AA	1260	G	C6-N1	-5.16	1.35	1.39
53	BA	331	C	N3-C4	-5.16	1.30	1.33
53	BA	485	C	C4-N4	-5.16	1.29	1.33
53	BA	798	G	C2-N2	-5.16	1.29	1.34
53	BA	1828	G	C2-N2	-5.16	1.29	1.34
53	BA	2556	C	N3-C4	-5.16	1.30	1.33
53	BA	2793	C	C4-N4	-5.16	1.29	1.33
21	AA	810	C	C4-N4	-5.16	1.29	1.33
21	AA	1047	G	N1-C2	-5.16	1.33	1.37
53	BA	1655	A	C6-N1	-5.16	1.31	1.35
53	BA	1028	A	C5-C4	-5.15	1.35	1.38
53	BA	1216	G	C2-N2	-5.15	1.29	1.34
21	AA	278	G	C2-N2	-5.15	1.29	1.34
21	AA	694	A	C6-N6	-5.15	1.29	1.33
22	A1	39	G	C2-N2	-5.15	1.29	1.34
53	BA	407	G	C2-N2	-5.15	1.29	1.34
53	BA	928	A	C6-N1	-5.15	1.31	1.35
53	BA	2115	G	C2-N2	-5.15	1.29	1.34
21	AA	305	G	C2-N2	-5.15	1.29	1.34
53	BA	274	C	C4-N4	-5.15	1.29	1.33
53	BA	2682	A	C5-C4	-5.15	1.35	1.38
22	A1	44	G	C2-N2	-5.15	1.29	1.34
21	AA	1373	G	C2-N2	-5.15	1.29	1.34
53	BA	41	C	C4-N4	-5.15	1.29	1.33
53	BA	1001	A	N9-C4	-5.15	1.34	1.37
53	BA	2487	G	C6-N1	-5.15	1.35	1.39
21	AA	563	A	C6-N6	-5.15	1.29	1.33
21	AA	1208	C	C4-N4	-5.15	1.29	1.33
53	BA	899	A	C6-N1	-5.15	1.31	1.35
21	AA	1198	G	C2-N2	-5.14	1.29	1.34
53	BA	400	G	N1-C2	-5.14	1.33	1.37
53	BA	806	C	N3-C4	-5.14	1.30	1.33
53	BA	1278	C	N3-C4	-5.14	1.30	1.33
53	BA	1423	G	C6-N1	-5.14	1.35	1.39
53	BA	1721	G	C6-N1	-5.14	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	61	C	C4-N4	-5.14	1.29	1.33
53	BA	1028	A	C6-N6	-5.14	1.29	1.33
53	BA	1577	C	N3-C4	-5.14	1.30	1.33
53	BA	2088	A	C5-C4	-5.14	1.35	1.38
21	AA	1510	C	C4-N4	-5.14	1.29	1.33
53	BA	379	G	C6-N1	-5.14	1.35	1.39
53	BA	939	G	C2-N2	-5.14	1.29	1.34
53	BA	833	A	C6-N1	-5.14	1.31	1.35
53	BA	875	G	C2-N2	-5.14	1.29	1.34
21	AA	1089	G	C2-N2	-5.14	1.29	1.34
53	BA	132	G	C2-N2	-5.14	1.29	1.34
53	BA	1327	A	C6-N1	-5.14	1.31	1.35
21	AA	696	A	C6-N1	-5.13	1.31	1.35
21	AA	450	G	C2-N2	-5.13	1.29	1.34
21	AA	1318	A	C6-N1	-5.13	1.31	1.35
53	BA	740	C	C4-N4	-5.13	1.29	1.33
53	BA	1631	G	C2-N2	-5.13	1.29	1.34
53	BA	843	G	C2-N2	-5.13	1.29	1.34
53	BA	537	G	C2-N2	-5.13	1.29	1.34
53	BA	628	G	C6-N1	-5.13	1.35	1.39
53	BA	2578	G	N1-C2	-5.13	1.33	1.37
53	BA	2610	C	C4-N4	-5.13	1.29	1.33
21	AA	974	A	C6-N6	-5.13	1.29	1.33
21	AA	1204	A	C6-N1	-5.13	1.31	1.35
53	BA	673	C	C4-N4	-5.13	1.29	1.33
53	BA	2247	A	C6-N1	-5.13	1.31	1.35
53	BA	691	C	C4-N4	-5.12	1.29	1.33
53	BA	708	G	C6-N1	-5.12	1.35	1.39
53	BA	885	C	N3-C4	-5.12	1.30	1.33
21	AA	910	C	N3-C4	-5.12	1.30	1.33
53	BA	2883	A	C6-N1	-5.12	1.31	1.35
21	AA	1317	C	C4-N4	-5.12	1.29	1.33
53	BA	2304	G	C6-N1	-5.12	1.35	1.39
21	AA	79	G	C2-N2	-5.12	1.29	1.34
21	AA	554	A	C6-N1	-5.12	1.31	1.35
53	BA	2674	G	C6-N1	-5.12	1.35	1.39
21	AA	716	A	C6-N1	-5.12	1.31	1.35
21	AA	945	G	C2-N2	-5.12	1.29	1.34
53	BA	2742	G	C2-N2	-5.12	1.29	1.34
53	BA	2446	G	N1-C2	-5.11	1.33	1.37
53	BA	401	A	C5-C4	-5.11	1.35	1.38
53	BA	587	C	N3-C4	-5.11	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	726	C	C4-N4	-5.11	1.29	1.33
53	BA	22	C	N3-C4	-5.11	1.30	1.33
53	BA	1749	A	C5-C4	-5.11	1.35	1.38
53	BA	678	C	C4-N4	-5.11	1.29	1.33
21	AA	241	G	N1-C2	-5.11	1.33	1.37
53	BA	2421	G	C2-N2	-5.11	1.29	1.34
53	BA	2803	G	C2-N2	-5.11	1.29	1.34
53	BA	2879	A	C6-N6	-5.11	1.29	1.33
53	BA	729	G	N1-C2	-5.11	1.33	1.37
53	BA	1126	A	C5-C4	-5.10	1.35	1.38
53	BA	1236	G	C6-N1	-5.10	1.35	1.39
53	BA	1525	A	C6-N1	-5.10	1.31	1.35
53	BA	2509	G	C6-N1	-5.10	1.35	1.39
53	BA	1640	A	C5-C4	-5.10	1.35	1.38
53	BA	127	A	C6-N1	-5.10	1.31	1.35
53	BA	866	A	C6-N6	-5.10	1.29	1.33
53	BA	1612	C	C4-N4	-5.10	1.29	1.33
53	BA	2673	G	C2-N2	-5.10	1.29	1.34
21	AA	148	G	C2-N2	-5.10	1.29	1.34
21	AA	295	C	N3-C4	-5.10	1.30	1.33
53	BA	2658	C	C4-N4	-5.10	1.29	1.33
54	BB	36	C	C4-N4	-5.10	1.29	1.33
53	BA	1665	A	C6-N1	-5.10	1.31	1.35
53	BA	1895	C	C4-N4	-5.10	1.29	1.33
53	BA	1116	G	C6-N1	-5.09	1.35	1.39
53	BA	393	C	N3-C4	-5.09	1.30	1.33
53	BA	241	A	C6-N1	-5.09	1.31	1.35
53	BA	1907	G	C6-N1	-5.09	1.35	1.39
53	BA	1980	G	C2-N2	-5.09	1.29	1.34
53	BA	1674	G	C2-N2	-5.09	1.29	1.34
53	BA	1715	G	C6-N1	-5.09	1.35	1.39
21	AA	771	G	C2-N2	-5.09	1.29	1.34
53	BA	279	A	C6-N6	-5.09	1.29	1.33
21	AA	513	C	C4-N4	-5.09	1.29	1.33
21	AA	1013	G	C2-N2	-5.09	1.29	1.34
21	AA	1333	A	C5-C4	-5.09	1.35	1.38
53	BA	1244	A	C6-N6	-5.09	1.29	1.33
21	AA	184	G	N1-C2	-5.08	1.33	1.37
53	BA	1420	A	C6-N1	-5.08	1.31	1.35
53	BA	819	A	C5-C4	-5.08	1.35	1.38
53	BA	1192	G	N1-C2	-5.08	1.33	1.37
53	BA	2339	C	N3-C4	-5.08	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1196	A	C6-N6	-5.08	1.29	1.33
53	BA	1324	G	C2-N2	-5.08	1.29	1.34
53	BA	2168	G	C2-N2	-5.08	1.29	1.34
21	AA	160	A	C6-N1	-5.08	1.31	1.35
21	AA	1268	G	C2-N2	-5.08	1.29	1.34
21	AA	175	C	C4-N4	-5.08	1.29	1.33
53	BA	1703	G	C2-N2	-5.08	1.29	1.34
53	BA	2895	G	C6-N1	-5.08	1.35	1.39
21	AA	284	C	N3-C4	-5.08	1.30	1.33
53	BA	1783	A	C6-N1	-5.08	1.31	1.35
21	AA	144	G	N1-C2	-5.07	1.33	1.37
53	BA	508	A	C5-C4	-5.07	1.35	1.38
53	BA	1175	A	C5-C4	-5.07	1.35	1.38
21	AA	77	A	C6-N6	-5.07	1.29	1.33
21	AA	1397	C	C4-N4	-5.07	1.29	1.33
53	BA	2138	G	C2-N2	-5.07	1.29	1.34
21	AA	259	G	C2-N2	-5.07	1.29	1.34
21	AA	584	G	C2-N2	-5.07	1.29	1.34
53	BA	371	A	C5-C4	-5.07	1.35	1.38
53	BA	2483	C	N3-C4	-5.07	1.30	1.33
53	BA	2902	C	N3-C4	-5.07	1.30	1.33
21	AA	1289	A	C6-N1	-5.07	1.32	1.35
53	BA	1999	C	N3-C4	-5.07	1.30	1.33
54	BB	81	G	O3'-P	-5.07	1.55	1.61
21	AA	839	C	C4-N4	-5.07	1.29	1.33
21	AA	1514	G	C6-N1	-5.07	1.36	1.39
22	A1	48	C	N3-C4	-5.07	1.30	1.33
53	BA	1511	G	C6-N1	-5.07	1.36	1.39
53	BA	1710	G	N1-C2	-5.07	1.33	1.37
53	BA	2638	G	N1-C2	-5.07	1.33	1.37
53	BA	1595	C	N3-C4	-5.06	1.30	1.33
53	BA	1958	C	C4-N4	-5.06	1.29	1.33
53	BA	1985	C	C4-N4	-5.06	1.29	1.33
53	BA	1171	G	C2-N2	-5.06	1.29	1.34
53	BA	1332	G	C2-N2	-5.06	1.29	1.34
53	BA	1686	C	C4-N4	-5.06	1.29	1.33
53	BA	2417	C	N3-C4	-5.06	1.30	1.33
53	BA	2478	A	C5-C4	-5.06	1.35	1.38
53	BA	2495	G	N1-C2	-5.06	1.33	1.37
53	BA	368	A	C6-N1	-5.06	1.32	1.35
53	BA	624	C	C4-N4	-5.06	1.29	1.33
53	BA	996	A	C6-N1	-5.06	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	43	G	C6-N1	-5.06	1.36	1.39
53	BA	47	C	C4-N4	-5.06	1.29	1.33
53	BA	1136	G	C6-N1	-5.06	1.36	1.39
53	BA	1637	A	C6-N1	-5.06	1.32	1.35
21	AA	505	G	N1-C2	-5.06	1.33	1.37
21	AA	574	A	C6-N6	-5.06	1.29	1.33
21	AA	742	G	C2-N2	-5.06	1.29	1.34
21	AA	1370	G	C2-N2	-5.06	1.29	1.34
21	AA	192	A	C6-N1	-5.05	1.32	1.35
21	AA	1273	C	C4-N4	-5.05	1.29	1.33
53	BA	2631	G	C2-N2	-5.05	1.29	1.34
21	AA	152	A	C6-N6	-5.05	1.29	1.33
53	BA	2333	A	C5-C4	-5.05	1.35	1.38
21	AA	1337	G	C2-N2	-5.05	1.29	1.34
53	BA	672	C	C4-N4	-5.05	1.29	1.33
53	BA	776	G	C2-N2	-5.05	1.29	1.34
54	BB	68	C	C4-N4	-5.05	1.29	1.33
21	AA	1379	G	C2-N2	-5.04	1.29	1.34
53	BA	637	A	C5-C4	-5.04	1.35	1.38
21	AA	200	G	N1-C2	-5.04	1.33	1.37
21	AA	1210	C	N3-C4	-5.04	1.30	1.33
53	BA	559	G	C2-N2	-5.04	1.29	1.34
53	BA	1261	C	C4-N4	-5.04	1.29	1.33
53	BA	2813	A	C5-C4	-5.04	1.35	1.38
21	AA	301	G	C2-N2	-5.04	1.29	1.34
53	BA	175	G	N1-C2	-5.04	1.33	1.37
53	BA	785	G	C2-N2	-5.04	1.29	1.34
53	BA	380	G	N1-C2	-5.04	1.33	1.37
53	BA	1597	A	C5-C4	-5.04	1.35	1.38
53	BA	2444	G	C6-N1	-5.04	1.36	1.39
53	BA	1315	C	N3-C4	-5.04	1.30	1.33
21	AA	396	C	C4-N4	-5.03	1.29	1.33
21	AA	1036	A	C6-N1	-5.03	1.32	1.35
53	BA	757	G	C2-N2	-5.03	1.29	1.34
53	BA	1790	C	N3-C4	-5.03	1.30	1.33
21	AA	849	G	C6-N1	-5.03	1.36	1.39
53	BA	194	G	C6-N1	-5.03	1.36	1.39
53	BA	1808	A	C6-N1	-5.03	1.32	1.35
54	BB	44	G	N1-C2	-5.03	1.33	1.37
21	AA	1312	G	N1-C2	-5.03	1.33	1.37
53	BA	1669	A	C6-N6	-5.03	1.29	1.33
53	BA	2047	C	C4-N4	-5.03	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	2854	G	N1-C2	-5.03	1.33	1.37
21	AA	90	C	C4-N4	-5.03	1.29	1.33
21	AA	1452	C	N3-C4	-5.03	1.30	1.33
21	AA	124	C	C4-N4	-5.03	1.29	1.33
21	AA	1239	A	C6-N1	-5.03	1.32	1.35
53	BA	1598	A	C6-N1	-5.03	1.32	1.35
21	AA	824	G	C2-N2	-5.03	1.29	1.34
21	AA	153	C	N3-C4	-5.02	1.30	1.33
21	AA	1305	G	N1-C2	-5.02	1.33	1.37
53	BA	1125	G	C6-N1	-5.02	1.36	1.39
21	AA	351	G	C6-N1	-5.02	1.36	1.39
53	BA	344	A	C5-C4	-5.02	1.35	1.38
53	BA	1387	A	C6-N1	-5.02	1.32	1.35
21	AA	1305	G	C2-N2	-5.02	1.29	1.34
53	BA	147	C	C4-N4	-5.02	1.29	1.33
53	BA	743	A	C6-N1	-5.02	1.32	1.35
53	BA	2425	A	C5-C4	-5.02	1.35	1.38
22	A1	9	A	C6-N1	-5.02	1.32	1.35
53	BA	880	G	C6-N1	-5.02	1.36	1.39
53	BA	1337	G	N1-C2	-5.02	1.33	1.37
53	BA	424	G	C2-N2	-5.01	1.29	1.34
53	BA	2242	G	C6-N1	-5.01	1.36	1.39
21	AA	285	C	N3-C4	-5.01	1.30	1.33
53	BA	1500	G	C6-N1	-5.01	1.36	1.39
53	BA	2006	C	C4-C5	-5.01	1.39	1.43
54	BB	63	C	C4-N4	-5.01	1.29	1.33
53	BA	705	A	C6-N1	-5.01	1.32	1.35
53	BA	924	G	N1-C2	-5.01	1.33	1.37
53	BA	988	A	C6-N1	-5.01	1.32	1.35
53	BA	1287	A	C6-N6	-5.01	1.29	1.33
53	BA	1290	C	N3-C4	-5.01	1.30	1.33
53	BA	502	A	C6-N1	-5.01	1.32	1.35
53	BA	2574	G	C2-N2	-5.01	1.29	1.34
21	AA	27	G	C6-N1	-5.01	1.36	1.39
53	BA	198	C	C4-N4	-5.01	1.29	1.33
21	AA	1045	C	N3-C4	-5.00	1.30	1.33
53	BA	1138	G	N1-C2	-5.00	1.33	1.37
21	AA	901	A	C5-C4	-5.00	1.35	1.38
53	BA	15	G	C2-N2	-5.00	1.29	1.34
53	BA	838	C	N3-C4	-5.00	1.30	1.33
53	BA	2505	G	N1-C2	-5.00	1.33	1.37
21	AA	69	G	C6-N1	-5.00	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	94	A	C6-N6	-5.00	1.29	1.33
53	BA	2472	G	C2-N2	-5.00	1.29	1.34
53	BA	2828	G	C2-N2	-5.00	1.29	1.34

All (8093) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	323	C	O4'-C1'-N1	14.98	120.18	108.20
53	BA	1932	A	N1-C6-N6	-13.12	110.73	118.60
53	BA	800	A	N1-C6-N6	-12.78	110.93	118.60
21	AA	1502	A	N1-C6-N6	-12.44	111.14	118.60
53	BA	219	A	N1-C6-N6	-12.42	111.15	118.60
53	BA	344	A	N1-C6-N6	-12.40	111.16	118.60
22	A1	59	U	O4'-C1'-N1	12.38	118.10	108.20
21	AA	1257	A	N1-C6-N6	-12.30	111.22	118.60
53	BA	2889	C	O4'-C1'-N1	12.30	118.04	108.20
53	BA	1791	A	N1-C6-N6	-12.28	111.23	118.60
53	BA	2388	A	N1-C6-N6	-12.21	111.27	118.60
53	BA	1591	A	N1-C6-N6	-12.21	111.27	118.60
53	BA	2212	A	N1-C6-N6	-12.17	111.30	118.60
53	BA	1469	A	N1-C6-N6	-12.11	111.34	118.60
54	BB	37	C	O4'-C1'-N1	12.11	117.88	108.20
53	BA	752	A	O4'-C1'-N9	12.02	117.82	108.20
21	AA	195	A	N1-C6-N6	-12.01	111.39	118.60
21	AA	1534	A	N1-C6-N6	-11.96	111.43	118.60
53	BA	38	A	N1-C6-N6	-11.85	111.49	118.60
53	BA	165	A	N1-C6-N6	-11.85	111.49	118.60
53	BA	1969	A	N1-C6-N6	-11.84	111.49	118.60
21	AA	621	A	N1-C6-N6	-11.84	111.50	118.60
18	AS	2	ARG	NE-CZ-NH2	11.84	126.22	120.30
53	BA	2033	A	N1-C6-N6	-11.82	111.51	118.60
53	BA	412	A	N1-C6-N6	-11.81	111.51	118.60
53	BA	743	A	N1-C6-N6	-11.81	111.51	118.60
21	AA	383	A	N1-C6-N6	-11.80	111.52	118.60
53	BA	2516	A	N1-C6-N6	-11.79	111.53	118.60
53	BA	1453	A	N1-C6-N6	-11.73	111.56	118.60
21	AA	865	A	N1-C6-N6	-11.67	111.60	118.60
53	BA	103	A	N1-C6-N6	-11.65	111.61	118.60
21	AA	194	C	N1-C2-O2	11.59	125.85	118.90
21	AA	190	A	N1-C6-N6	-11.57	111.66	118.60
21	AA	1360	A	N1-C6-N6	-11.56	111.67	118.60
21	AA	630	A	N1-C6-N6	-11.52	111.69	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	886	A	N1-C6-N6	-11.50	111.70	118.60
53	BA	1890	A	N1-C6-N6	-11.50	111.70	118.60
53	BA	2448	A	N1-C6-N6	-11.50	111.70	118.60
21	AA	1311	A	N1-C6-N6	-11.48	111.71	118.60
53	BA	1275	A	N1-C6-N6	-11.48	111.71	118.60
21	AA	1288	A	N1-C6-N6	-11.48	111.71	118.60
53	BA	2882	A	N1-C6-N6	-11.47	111.72	118.60
21	AA	389	A	N1-C6-N6	-11.47	111.72	118.60
21	AA	468	A	N1-C6-N6	-11.46	111.73	118.60
53	BA	514	A	N1-C6-N6	-11.44	111.73	118.60
21	AA	602	A	N1-C6-N6	-11.44	111.74	118.60
53	BA	1569	A	N1-C6-N6	-11.44	111.74	118.60
53	BA	119	A	N1-C6-N6	-11.44	111.74	118.60
53	BA	199	A	N1-C6-N6	-11.42	111.75	118.60
21	AA	937	A	N1-C6-N6	-11.40	111.76	118.60
21	AA	499	A	N1-C6-N6	-11.38	111.77	118.60
53	BA	666	A	N1-C6-N6	-11.37	111.78	118.60
53	BA	2009	A	N1-C6-N6	-11.37	111.78	118.60
21	AA	635	A	N1-C6-N6	-11.34	111.80	118.60
53	BA	2278	A	N1-C6-N6	-11.33	111.80	118.60
53	BA	2600	A	N1-C6-N6	-11.33	111.80	118.60
53	BA	415	A	N1-C6-N6	-11.32	111.81	118.60
53	BA	1010	A	N1-C6-N6	-11.30	111.82	118.60
53	BA	2406	A	N1-C6-N6	-11.30	111.82	118.60
53	BA	1319	C	O4'-C1'-N1	11.29	117.23	108.20
21	AA	1021	A	N1-C6-N6	-11.26	111.84	118.60
53	BA	2147	A	N1-C6-N6	-11.25	111.85	118.60
53	BA	984	A	N1-C6-N6	-11.22	111.87	118.60
21	AA	1213	A	N1-C6-N6	-11.21	111.87	118.60
54	BB	50	A	N1-C6-N6	-11.21	111.87	118.60
53	BA	2425	A	N1-C6-N6	-11.21	111.88	118.60
53	BA	1274	A	N1-C6-N6	-11.21	111.88	118.60
53	BA	1378	A	N1-C6-N6	-11.21	111.88	118.60
53	BA	849	A	N1-C6-N6	-11.20	111.88	118.60
21	AA	1394	A	N1-C6-N6	-11.19	111.89	118.60
53	BA	479	A	N1-C6-N6	-11.18	111.89	118.60
21	AA	610	U	O4'-C1'-N1	11.16	117.13	108.20
53	BA	56	A	N1-C6-N6	-11.15	111.91	118.60
24	BC	237	ARG	NE-CZ-NH1	11.15	125.88	120.30
53	BA	508	A	N1-C6-N6	-11.14	111.91	118.60
21	AA	1030	U	O4'-C1'-N1	11.14	117.11	108.20
53	BA	705	A	N1-C6-N6	-11.14	111.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1086	A	N1-C6-N6	-11.13	111.92	118.60
21	AA	831	A	N1-C6-N6	-11.12	111.93	118.60
53	BA	1854	A	N1-C6-N6	-11.11	111.93	118.60
53	BA	2418	A	N1-C6-N6	-11.10	111.94	118.60
53	BA	2476	A	N1-C6-N6	-11.08	111.95	118.60
21	AA	1046	A	N1-C6-N6	-11.07	111.96	118.60
21	AA	1363	A	N1-C6-N6	-11.06	111.96	118.60
21	AA	1531	A	N1-C6-N6	-11.06	111.97	118.60
53	BA	2033	A	O4'-C1'-N9	11.02	117.02	108.20
53	BA	2266	A	N1-C6-N6	-11.02	111.99	118.60
21	AA	814	A	N1-C6-N6	-11.01	111.99	118.60
53	BA	668	A	N1-C6-N6	-11.01	111.99	118.60
21	AA	320	A	N1-C6-N6	-11.00	112.00	118.60
31	BJ	27	ARG	NE-CZ-NH1	10.98	125.79	120.30
54	BB	94	A	N1-C6-N6	-10.98	112.01	118.60
21	AA	718	A	N1-C6-N6	-10.97	112.02	118.60
21	AA	8	A	N1-C6-N6	-10.96	112.02	118.60
53	BA	574	A	N1-C6-N6	-10.96	112.03	118.60
53	BA	127	A	N1-C6-N6	-10.95	112.03	118.60
53	BA	1241	A	N1-C6-N6	-10.94	112.03	118.60
53	BA	2589	A	N1-C6-N6	-10.94	112.03	118.60
21	AA	182	A	N1-C6-N6	-10.91	112.06	118.60
21	AA	1067	A	N1-C6-N6	-10.91	112.06	118.60
53	BA	1640	A	N1-C6-N6	-10.89	112.06	118.60
21	AA	994	A	N1-C6-N6	-10.89	112.07	118.60
53	BA	2590	A	N1-C6-N6	-10.88	112.07	118.60
53	BA	160	A	N1-C6-N6	-10.83	112.10	118.60
53	BA	2478	A	N1-C6-N6	-10.82	112.11	118.60
53	BA	784	G	O4'-C1'-N9	10.82	116.85	108.20
21	AA	152	A	N1-C6-N6	-10.81	112.11	118.60
53	BA	2675	A	N1-C6-N6	-10.80	112.12	118.60
21	AA	282	A	N1-C6-N6	-10.80	112.12	118.60
54	BB	45	A	N1-C6-N6	-10.80	112.12	118.60
21	AA	520	A	N1-C6-N6	-10.79	112.12	118.60
53	BA	751	A	N1-C6-N6	-10.79	112.12	118.60
21	AA	1093	A	N1-C6-N6	-10.79	112.13	118.60
53	BA	1940	U	O4'-C1'-N1	10.79	116.83	108.20
53	BA	1387	A	N1-C6-N6	-10.78	112.13	118.60
53	BA	2639	A	N1-C6-N6	-10.77	112.14	118.60
4	AE	28	ARG	NE-CZ-NH1	10.76	125.68	120.30
53	BA	572	A	N1-C6-N6	-10.75	112.15	118.60
21	AA	706	A	N1-C6-N6	-10.74	112.15	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	554	A	N1-C6-N6	-10.73	112.16	118.60
53	BA	1690	A	N1-C6-N6	-10.72	112.17	118.60
53	BA	1590	A	N1-C6-N6	-10.71	112.17	118.60
21	AA	151	A	N1-C6-N6	-10.69	112.19	118.60
21	AA	1251	A	N1-C6-N6	-10.69	112.19	118.60
53	BA	1103	A	N1-C6-N6	-10.68	112.19	118.60
53	BA	497	A	N1-C6-N6	-10.65	112.21	118.60
53	BA	1021	A	N1-C6-N6	-10.65	112.21	118.60
21	AA	194	C	N3-C2-O2	-10.64	114.45	121.90
54	BB	37	C	N3-C2-O2	-10.64	114.45	121.90
53	BA	49	A	O4'-C1'-N9	10.63	116.70	108.20
53	BA	1535	A	N1-C6-N6	-10.63	112.22	118.60
53	BA	1717	A	N1-C6-N6	-10.62	112.23	118.60
21	AA	28	A	N1-C6-N6	-10.62	112.23	118.60
21	AA	452	A	N1-C6-N6	-10.61	112.23	118.60
53	BA	2352	A	N1-C6-N6	-10.61	112.23	118.60
53	BA	453	A	N1-C6-N6	-10.60	112.24	118.60
53	BA	1308	A	N1-C6-N6	-10.60	112.24	118.60
21	AA	179	A	N1-C6-N6	-10.59	112.25	118.60
53	BA	1889	A	N1-C6-N6	-10.59	112.25	118.60
11	AL	93	ARG	NE-CZ-NH1	10.58	125.59	120.30
21	AA	704	A	N1-C6-N6	-10.58	112.25	118.60
40	BS	99	ARG	NE-CZ-NH1	10.56	125.58	120.30
21	AA	155	A	N1-C6-N6	-10.55	112.27	118.60
24	BC	181	ARG	NE-CZ-NH1	10.55	125.57	120.30
23	A2	82	A	N1-C6-N6	-10.54	112.27	118.60
21	AA	968	A	N1-C6-N6	-10.54	112.28	118.60
53	BA	2126	A	O4'-C1'-N9	10.54	116.63	108.20
53	BA	1937	A	N1-C6-N6	-10.53	112.28	118.60
53	BA	422	A	N1-C6-N6	-10.53	112.28	118.60
53	BA	300	A	N1-C6-N6	-10.52	112.29	118.60
21	AA	1227	A	N1-C6-N6	-10.52	112.29	118.60
53	BA	1496	A	N1-C6-N6	-10.52	112.29	118.60
53	BA	1265	A	N1-C6-N6	-10.49	112.30	118.60
53	BA	1505	A	N1-C6-N6	-10.49	112.30	118.60
21	AA	1004	A	N1-C6-N6	-10.49	112.31	118.60
21	AA	749	A	N1-C6-N6	-10.49	112.31	118.60
50	B2	34	ARG	NE-CZ-NH1	10.48	125.54	120.30
53	BA	941	A	N1-C6-N6	-10.47	112.31	118.60
21	AA	183	C	O4'-C1'-N1	10.47	116.58	108.20
53	BA	2727	A	N1-C6-N6	-10.47	112.32	118.60
21	AA	223	A	N1-C6-N6	-10.46	112.32	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2071	A	N1-C6-N6	-10.46	112.32	118.60
21	AA	629	A	N1-C6-N6	-10.46	112.32	118.60
21	AA	98	A	N1-C6-N6	-10.45	112.33	118.60
53	BA	556	A	N1-C6-N6	-10.41	112.36	118.60
53	BA	2850	A	N1-C6-N6	-10.41	112.36	118.60
53	BA	2336	A	N1-C6-N6	-10.40	112.36	118.60
53	BA	988	A	N1-C6-N6	-10.39	112.37	118.60
53	BA	1384	A	N1-C6-N6	-10.38	112.37	118.60
53	BA	1610	A	O4'-C1'-N9	10.38	116.50	108.20
13	AN	63	ARG	NE-CZ-NH1	10.36	125.48	120.30
21	AA	915	A	N1-C6-N6	-10.36	112.39	118.60
53	BA	181	A	N1-C6-N6	-10.35	112.39	118.60
53	BA	1755	A	N1-C6-N6	-10.35	112.39	118.60
53	BA	401	A	N1-C6-N6	-10.34	112.39	118.60
53	BA	44	A	N1-C6-N6	-10.32	112.41	118.60
39	BR	80	ARG	NE-CZ-NH2	10.32	125.46	120.30
53	BA	322	A	N1-C6-N6	-10.31	112.41	118.60
21	AA	1499	A	N1-C6-N6	-10.31	112.42	118.60
21	AA	777	A	N1-C6-N6	-10.29	112.42	118.60
21	AA	1433	A	N1-C6-N6	-10.29	112.43	118.60
53	BA	2700	A	N1-C6-N6	-10.29	112.43	118.60
27	BF	124	ARG	NE-CZ-NH2	10.28	125.44	120.30
11	AL	82	ARG	NE-CZ-NH1	10.28	125.44	120.30
21	AA	1430	A	N1-C6-N6	-10.27	112.44	118.60
53	BA	449	A	N1-C6-N6	-10.26	112.44	118.60
53	BA	1253	A	N1-C6-N6	-10.26	112.44	118.60
53	BA	2738	A	N1-C6-N6	-10.26	112.44	118.60
3	AD	127	ARG	NE-CZ-NH1	10.26	125.43	120.30
23	A2	79	A	N1-C6-N6	-10.26	112.45	118.60
21	AA	329	A	N1-C6-N6	-10.25	112.45	118.60
53	BA	2564	A	N1-C6-N6	-10.25	112.45	118.60
53	BA	2679	A	N1-C6-N6	-10.25	112.45	118.60
36	BO	81	ARG	NE-CZ-NH1	10.25	125.42	120.30
21	AA	1171	A	N1-C6-N6	-10.23	112.46	118.60
53	BA	1046	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	1508	A	N1-C6-N6	-10.22	112.47	118.60
53	BA	2468	A	N1-C6-N6	-10.22	112.47	118.60
21	AA	1287	A	N1-C6-N6	-10.22	112.47	118.60
53	BA	2665	A	N1-C6-N6	-10.22	112.47	118.60
53	BA	1805	A	N1-C6-N6	-10.21	112.47	118.60
53	BA	1439	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	2542	A	N1-C6-N6	-10.20	112.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1858	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	223	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	677	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	753	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	222	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	1392	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	685	A	C5-C6-N1	10.19	122.80	117.70
53	BA	928	A	N1-C6-N6	-10.19	112.49	118.60
53	BA	1586	A	N1-C6-N6	-10.16	112.50	118.60
53	BA	1783	A	N1-C6-N6	-10.14	112.51	118.60
21	AA	415	A	N1-C6-N6	-10.14	112.51	118.60
21	AA	802	A	N1-C6-N6	-10.14	112.52	118.60
21	AA	199	A	N1-C6-N6	-10.14	112.52	118.60
21	AA	1042	A	N1-C6-N6	-10.14	112.52	118.60
53	BA	1759	A	N1-C6-N6	-10.13	112.52	118.60
21	AA	965	U	O4'-C1'-N1	10.12	116.30	108.20
53	BA	1580	A	N1-C6-N6	-10.13	112.53	118.60
53	BA	156	A	N1-C6-N6	-10.12	112.53	118.60
53	BA	63	A	N1-C6-N6	-10.12	112.53	118.60
21	AA	1256	A	N1-C6-N6	-10.12	112.53	118.60
53	BA	2135	A	N1-C6-N6	-10.12	112.53	118.60
53	BA	1583	A	N1-C6-N6	-10.11	112.54	118.60
22	A1	73	A	N1-C6-N6	-10.10	112.54	118.60
53	BA	1901	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	560	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	864	A	N1-C6-N6	-10.10	112.54	118.60
53	BA	111	A	N1-C6-N6	-10.09	112.54	118.60
53	BA	2003	A	N1-C6-N6	-10.08	112.55	118.60
53	BA	2750	A	N1-C6-N6	-10.08	112.55	118.60
53	BA	207	A	N1-C6-N6	-10.08	112.55	118.60
53	BA	1912	A	N1-C6-N6	-10.08	112.55	118.60
53	BA	2211	A	N1-C6-N6	-10.07	112.56	118.60
53	BA	2117	A	N1-C6-N6	-10.06	112.56	118.60
21	AA	532	A	N1-C6-N6	-10.06	112.56	118.60
34	BM	55	ARG	NE-CZ-NH1	10.06	125.33	120.30
53	BA	1287	A	N1-C6-N6	-10.05	112.57	118.60
53	BA	721	A	N1-C6-N6	-10.05	112.57	118.60
21	AA	1289	A	N1-C6-N6	-10.05	112.57	118.60
53	BA	2267	A	N1-C6-N6	-10.04	112.58	118.60
53	BA	1205	A	N1-C6-N6	-10.04	112.58	118.60
2	AC	171	ARG	NE-CZ-NH1	10.03	125.31	120.30
21	AA	1169	A	N1-C6-N6	-10.03	112.58	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1230	A	N1-C6-N6	-10.03	112.58	118.60
21	AA	1396	A	N1-C6-N6	-10.02	112.59	118.60
53	BA	614	A	O4'-C1'-N9	10.02	116.22	108.20
53	BA	1606	C	N3-C2-O2	-10.02	114.89	121.90
21	AA	573	A	N1-C6-N6	-10.02	112.59	118.60
53	BA	866	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	1332	A	N1-C6-N6	-10.01	112.60	118.60
24	BC	269	ARG	NE-CZ-NH1	10.01	125.30	120.30
53	BA	1451	C	N3-C2-O2	-10.01	114.90	121.90
53	BA	83	A	N1-C6-N6	-10.00	112.60	118.60
53	BA	2820	A	N1-C6-N6	-9.99	112.60	118.60
53	BA	1469	A	C5-C6-N1	9.99	122.69	117.70
53	BA	2309	A	N1-C6-N6	-9.99	112.61	118.60
53	BA	1454	C	N3-C2-O2	-9.98	114.92	121.90
21	AA	681	A	N1-C6-N6	-9.98	112.61	118.60
53	BA	21	A	N1-C6-N6	-9.97	112.61	118.60
53	BA	1502	A	N1-C6-N6	-9.97	112.61	118.60
53	BA	2461	A	N1-C6-N6	-9.97	112.61	118.60
53	BA	197	A	N1-C6-N6	-9.97	112.62	118.60
21	AA	1204	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	572	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	10	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	642	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	493	A	O4'-C1'-N9	9.94	116.15	108.20
53	BA	504	A	N1-C6-N6	-9.94	112.63	118.60
53	BA	1603	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	815	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	33	A	N1-C6-N6	-9.93	112.64	118.60
53	BA	547	A	N1-C6-N6	-9.93	112.64	118.60
21	AA	648	A	N1-C6-N6	-9.92	112.65	118.60
21	AA	1346	A	N1-C6-N6	-9.92	112.65	118.60
53	BA	457	A	N1-C6-N6	-9.92	112.64	118.60
31	BJ	116	ARG	NE-CZ-NH1	9.92	125.26	120.30
21	AA	306	A	N1-C6-N6	-9.91	112.65	118.60
53	BA	685	A	N1-C6-N6	-9.91	112.65	118.60
53	BA	1383	A	N1-C6-N6	-9.91	112.66	118.60
21	AA	675	A	N1-C6-N6	-9.91	112.66	118.60
53	BA	1952	A	N1-C6-N6	-9.90	112.66	118.60
21	AA	71	A	N1-C6-N6	-9.90	112.66	118.60
8	AI	11	ARG	NE-CZ-NH1	9.90	125.25	120.30
53	BA	793	A	N1-C6-N6	-9.89	112.66	118.60
21	AA	974	A	C5-C6-N1	9.89	122.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	101	A	N1-C6-N6	-9.88	112.67	118.60
21	AA	1252	A	C5-C6-N1	9.88	122.64	117.70
21	AA	1216	A	N1-C6-N6	-9.87	112.68	118.60
53	BA	2333	A	N1-C6-N6	-9.87	112.68	118.60
53	BA	311	A	N1-C6-N6	-9.87	112.68	118.60
21	AA	983	A	N1-C6-N6	-9.87	112.68	118.60
53	BA	1794	A	N1-C6-N6	-9.87	112.68	118.60
53	BA	1749	A	N1-C6-N6	-9.86	112.69	118.60
46	BY	29	ARG	NE-CZ-NH2	9.86	125.23	120.30
53	BA	310	A	N1-C6-N6	-9.86	112.69	118.60
53	BA	1489	C	O4'-C1'-N1	9.86	116.08	108.20
54	BB	73	A	N1-C6-N6	-9.86	112.69	118.60
53	BA	781	A	N1-C6-N6	-9.85	112.69	118.60
6	AG	110	ARG	NE-CZ-NH1	9.85	125.22	120.30
53	BA	173	A	N1-C6-N6	-9.84	112.69	118.60
21	AA	1408	A	N1-C6-N6	-9.84	112.70	118.60
53	BA	2052	A	N1-C6-N6	-9.84	112.70	118.60
53	BA	1353	A	N1-C6-N6	-9.83	112.70	118.60
9	AJ	37	ARG	NE-CZ-NH1	9.82	125.21	120.30
21	AA	1191	A	N1-C6-N6	-9.82	112.70	118.60
21	AA	65	A	N1-C6-N6	-9.82	112.71	118.60
53	BA	439	A	N1-C6-N6	-9.82	112.71	118.60
53	BA	910	A	N1-C6-N6	-9.82	112.71	118.60
53	BA	2052	A	C5-C6-N1	9.82	122.61	117.70
53	BA	348	A	N1-C6-N6	-9.81	112.71	118.60
42	BU	93	ARG	NE-CZ-NH1	9.81	125.20	120.30
54	BB	15	A	N1-C6-N6	-9.81	112.72	118.60
50	B2	28	ARG	NE-CZ-NH1	9.80	125.20	120.30
53	BA	279	A	C5-C6-N1	9.80	122.60	117.70
54	BB	46	A	N1-C6-N6	-9.79	112.72	118.60
21	AA	1492	A	N1-C6-N6	-9.79	112.73	118.60
21	AA	1398	A	N1-C6-N6	-9.78	112.73	118.60
53	BA	1754	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	767	A	N1-C6-N6	-9.77	112.74	118.60
54	BB	29	A	N1-C6-N6	-9.76	112.75	118.60
53	BA	1966	A	N1-C6-N6	-9.75	112.75	118.60
54	BB	34	A	N1-C6-N6	-9.74	112.75	118.60
53	BA	896	A	O4'-C1'-N9	9.74	115.99	108.20
53	BA	1960	A	N1-C6-N6	-9.74	112.76	118.60
53	BA	1301	A	N1-C6-N6	-9.73	112.76	118.60
53	BA	716	A	N1-C6-N6	-9.73	112.76	118.60
53	BA	582	A	N1-C6-N6	-9.72	112.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	465	A	N1-C6-N6	-9.71	112.77	118.60
21	AA	195	A	C5-C6-N1	9.71	122.56	117.70
21	AA	609	A	N1-C6-N6	-9.71	112.78	118.60
53	BA	2705	A	N1-C6-N6	-9.71	112.78	118.60
21	AA	766	A	N1-C6-N6	-9.70	112.78	118.60
21	AA	574	A	N1-C6-N6	-9.70	112.78	118.60
53	BA	1525	A	N1-C6-N6	-9.69	112.78	118.60
53	BA	2097	A	N1-C6-N6	-9.69	112.78	118.60
21	AA	1214	C	N1-C2-O2	9.68	124.71	118.90
53	BA	2114	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	1362	A	N1-C6-N6	-9.68	112.79	118.60
50	B2	33	ARG	NE-CZ-NH1	9.68	125.14	120.30
53	BA	1549	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	1214	C	N3-C2-O2	-9.68	115.13	121.90
53	BA	502	A	N1-C6-N6	-9.67	112.80	118.60
53	BA	231	A	N1-C6-N6	-9.66	112.80	118.60
21	AA	563	A	C5-C6-N1	9.66	122.53	117.70
31	BJ	13	ARG	NE-CZ-NH1	9.66	125.13	120.30
53	BA	734	A	N1-C6-N6	-9.66	112.80	118.60
53	BA	2734	A	N1-C6-N6	-9.66	112.80	118.60
53	BA	1395	A	N1-C6-N6	-9.66	112.81	118.60
22	A1	16	C	N3-C2-O2	-9.65	115.14	121.90
21	AA	559	A	O4'-C1'-N9	9.65	115.92	108.20
21	AA	1333	A	N1-C6-N6	-9.65	112.81	118.60
53	BA	655	A	N1-C6-N6	-9.65	112.81	118.60
53	BA	1032	A	N1-C6-N6	-9.64	112.82	118.60
21	AA	1428	A	N1-C6-N6	-9.64	112.82	118.60
53	BA	1067	A	N1-C6-N6	-9.64	112.82	118.60
53	BA	2298	A	N1-C6-N6	-9.64	112.82	118.60
5	AF	86	ARG	NE-CZ-NH1	9.62	125.11	120.30
53	BA	1913	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	448	A	N1-C6-N6	-9.62	112.83	118.60
27	BF	79	ARG	NE-CZ-NH2	9.62	125.11	120.30
53	BA	2598	A	N1-C6-N6	-9.62	112.83	118.60
53	BA	73	A	N1-C6-N6	-9.61	112.83	118.60
53	BA	94	A	N1-C6-N6	-9.61	112.83	118.60
53	BA	2092	U	O4'-C1'-N1	9.61	115.89	108.20
53	BA	279	A	N1-C6-N6	-9.61	112.83	118.60
22	A1	35	A	N1-C6-N6	-9.61	112.84	118.60
53	BA	2518	A	N1-C6-N6	-9.61	112.84	118.60
53	BA	2800	A	N1-C6-N6	-9.60	112.84	118.60
53	BA	2682	A	C5-C6-N1	9.60	122.50	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	368	A	N1-C6-N6	-9.60	112.84	118.60
21	AA	1055	A	N1-C6-N6	-9.60	112.84	118.60
53	BA	1321	A	N1-C6-N6	-9.60	112.84	118.60
53	BA	981	A	N1-C6-N6	-9.60	112.84	118.60
53	BA	2654	A	N1-C6-N6	-9.60	112.84	118.60
53	BA	53	A	N1-C6-N6	-9.59	112.85	118.60
53	BA	1866	A	N1-C6-N6	-9.58	112.85	118.60
8	AI	84	ARG	NE-CZ-NH1	9.57	125.09	120.30
53	BA	1829	A	N1-C6-N6	-9.57	112.86	118.60
53	BA	1302	A	N1-C6-N6	-9.56	112.86	118.60
43	BV	21	ARG	NE-CZ-NH1	9.56	125.08	120.30
53	BA	294	A	N1-C6-N6	-9.56	112.86	118.60
21	AA	754	C	N3-C2-O2	-9.56	115.21	121.90
53	BA	963	U	O4'-C1'-N1	9.56	115.85	108.20
53	BA	1322	A	C5-C6-N1	9.56	122.48	117.70
53	BA	2176	A	N1-C6-N6	-9.56	112.87	118.60
53	BA	1981	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	344	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	1306	A	N1-C6-N6	-9.55	112.87	118.60
53	BA	905	A	N1-C6-N6	-9.55	112.87	118.60
53	BA	2711	A	N1-C6-N6	-9.55	112.87	118.60
53	BA	1677	A	N1-C6-N6	-9.55	112.87	118.60
53	BA	825	A	N1-C6-N6	-9.55	112.87	118.60
53	BA	2825	G	O4'-C1'-N9	9.55	115.84	108.20
53	BA	1848	A	N1-C6-N6	-9.54	112.88	118.60
21	AA	139	A	N1-C6-N6	-9.54	112.88	118.60
53	BA	1453	A	C5-C6-N1	9.54	122.47	117.70
53	BA	2468	A	C5-C6-N1	9.54	122.47	117.70
21	AA	974	A	N1-C6-N6	-9.54	112.88	118.60
53	BA	2425	A	C5-C6-N1	9.53	122.47	117.70
53	BA	1637	A	N1-C6-N6	-9.53	112.88	118.60
21	AA	968	A	C5-C6-N1	9.52	122.46	117.70
21	AA	345	C	N3-C2-O2	-9.52	115.24	121.90
21	AA	1150	A	N1-C6-N6	-9.52	112.89	118.60
14	AO	53	ARG	NE-CZ-NH1	9.51	125.06	120.30
43	BV	93	ARG	NE-CZ-NH1	9.51	125.06	120.30
53	BA	1347	A	N1-C6-N6	-9.50	112.90	118.60
21	AA	246	A	N1-C6-N6	-9.50	112.90	118.60
21	AA	435	A	N1-C6-N6	-9.49	112.90	118.60
21	AA	535	A	N1-C6-N6	-9.49	112.91	118.60
4	AE	19	ARG	NE-CZ-NH1	9.48	125.04	120.30
53	BA	2503	A	N1-C6-N6	-9.48	112.91	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	BQ	69	ARG	NE-CZ-NH1	9.47	125.04	120.30
21	AA	860	A	N1-C6-N6	-9.47	112.92	118.60
53	BA	1156	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	72	A	N1-C6-N6	-9.46	112.92	118.60
22	A1	58	A	N1-C6-N6	-9.46	112.92	118.60
53	BA	2169	A	N1-C6-N6	-9.46	112.92	118.60
53	BA	1579	A	N1-C6-N6	-9.46	112.93	118.60
21	AA	665	A	N1-C6-N6	-9.45	112.93	118.60
53	BA	1853	A	N1-C6-N6	-9.45	112.93	118.60
53	BA	1789	A	N1-C6-N6	-9.45	112.93	118.60
53	BA	613	A	N1-C6-N6	-9.45	112.93	118.60
53	BA	1758	U	O4'-C1'-N1	9.45	115.76	108.20
53	BA	943	A	N1-C6-N6	-9.44	112.93	118.60
53	BA	2886	A	N1-C6-N6	-9.44	112.93	118.60
21	AA	1493	A	C5-C6-N1	9.44	122.42	117.70
53	BA	1679	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	441	A	N1-C6-N6	-9.44	112.94	118.60
53	BA	2453	A	N1-C6-N6	-9.43	112.94	118.60
23	A2	91	A	N1-C6-N6	-9.43	112.94	118.60
49	B1	5	ARG	NE-CZ-NH1	9.43	125.01	120.30
53	BA	1268	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	327	A	N1-C6-N6	-9.43	112.94	118.60
53	BA	152	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	995	C	N3-C2-O2	-9.41	115.31	121.90
14	AO	16	ARG	NE-CZ-NH1	9.40	125.00	120.30
21	AA	845	A	N1-C6-N6	-9.40	112.96	118.60
53	BA	1528	A	N1-C6-N6	-9.40	112.96	118.60
53	BA	637	A	N1-C6-N6	-9.39	112.96	118.60
21	AA	53	A	N1-C6-N6	-9.39	112.96	118.60
53	BA	960	A	N1-C6-N6	-9.39	112.97	118.60
53	BA	2134	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	1500	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	181	A	N1-C6-N6	-9.38	112.97	118.60
22	A1	6	A	N1-C6-N6	-9.38	112.97	118.60
53	BA	466	A	N1-C6-N6	-9.38	112.97	118.60
53	BA	2328	A	N1-C6-N6	-9.38	112.97	118.60
53	BA	1048	A	N1-C6-N6	-9.38	112.97	118.60
53	BA	2560	A	N1-C6-N6	-9.38	112.97	118.60
21	AA	1368	A	N1-C6-N6	-9.38	112.97	118.60
53	BA	592	A	N1-C6-N6	-9.38	112.97	118.60
53	BA	2009	A	C5-C6-N1	9.37	122.38	117.70
53	BA	2634	A	N1-C6-N6	-9.36	112.98	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BN	45	ARG	NE-CZ-NH1	9.36	124.98	120.30
21	AA	130	A	N1-C6-N6	-9.36	112.98	118.60
21	AA	1440	U	O4'-C1'-N1	9.36	115.69	108.20
53	BA	1780	A	N1-C6-N6	-9.36	112.99	118.60
53	BA	270	A	N1-C6-N6	-9.35	112.99	118.60
53	BA	2058	A	N1-C6-N6	-9.34	112.99	118.60
21	AA	189	A	N1-C6-N6	-9.34	113.00	118.60
53	BA	2748	A	N1-C6-N6	-9.34	113.00	118.60
53	BA	280	U	O4'-C1'-N1	9.34	115.67	108.20
53	BA	412	A	C4-C5-C6	-9.34	112.33	117.00
53	BA	1427	A	N1-C6-N6	-9.34	113.00	118.60
21	AA	1465	A	N1-C6-N6	-9.33	113.00	118.60
21	AA	1377	A	N1-C6-N6	-9.32	113.01	118.60
53	BA	727	A	N1-C6-N6	-9.32	113.01	118.60
4	AE	68	ARG	NE-CZ-NH1	9.32	124.96	120.30
21	AA	1298	U	O4'-C1'-N1	9.32	115.65	108.20
53	BA	6	A	N1-C6-N6	-9.31	113.01	118.60
53	BA	945	A	N1-C6-N6	-9.31	113.01	118.60
53	BA	213	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	663	A	N1-C6-N6	-9.31	113.02	118.60
53	BA	1095	A	N1-C6-N6	-9.30	113.02	118.60
53	BA	1385	A	N1-C6-N6	-9.30	113.02	118.60
21	AA	81	A	N1-C6-N6	-9.29	113.02	118.60
53	BA	456	C	N3-C2-O2	-9.29	115.39	121.90
53	BA	1596	A	N1-C6-N6	-9.29	113.02	118.60
53	BA	2879	A	N1-C6-N6	-9.29	113.02	118.60
21	AA	794	A	N1-C6-N6	-9.29	113.02	118.60
53	BA	1885	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	129	A	N1-C6-N6	-9.29	113.03	118.60
53	BA	472	A	N1-C6-N6	-9.29	113.03	118.60
53	BA	2327	A	N1-C6-N6	-9.29	113.03	118.60
53	BA	2183	A	N1-C6-N6	-9.28	113.03	118.60
21	AA	92	U	O4'-C1'-N1	9.28	115.62	108.20
21	AA	1257	A	C5-C6-N1	9.28	122.34	117.70
53	BA	204	A	N1-C6-N6	-9.28	113.03	118.60
53	BA	1937	A	C4-C5-C6	-9.28	112.36	117.00
53	BA	1998	A	N1-C6-N6	-9.28	113.03	118.60
53	BA	706	A	C5-C6-N1	9.27	122.34	117.70
21	AA	279	A	N1-C6-N6	-9.27	113.04	118.60
21	AA	1111	A	N1-C6-N6	-9.27	113.04	118.60
53	BA	654	A	N1-C6-N6	-9.27	113.04	118.60
21	AA	1155	A	N1-C6-N6	-9.27	113.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	420	C	N3-C2-O2	-9.27	115.41	121.90
53	BA	1366	A	N1-C6-N6	-9.26	113.04	118.60
21	AA	174	A	C5-C6-N1	9.26	122.33	117.70
53	BA	742	A	N1-C6-N6	-9.26	113.05	118.60
53	BA	861	A	N1-C6-N6	-9.25	113.05	118.60
10	AK	36	ARG	NE-CZ-NH1	9.25	124.92	120.30
53	BA	94	A	C5-C6-N1	9.25	122.33	117.70
53	BA	1762	A	N1-C6-N6	-9.25	113.05	118.60
21	AA	149	A	N1-C6-N6	-9.24	113.05	118.60
53	BA	345	A	N1-C6-N6	-9.24	113.06	118.60
53	BA	1669	A	C5-C6-N1	9.24	122.32	117.70
53	BA	2358	A	N1-C6-N6	-9.24	113.06	118.60
53	BA	1640	A	C5-C6-N1	9.24	122.32	117.70
53	BA	1652	A	N1-C6-N6	-9.24	113.06	118.60
13	AN	81	ARG	NE-CZ-NH1	9.23	124.92	120.30
53	BA	982	C	N3-C2-O2	-9.23	115.44	121.90
53	BA	802	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	167	A	N1-C6-N6	-9.22	113.07	118.60
53	BA	402	A	C5-C6-N1	9.21	122.31	117.70
21	AA	152	A	C5-C6-N1	9.21	122.31	117.70
21	AA	574	A	C5-C6-N1	9.21	122.31	117.70
21	AA	192	A	N1-C6-N6	-9.21	113.08	118.60
21	AA	1246	A	N1-C6-N6	-9.21	113.07	118.60
53	BA	71	A	N1-C6-N6	-9.21	113.08	118.60
43	BV	9	ARG	NE-CZ-NH1	9.20	124.90	120.30
54	BB	37	C	N1-C2-O2	9.21	124.42	118.90
53	BA	2033	A	O3'-P-O5'	-9.20	86.51	104.00
22	A1	74	C	O4'-C1'-N1	9.20	115.56	108.20
53	BA	2372	U	O4'-C1'-N1	9.20	115.56	108.20
21	AA	408	A	N1-C6-N6	-9.20	113.08	118.60
53	BA	833	A	N1-C6-N6	-9.20	113.08	118.60
53	BA	1618	A	N1-C6-N6	-9.19	113.08	118.60
13	AN	9	ARG	NE-CZ-NH1	9.19	124.89	120.30
32	BK	30	ARG	NE-CZ-NH1	9.19	124.89	120.30
21	AA	1398	A	C5-C6-N1	9.18	122.29	117.70
53	BA	340	A	C5-C6-N1	9.18	122.29	117.70
53	BA	1320	C	N3-C2-O2	-9.18	115.47	121.90
53	BA	1050	A	N1-C6-N6	-9.18	113.09	118.60
21	AA	1101	A	N1-C6-N6	-9.17	113.10	118.60
54	BB	36	C	N3-C2-O2	-9.17	115.48	121.90
21	AA	1004	A	C5-C6-N1	9.17	122.29	117.70
53	BA	2602	A	N1-C6-N6	-9.17	113.10	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	50	A	C5-C6-N1	9.17	122.28	117.70
21	AA	510	A	N1-C6-N6	-9.17	113.10	118.60
53	BA	2821	A	N1-C6-N6	-9.16	113.10	118.60
21	AA	1102	A	N1-C6-N6	-9.16	113.10	118.60
21	AA	901	A	N1-C6-N6	-9.15	113.11	118.60
53	BA	192	C	N3-C2-O2	-9.15	115.49	121.90
53	BA	1977	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	958	A	C5-C6-N1	9.15	122.27	117.70
53	BA	195	A	C5-C6-N1	9.14	122.27	117.70
53	BA	508	A	C5-C6-N1	9.14	122.27	117.70
53	BA	637	A	C5-C6-N1	9.14	122.27	117.70
53	BA	1745	A	C5-C6-N1	9.14	122.27	117.70
53	BA	1815	A	N1-C6-N6	-9.14	113.11	118.60
53	BA	456	C	N1-C2-O2	9.14	124.38	118.90
22	A1	16	C	O4'-C1'-N1	9.13	115.51	108.20
35	BN	17	ARG	NE-CZ-NH1	9.13	124.87	120.30
53	BA	2033	A	C5-C6-N1	9.13	122.27	117.70
26	BE	114	ARG	NE-CZ-NH1	9.13	124.86	120.30
53	BA	821	A	N1-C6-N6	-9.12	113.12	118.60
21	AA	716	A	N1-C6-N6	-9.12	113.13	118.60
53	BA	2482	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	1110	A	N1-C6-N6	-9.12	113.13	118.60
28	BG	54	ARG	NE-CZ-NH1	9.12	124.86	120.30
53	BA	689	A	N1-C6-N6	-9.11	113.13	118.60
53	BA	1322	A	N1-C6-N6	-9.12	113.13	118.60
53	BA	2829	A	N1-C6-N6	-9.11	113.13	118.60
21	AA	1036	A	N1-C6-N6	-9.11	113.13	118.60
53	BA	453	A	C5-C6-N1	9.11	122.25	117.70
21	AA	975	A	N1-C6-N6	-9.11	113.14	118.60
21	AA	1067	A	C5-C6-N1	9.11	122.25	117.70
31	BJ	69	ARG	NE-CZ-NH1	9.10	124.85	120.30
53	BA	160	A	C5-C6-N1	9.10	122.25	117.70
53	BA	146	A	N1-C6-N6	-9.10	113.14	118.60
53	BA	699	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	563	A	N1-C6-N6	-9.10	113.14	118.60
53	BA	1420	A	O4'-C1'-N9	9.10	115.48	108.20
21	AA	575	G	O4'-C1'-N9	9.10	115.48	108.20
53	BA	925	A	N1-C6-N6	-9.10	113.14	118.60
53	BA	1489	C	N3-C2-O2	-9.10	115.53	121.90
53	BA	2158	A	C5-C6-N1	9.10	122.25	117.70
53	BA	2407	A	N1-C6-N6	-9.09	113.14	118.60
53	BA	420	C	N1-C2-O2	9.09	124.35	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2369	A	N1-C6-N6	-9.09	113.15	118.60
21	AA	977	A	N1-C6-N6	-9.08	113.15	118.60
53	BA	706	A	N1-C6-N6	-9.08	113.15	118.60
55	B5	122	ARG	NE-CZ-NH1	9.08	124.84	120.30
21	AA	495	A	N1-C6-N6	-9.08	113.15	118.60
53	BA	933	A	N1-C6-N6	-9.08	113.15	118.60
21	AA	238	A	N1-C6-N6	-9.07	113.16	118.60
53	BA	221	A	C5-C6-N1	9.07	122.24	117.70
15	AP	70	ARG	NE-CZ-NH1	9.07	124.84	120.30
21	AA	371	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	1163	A	N1-C6-N6	-9.07	113.16	118.60
53	BA	990	A	C1'-O4'-C4'	-9.07	102.65	109.90
53	BA	1890	A	C5-C6-N1	9.07	122.23	117.70
21	AA	174	A	N1-C6-N6	-9.06	113.16	118.60
53	BA	2835	A	N1-C6-N6	-9.06	113.16	118.60
53	BA	195	A	N1-C6-N6	-9.06	113.17	118.60
53	BA	2321	U	O4'-C1'-N1	9.05	115.44	108.20
15	AP	8	ARG	NE-CZ-NH1	9.05	124.83	120.30
53	BA	613	A	C5-C6-N1	9.05	122.23	117.70
53	BA	2753	A	N1-C6-N6	-9.05	113.17	118.60
35	BN	69	ARG	NE-CZ-NH1	9.04	124.82	120.30
33	BL	21	ARG	NE-CZ-NH2	9.04	124.82	120.30
53	BA	371	A	C5-C6-N1	9.04	122.22	117.70
53	BA	1610	A	C5-C6-N1	9.04	122.22	117.70
21	AA	338	A	C5-C6-N1	9.03	122.22	117.70
38	BQ	91	ARG	NE-CZ-NH1	9.03	124.82	120.30
53	BA	1126	A	C5-C6-N1	9.03	122.22	117.70
21	AA	1283	U	O4'-C1'-N1	9.03	115.42	108.20
21	AA	1434	A	N1-C6-N6	-9.03	113.19	118.60
53	BA	2005	A	C5-C6-N1	9.03	122.21	117.70
53	BA	2395	C	O4'-C1'-N1	9.02	115.42	108.20
21	AA	274	A	N1-C6-N6	-9.02	113.19	118.60
53	BA	1609	A	N1-C6-N6	-9.02	113.19	118.60
53	BA	1551	A	N1-C6-N6	-9.02	113.19	118.60
53	BA	2632	A	N1-C6-N6	-9.02	113.19	118.60
53	BA	947	A	N1-C6-N6	-9.01	113.19	118.60
21	AA	1250	A	N1-C6-N6	-9.01	113.19	118.60
53	BA	196	A	N1-C6-N6	-9.01	113.20	118.60
53	BA	346	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	1318	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	282	A	C5-C6-N1	9.00	122.20	117.70
53	BA	2886	A	C5-C6-N1	9.00	122.20	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2426	A	N1-C6-N6	-8.99	113.20	118.60
5	AF	38	ARG	NE-CZ-NH1	8.99	124.79	120.30
21	AA	782	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	373	A	C5-C6-N1	8.99	122.19	117.70
21	AA	1357	A	N1-C6-N6	-8.99	113.21	118.60
17	AR	72	ARG	NE-CZ-NH2	8.98	124.79	120.30
53	BA	1509	A	N1-C6-N6	-8.98	113.21	118.60
53	BA	1938	A	N1-C6-N6	-8.98	113.21	118.60
53	BA	2860	A	N1-C6-N6	-8.98	113.21	118.60
53	BA	1142	A	N1-C6-N6	-8.98	113.21	118.60
53	BA	2274	A	C5-C6-N1	8.98	122.19	117.70
53	BA	2071	A	C5-C6-N1	8.97	122.19	117.70
54	BB	104	A	N1-C6-N6	-8.97	113.22	118.60
53	BA	1669	A	N1-C6-N6	-8.97	113.22	118.60
53	BA	1928	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	547	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	1016	A	N1-C6-N6	-8.96	113.22	118.60
53	BA	52	A	N1-C6-N6	-8.96	113.22	118.60
53	BA	1301	A	C5-C6-N1	8.96	122.18	117.70
53	BA	1772	A	N1-C6-N6	-8.96	113.22	118.60
53	BA	2093	G	O4'-C1'-N9	8.96	115.37	108.20
22	A1	74	C	N3-C2-O2	-8.96	115.63	121.90
53	BA	982	C	N1-C2-O2	8.96	124.27	118.90
54	BB	66	A	C5-C6-N1	8.95	122.17	117.70
1	AB	224	ARG	NE-CZ-NH1	8.95	124.77	120.30
21	AA	1374	A	N1-C6-N6	-8.94	113.23	118.60
53	BA	1336	A	N1-C6-N6	-8.94	113.24	118.60
21	AA	1429	A	N1-C6-N6	-8.94	113.24	118.60
26	BE	162	ARG	NE-CZ-NH1	8.94	124.77	120.30
21	AA	72	A	C5-C6-N1	8.94	122.17	117.70
21	AA	767	A	C5-C6-N1	8.93	122.17	117.70
21	AA	1146	A	N1-C6-N6	-8.93	113.24	118.60
10	AK	92	ARG	NE-CZ-NH1	8.93	124.77	120.30
21	AA	607	A	N1-C6-N6	-8.93	113.24	118.60
21	AA	1180	A	N1-C6-N6	-8.93	113.24	118.60
25	BD	59	ARG	NE-CZ-NH1	8.93	124.77	120.30
8	AI	121	ARG	NE-CZ-NH1	8.93	124.77	120.30
53	BA	2051	A	N1-C6-N6	-8.93	113.24	118.60
53	BA	2070	A	N1-C6-N6	-8.93	113.24	118.60
53	BA	670	A	N1-C6-N6	-8.93	113.24	118.60
21	AA	900	A	N1-C6-N6	-8.93	113.25	118.60
53	BA	2101	A	N1-C6-N6	-8.93	113.25	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2879	A	C5-C6-N1	8.93	122.16	117.70
21	AA	533	A	N1-C6-N6	-8.92	113.25	118.60
25	BD	77	ARG	NE-CZ-NH1	8.92	124.76	120.30
53	BA	1616	A	N1-C6-N6	-8.92	113.25	118.60
53	BA	1434	A	O4'-C1'-N9	8.92	115.34	108.20
18	AS	77	ARG	NE-CZ-NH1	8.92	124.76	120.30
21	AA	819	A	N1-C6-N6	-8.91	113.25	118.60
21	AA	422	C	O4'-C1'-N1	8.90	115.32	108.20
53	BA	654	A	O4'-C1'-N9	8.90	115.32	108.20
21	AA	509	A	N1-C6-N6	-8.90	113.26	118.60
53	BA	323	C	N3-C2-O2	-8.90	115.67	121.90
53	BA	1978	A	N1-C6-N6	-8.89	113.26	118.60
21	AA	697	U	O4'-C1'-N1	8.89	115.31	108.20
53	BA	1133	A	N1-C6-N6	-8.89	113.27	118.60
53	BA	2377	A	N1-C6-N6	-8.89	113.27	118.60
53	BA	1048	A	C5-C6-N1	8.88	122.14	117.70
21	AA	152	A	C4-C5-C6	-8.88	112.56	117.00
8	AI	10	ARG	NE-CZ-NH1	8.88	124.74	120.30
21	AA	819	A	C5-C6-N1	8.88	122.14	117.70
53	BA	2317	A	N1-C6-N6	-8.88	113.27	118.60
53	BA	227	A	N1-C6-N6	-8.88	113.28	118.60
21	AA	1275	A	N1-C6-N6	-8.87	113.28	118.60
53	BA	1801	A	N1-C6-N6	-8.87	113.28	118.60
53	BA	2883	A	N1-C6-N6	-8.86	113.28	118.60
53	BA	2340	A	N1-C6-N6	-8.86	113.28	118.60
53	BA	103	A	C5-C6-N1	8.86	122.13	117.70
53	BA	1134	A	N1-C6-N6	-8.86	113.29	118.60
53	BA	1431	A	N1-C6-N6	-8.86	113.29	118.60
53	BA	781	A	C5-C6-N1	8.85	122.13	117.70
53	BA	626	A	N1-C6-N6	-8.85	113.29	118.60
54	BB	78	A	N1-C6-N6	-8.85	113.29	118.60
53	BA	631	A	C5-C6-N1	8.85	122.12	117.70
53	BA	2418	A	C4-C5-C6	-8.85	112.58	117.00
53	BA	1014	A	N1-C6-N6	-8.85	113.29	118.60
53	BA	2158	A	N1-C6-N6	-8.84	113.30	118.60
53	BA	2614	A	N1-C6-N6	-8.84	113.30	118.60
53	BA	1000	A	C5-C6-N1	8.84	122.12	117.70
53	BA	1204	A	N1-C6-N6	-8.84	113.30	118.60
53	BA	2889	C	N1-C2-O2	8.84	124.20	118.90
53	BA	89	A	N1-C6-N6	-8.83	113.30	118.60
53	BA	1439	A	O4'-C1'-N9	8.83	115.26	108.20
21	AA	1216	A	C5-C6-N1	8.82	122.11	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	BQ	49	ARG	NE-CZ-NH1	8.82	124.71	120.30
53	BA	845	A	N1-C6-N6	-8.82	113.31	118.60
53	BA	2657	A	N1-C6-N6	-8.82	113.31	118.60
11	AL	85	ARG	NE-CZ-NH1	8.82	124.71	120.30
53	BA	221	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	780	A	N1-C6-N6	-8.81	113.31	118.60
53	BA	633	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	179	A	C5-C6-N1	8.81	122.10	117.70
53	BA	1744	A	N1-C6-N6	-8.81	113.31	118.60
53	BA	1810	A	N1-C6-N6	-8.80	113.32	118.60
53	BA	1490	A	N1-C6-N6	-8.80	113.32	118.60
53	BA	1544	A	C5-C6-N1	8.80	122.10	117.70
21	AA	938	A	N1-C6-N6	-8.79	113.32	118.60
21	AA	98	A	C5-C6-N1	8.79	122.10	117.70
21	AA	466	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	1285	A	N1-C6-N6	-8.79	113.32	118.60
53	BA	783	A	N1-C6-N6	-8.79	113.32	118.60
22	A1	41	A	N1-C6-N6	-8.79	113.33	118.60
12	AM	92	ARG	NE-CZ-NH2	8.79	124.69	120.30
21	AA	1022	A	N1-C6-N6	-8.79	113.33	118.60
53	BA	2668	G	O4'-C1'-N9	8.79	115.23	108.20
21	AA	1377	A	C5-C6-N1	8.79	122.09	117.70
53	BA	1169	A	N1-C6-N6	-8.79	113.33	118.60
53	BA	2451	A	N1-C6-N6	-8.79	113.33	118.60
54	BB	58	A	C5-C6-N1	8.79	122.09	117.70
54	BB	109	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	382	A	N1-C6-N6	-8.79	113.33	118.60
53	BA	2433	A	N1-C6-N6	-8.79	113.33	118.60
53	BA	1287	A	C5-C6-N1	8.78	122.09	117.70
53	BA	2530	A	N1-C6-N6	-8.78	113.33	118.60
8	AI	94	ARG	NE-CZ-NH1	8.77	124.69	120.30
9	AJ	89	ARG	NE-CZ-NH1	8.77	124.68	120.30
21	AA	19	A	N1-C6-N6	-8.77	113.34	118.60
53	BA	2813	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	913	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	210	C	N3-C2-O2	-8.76	115.77	121.90
37	BP	100	ARG	NE-CZ-NH1	8.76	124.68	120.30
53	BA	2126	A	N1-C6-N6	-8.76	113.34	118.60
53	BA	2837	A	C4-C5-C6	-8.76	112.62	117.00
21	AA	174	A	C4-C5-C6	-8.76	112.62	117.00
53	BA	478	A	N1-C6-N6	-8.76	113.34	118.60
53	BA	2333	A	C5-C6-N1	8.76	122.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1031	C	N3-C2-O2	-8.76	115.77	121.90
53	BA	1039	A	N1-C6-N6	-8.76	113.35	118.60
21	AA	1311	A	C5-C6-N1	8.76	122.08	117.70
53	BA	1900	A	N1-C6-N6	-8.76	113.35	118.60
2	AC	10	ARG	NE-CZ-NH1	8.75	124.68	120.30
21	AA	1480	A	N1-C6-N6	-8.75	113.35	118.60
53	BA	920	A	C4-C5-C6	-8.75	112.62	117.00
53	BA	2108	A	N1-C6-N6	-8.75	113.35	118.60
53	BA	340	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	171	A	N1-C6-N6	-8.74	113.35	118.60
21	AA	330	C	N3-C2-O2	-8.74	115.78	121.90
21	AA	1093	A	C4-C5-C6	-8.74	112.63	117.00
53	BA	676	A	N1-C6-N6	-8.74	113.35	118.60
53	BA	980	A	N1-C6-N6	-8.74	113.35	118.60
53	BA	2518	A	C5-C6-N1	8.74	122.07	117.70
21	AA	190	A	C5-C6-N1	8.74	122.07	117.70
53	BA	2639	A	C5-C6-N1	8.74	122.07	117.70
53	BA	2721	A	N1-C6-N6	-8.74	113.36	118.60
53	BA	2733	A	N1-C6-N6	-8.74	113.36	118.60
21	AA	959	A	N1-C6-N6	-8.74	113.36	118.60
22	A1	60	C	N3-C2-O2	-8.74	115.78	121.90
53	BA	144	A	N1-C6-N6	-8.73	113.36	118.60
53	BA	449	A	C5-C6-N1	8.73	122.06	117.70
21	AA	949	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	1196	A	C5-C6-N1	8.73	122.06	117.70
53	BA	2666	C	O4'-C1'-N1	8.73	115.18	108.20
53	BA	1286	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	793	U	O4'-C1'-N1	8.72	115.18	108.20
53	BA	1265	A	C5-C6-N1	8.72	122.06	117.70
53	BA	1901	A	C4-C5-C6	-8.72	112.64	117.00
53	BA	73	A	C5-C6-N1	8.72	122.06	117.70
53	BA	344	A	C5-C6-N1	8.71	122.06	117.70
53	BA	1147	A	N1-C6-N6	-8.71	113.37	118.60
53	BA	2541	A	N1-C6-N6	-8.71	113.37	118.60
21	AA	1364	U	O4'-C1'-N1	8.71	115.17	108.20
53	BA	1635	A	N1-C6-N6	-8.71	113.37	118.60
53	BA	1730	C	N3-C2-O2	-8.71	115.80	121.90
53	BA	1579	A	C5-C6-N1	8.71	122.05	117.70
21	AA	199	A	C5-C6-N1	8.71	122.05	117.70
21	AA	648	A	C5-C6-N1	8.71	122.05	117.70
53	BA	2274	A	N1-C6-N6	-8.71	113.38	118.60
53	BA	2042	A	N1-C6-N6	-8.70	113.38	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2889	C	N3-C2-O2	-8.70	115.81	121.90
53	BA	1580	A	C4-C5-C6	-8.70	112.65	117.00
53	BA	2346	A	N1-C6-N6	-8.70	113.38	118.60
53	BA	2682	A	C4-C5-C6	-8.69	112.65	117.00
21	AA	901	A	C5-C6-N1	8.69	122.04	117.70
53	BA	608	A	C5-C6-N1	8.69	122.04	117.70
9	AJ	48	ARG	NE-CZ-NH2	8.68	124.64	120.30
53	BA	1080	A	N1-C6-N6	-8.68	113.39	118.60
53	BA	1073	A	C5-C6-N1	8.68	122.04	117.70
53	BA	2288	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	461	A	C5-C6-N1	8.68	122.04	117.70
53	BA	789	A	N1-C6-N6	-8.67	113.40	118.60
53	BA	1672	A	N1-C6-N6	-8.67	113.40	118.60
53	BA	2273	A	N1-C6-N6	-8.67	113.40	118.60
53	BA	1028	A	C5-C6-N1	8.66	122.03	117.70
38	BQ	27	ARG	NE-CZ-NH1	8.66	124.63	120.30
53	BA	94	A	C4-C5-C6	-8.66	112.67	117.00
53	BA	233	A	N1-C6-N6	-8.66	113.40	118.60
53	BA	44	A	C5-C6-N1	8.66	122.03	117.70
53	BA	1134	A	C5-C6-N1	8.66	122.03	117.70
53	BA	2170	A	N1-C6-N6	-8.66	113.41	118.60
53	BA	2761	A	N1-C6-N6	-8.66	113.41	118.60
53	BA	1609	A	C5-C6-N1	8.65	122.03	117.70
21	AA	205	A	N1-C6-N6	-8.65	113.41	118.60
40	BS	8	ARG	NE-CZ-NH1	8.65	124.62	120.30
53	BA	819	A	C5-C6-N1	8.65	122.03	117.70
21	AA	66	A	N1-C6-N6	-8.65	113.41	118.60
54	BB	39	A	C5-C6-N1	8.65	122.02	117.70
21	AA	1502	A	C5-C6-N1	8.64	122.02	117.70
53	BA	838	C	N3-C2-O2	-8.64	115.85	121.90
21	AA	958	A	N1-C6-N6	-8.64	113.42	118.60
53	BA	256	A	N1-C6-N6	-8.64	113.42	118.60
53	BA	546	U	O4'-C1'-N1	8.64	115.11	108.20
53	BA	1495	A	N1-C6-N6	-8.64	113.42	118.60
53	BA	2281	A	C5-C6-N1	8.64	122.02	117.70
8	AI	79	ARG	NE-CZ-NH1	8.63	124.62	120.30
41	BT	69	ARG	NE-CZ-NH1	8.63	124.62	120.30
53	BA	1937	A	C5-C6-N1	8.63	122.02	117.70
21	AA	59	A	N1-C6-N6	-8.63	113.42	118.60
53	BA	1700	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	412	A	N1-C6-N6	-8.62	113.42	118.60
21	AA	1396	A	C5-C6-N1	8.63	122.01	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1188	A	N1-C6-N6	-8.62	113.43	118.60
53	BA	49	A	N1-C6-N6	-8.62	113.42	118.60
53	BA	74	A	N1-C6-N6	-8.62	113.42	118.60
53	BA	973	A	N1-C6-N6	-8.63	113.42	118.60
24	BC	42	ARG	NE-CZ-NH2	8.62	124.61	120.30
38	BQ	50	ARG	NE-CZ-NH1	8.62	124.61	120.30
53	BA	866	A	C5-C6-N1	8.62	122.01	117.70
53	BA	1630	A	N1-C6-N6	-8.62	113.43	118.60
53	BA	825	A	C4-C5-C6	-8.62	112.69	117.00
6	AG	4	ARG	NE-CZ-NH2	8.62	124.61	120.30
53	BA	1285	A	N1-C6-N6	-8.61	113.43	118.60
21	AA	1022	A	C5-C6-N1	8.61	122.00	117.70
21	AA	1441	A	N1-C6-N6	-8.61	113.43	118.60
53	BA	2821	A	C5-C6-N1	8.61	122.00	117.70
21	AA	1012	A	N1-C6-N6	-8.61	113.44	118.60
53	BA	142	A	C5-C6-N1	8.61	122.00	117.70
53	BA	2062	A	C5-C6-N1	8.61	122.00	117.70
21	AA	270	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	694	A	C5-C6-N1	8.60	122.00	117.70
21	AA	1080	A	N1-C6-N6	-8.60	113.44	118.60
53	BA	1359	A	N1-C6-N6	-8.60	113.44	118.60
53	BA	1067	A	C5-C6-N1	8.60	122.00	117.70
21	AA	934	C	N3-C2-O2	-8.60	115.88	121.90
21	AA	197	A	C5-C6-N1	8.59	122.00	117.70
21	AA	1196	A	N1-C6-N6	-8.59	113.44	118.60
53	BA	845	A	C4-C5-C6	-8.59	112.70	117.00
21	AA	1238	A	N1-C6-N6	-8.59	113.44	118.60
53	BA	2406	A	C5-C6-N1	8.59	121.99	117.70
21	AA	964	A	N1-C6-N6	-8.59	113.45	118.60
53	BA	933	A	C5-C6-N1	8.59	121.99	117.70
53	BA	849	A	C5-C6-N1	8.58	121.99	117.70
53	BA	877	A	C5-C6-N1	8.58	121.99	117.70
53	BA	1916	A	N1-C6-N6	-8.58	113.45	118.60
21	AA	704	A	C5-C6-N1	8.58	121.99	117.70
12	AM	100	ARG	NE-CZ-NH1	8.57	124.59	120.30
53	BA	990	A	O4'-C1'-N9	8.57	115.06	108.20
21	AA	329	A	C5-C6-N1	8.57	121.98	117.70
21	AA	630	A	C5-C6-N1	8.57	121.99	117.70
21	AA	66	A	C5-C6-N1	8.57	121.98	117.70
53	BA	1545	A	N1-C6-N6	-8.57	113.46	118.60
53	BA	2800	A	C5-C6-N1	8.57	121.98	117.70
53	BA	2386	A	N1-C6-N6	-8.57	113.46	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BL	78	ARG	NE-CZ-NH1	8.56	124.58	120.30
53	BA	324	A	C5-C6-N1	8.56	121.98	117.70
53	BA	2376	A	N1-C6-N6	-8.56	113.46	118.60
53	BA	2749	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	461	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	1441	A	C4-C5-C6	-8.56	112.72	117.00
23	A2	82	A	C5-C6-N1	8.55	121.98	117.70
47	BZ	15	ARG	NE-CZ-NH1	8.55	124.58	120.30
53	BA	1061	U	O4'-C1'-N1	8.55	115.04	108.20
45	BX	49	ARG	NE-CZ-NH1	8.55	124.58	120.30
53	BA	983	A	N1-C6-N6	-8.55	113.47	118.60
53	BA	794	A	N1-C6-N6	-8.55	113.47	118.60
53	BA	2564	A	C5-C6-N1	8.55	121.97	117.70
8	AI	40	ARG	NE-CZ-NH1	8.54	124.57	120.30
21	AA	364	A	N1-C6-N6	-8.54	113.47	118.60
53	BA	2765	A	O4'-C1'-N9	8.54	115.03	108.20
11	AL	85	ARG	NE-CZ-NH2	-8.54	116.03	120.30
53	BA	909	A	C4-C5-C6	-8.54	112.73	117.00
21	AA	160	A	N1-C6-N6	-8.54	113.48	118.60
53	BA	563	A	N1-C6-N6	-8.54	113.48	118.60
21	AA	1176	A	N1-C6-N6	-8.53	113.48	118.60
23	A2	79	A	C5-C6-N1	8.54	121.97	117.70
21	AA	1110	A	C5-C6-N1	8.53	121.97	117.70
21	AA	459	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	1269	A	N1-C6-N6	-8.53	113.48	118.60
53	BA	1133	A	C5-C6-N1	8.53	121.97	117.70
53	BA	1175	A	C5-C6-N1	8.53	121.96	117.70
21	AA	1229	A	N1-C6-N6	-8.53	113.48	118.60
53	BA	2675	A	C5-C6-N1	8.53	121.96	117.70
54	BB	57	A	N1-C6-N6	-8.53	113.48	118.60
53	BA	222	A	C5-C6-N1	8.52	121.96	117.70
53	BA	1384	A	C5-C6-N1	8.52	121.96	117.70
54	BB	34	A	C4-C5-C6	-8.52	112.74	117.00
53	BA	1489	C	N1-C2-O2	8.52	124.01	118.90
21	AA	16	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	695	A	C5-C6-N1	8.52	121.96	117.70
53	BA	2547	A	C5-C6-N1	8.52	121.96	117.70
53	BA	1169	A	C4-C5-C6	-8.52	112.74	117.00
21	AA	1500	A	C5-C6-N1	8.51	121.95	117.70
53	BA	2104	C	N3-C2-O2	-8.51	115.94	121.90
53	BA	693	A	N1-C6-N6	-8.51	113.50	118.60
53	BA	1938	A	O4'-C1'-N9	8.51	115.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2395	C	N3-C2-O2	-8.51	115.95	121.90
21	AA	663	A	C5-C6-N1	8.50	121.95	117.70
2	AC	155	ARG	NE-CZ-NH1	8.50	124.55	120.30
53	BA	1096	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	815	A	C5-C6-N1	8.50	121.95	117.70
43	BV	19	ARG	NE-CZ-NH1	8.50	124.55	120.30
53	BA	126	A	O4'-C1'-N9	8.49	115.00	108.20
53	BA	750	A	N1-C6-N6	-8.49	113.50	118.60
53	BA	792	A	N1-C6-N6	-8.49	113.50	118.60
53	BA	1761	C	N3-C2-O2	-8.49	115.96	121.90
51	B3	44	ARG	NE-CZ-NH1	8.49	124.54	120.30
21	AA	356	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	460	A	N1-C6-N6	-8.48	113.51	118.60
53	BA	1451	C	O4'-C1'-N1	8.48	114.98	108.20
53	BA	1307	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	583	A	C5-C6-N1	8.48	121.94	117.70
53	BA	1745	A	C4-C5-C6	-8.47	112.76	117.00
12	AM	86	ARG	NE-CZ-NH1	8.47	124.54	120.30
53	BA	1764	C	O4'-C1'-N1	8.47	114.98	108.20
53	BA	909	A	N1-C6-N6	-8.47	113.52	118.60
21	AA	747	A	N1-C6-N6	-8.46	113.52	118.60
21	AA	1183	U	O4'-C1'-N1	8.47	114.97	108.20
21	AA	1158	C	N3-C2-O2	-8.46	115.97	121.90
53	BA	1515	A	N1-C6-N6	-8.46	113.52	118.60
53	BA	2542	A	C5-C6-N1	8.46	121.93	117.70
2	AC	39	ARG	NE-CZ-NH1	8.46	124.53	120.30
53	BA	781	A	C4-C5-C6	-8.46	112.77	117.00
53	BA	631	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	1410	A	N1-C6-N6	-8.46	113.53	118.60
53	BA	1876	A	C5-C6-N1	8.46	121.93	117.70
21	AA	51	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	970	C	N3-C2-O2	-8.45	115.98	121.90
21	AA	1014	A	C5-C6-N1	8.45	121.93	117.70
53	BA	1070	A	N1-C6-N6	-8.45	113.53	118.60
53	BA	2510	C	N3-C2-O2	-8.45	115.99	121.90
53	BA	637	A	C4-C5-C6	-8.45	112.78	117.00
21	AA	753	A	N1-C6-N6	-8.44	113.53	118.60
53	BA	1213	A	C5-C6-N1	8.44	121.92	117.70
21	AA	704	A	C4-C5-C6	-8.44	112.78	117.00
53	BA	1247	A	N1-C6-N6	-8.44	113.54	118.60
53	BA	1668	A	N1-C6-N6	-8.44	113.54	118.60
53	BA	2117	A	C5-C6-N1	8.44	121.92	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2328	A	C4-C5-C6	-8.44	112.78	117.00
53	BA	2088	A	C5-C6-N1	8.44	121.92	117.70
22	A1	76	A	N1-C6-N6	-8.44	113.54	118.60
53	BA	2469	A	N1-C6-N6	-8.44	113.54	118.60
12	AM	97	ARG	NE-CZ-NH1	8.43	124.52	120.30
53	BA	2013	A	N1-C6-N6	-8.43	113.54	118.60
53	BA	2458	G	O4'-C1'-N9	8.43	114.94	108.20
53	BA	910	A	C5-C6-N1	8.43	121.92	117.70
21	AA	914	A	N1-C6-N6	-8.43	113.54	118.60
21	AA	946	A	N1-C6-N6	-8.43	113.55	118.60
53	BA	91	A	N1-C6-N6	-8.43	113.54	118.60
53	BA	1244	A	C5-C6-N1	8.43	121.91	117.70
12	AM	89	ARG	NE-CZ-NH1	8.42	124.51	120.30
21	AA	465	A	O4'-C1'-N9	8.42	114.94	108.20
21	AA	969	A	N1-C6-N6	-8.42	113.55	118.60
53	BA	975	A	C5-C6-N1	8.42	121.91	117.70
53	BA	1635	A	C5-C6-N1	8.42	121.91	117.70
21	AA	77	A	C5-C6-N1	8.42	121.91	117.70
21	AA	865	A	C5-C6-N1	8.42	121.91	117.70
53	BA	176	A	C5-C6-N1	8.42	121.91	117.70
53	BA	1970	A	N1-C6-N6	-8.42	113.55	118.60
21	AA	759	A	N1-C6-N6	-8.41	113.55	118.60
53	BA	718	A	O4'-C1'-N9	8.41	114.93	108.20
21	AA	172	A	N1-C6-N6	-8.41	113.55	118.60
45	BX	44	ARG	NE-CZ-NH1	8.41	124.51	120.30
53	BA	2005	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	48	C	N3-C2-O2	-8.41	116.01	121.90
53	BA	84	A	N1-C6-N6	-8.41	113.55	118.60
53	BA	844	A	C4-C5-C6	-8.41	112.80	117.00
53	BA	2311	A	C5-C6-N1	8.41	121.91	117.70
53	BA	2565	A	C5-C6-N1	8.41	121.91	117.70
21	AA	7	A	C5-C6-N1	8.41	121.90	117.70
21	AA	1157	A	N1-C6-N6	-8.41	113.56	118.60
53	BA	197	A	C5-C6-N1	8.41	121.90	117.70
53	BA	1413	A	N1-C6-N6	-8.41	113.56	118.60
54	BB	101	A	N1-C6-N6	-8.41	113.56	118.60
21	AA	50	A	N1-C6-N6	-8.40	113.56	118.60
26	BE	61	ARG	NE-CZ-NH1	8.40	124.50	120.30
21	AA	1092	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	250	A	O4'-C1'-N9	8.40	114.92	108.20
21	AA	130	A	C4-C5-C6	-8.40	112.80	117.00
24	BC	12	ARG	NE-CZ-NH1	8.40	124.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1957	C	N3-C2-O2	-8.40	116.02	121.90
53	BA	2030	A	N1-C6-N6	-8.39	113.56	118.60
53	BA	2147	A	C5-C6-N1	8.39	121.90	117.70
54	BB	29	A	C5-C6-N1	8.39	121.90	117.70
21	AA	872	A	N1-C6-N6	-8.39	113.56	118.60
22	A1	47	U	O4'-C1'-N1	8.39	114.91	108.20
21	AA	321	A	N1-C6-N6	-8.39	113.57	118.60
53	BA	975	A	N1-C6-N6	-8.39	113.56	118.60
53	BA	1668	A	C5-C6-N1	8.39	121.89	117.70
21	AA	1014	A	C4-C5-C6	-8.39	112.81	117.00
21	AA	1340	A	C4-C5-C6	-8.39	112.81	117.00
53	BA	2227	A	N1-C6-N6	-8.39	113.57	118.60
40	BS	11	ARG	NE-CZ-NH1	8.39	124.49	120.30
53	BA	2572	A	N1-C6-N6	-8.39	113.57	118.60
21	AA	298	A	C5-C6-N1	8.38	121.89	117.70
53	BA	28	A	N1-C6-N6	-8.38	113.57	118.60
53	BA	1029	A	N1-C6-N6	-8.38	113.57	118.60
53	BA	886	A	C5-C6-N1	8.38	121.89	117.70
53	BA	1127	A	O4'-C1'-N9	8.38	114.90	108.20
21	AA	794	A	C5-C6-N1	8.38	121.89	117.70
53	BA	203	A	N1-C6-N6	-8.38	113.57	118.60
53	BA	497	A	C5-C6-N1	8.38	121.89	117.70
21	AA	1267	C	N3-C2-O2	-8.37	116.04	121.90
21	AA	109	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	746	A	N1-C6-N6	-8.37	113.58	118.60
53	BA	404	A	C5-C6-N1	8.37	121.88	117.70
53	BA	2660	A	N1-C6-N6	-8.37	113.58	118.60
54	BB	39	A	N1-C6-N6	-8.37	113.58	118.60
53	BA	272	A	O4'-C1'-N9	8.37	114.89	108.20
53	BA	1522	A	N1-C6-N6	-8.36	113.58	118.60
45	BX	36	ARG	NE-CZ-NH2	8.36	124.48	120.30
53	BA	1932	A	C5-C6-N1	8.36	121.88	117.70
21	AA	983	A	C5-C6-N1	8.36	121.88	117.70
8	AI	112	ARG	NE-CZ-NH2	8.36	124.48	120.30
53	BA	2042	A	C5-C6-N1	8.36	121.88	117.70
53	BA	1147	A	C4-C5-C6	-8.36	112.82	117.00
53	BA	621	A	N1-C6-N6	-8.36	113.59	118.60
53	BA	2726	A	N1-C6-N6	-8.36	113.59	118.60
53	BA	1143	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	499	A	C5-C6-N1	8.35	121.88	117.70
53	BA	2163	A	N1-C6-N6	-8.35	113.59	118.60
53	BA	2191	A	N1-C6-N6	-8.35	113.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AQ	39	ARG	NE-CZ-NH1	8.35	124.47	120.30
21	AA	397	A	C5-C6-N1	8.35	121.88	117.70
21	AA	553	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	1126	U	O4'-C1'-N1	8.35	114.88	108.20
45	BX	2	ARG	NE-CZ-NH1	8.35	124.47	120.30
53	BA	2095	A	N1-C6-N6	-8.35	113.59	118.60
53	BA	5	A	N1-C6-N6	-8.35	113.59	118.60
53	BA	293	U	O4'-C1'-N1	8.35	114.88	108.20
53	BA	390	U	O4'-C1'-N1	8.35	114.88	108.20
53	BA	1569	A	C5-C6-N1	8.35	121.87	117.70
22	A1	74	C	N1-C2-O2	8.34	123.91	118.90
21	AA	119	A	C5-C6-N1	8.34	121.87	117.70
21	AA	729	A	N1-C6-N6	-8.34	113.59	118.60
21	AA	262	A	N1-C6-N6	-8.34	113.60	118.60
3	AD	80	ARG	NE-CZ-NH1	8.34	124.47	120.30
21	AA	183	C	N3-C2-O2	-8.34	116.06	121.90
21	AA	345	C	O4'-C1'-N1	8.34	114.87	108.20
21	AA	1201	A	N1-C6-N6	-8.34	113.60	118.60
53	BA	602	A	N1-C6-N6	-8.34	113.60	118.60
53	BA	1583	A	C5-C6-N1	8.34	121.87	117.70
35	BN	118	ARG	NE-CZ-NH1	8.33	124.47	120.30
53	BA	1272	A	N1-C6-N6	-8.33	113.60	118.60
47	BZ	37	ARG	NE-CZ-NH1	8.33	124.46	120.30
53	BA	1593	A	C4-C5-C6	-8.33	112.84	117.00
53	BA	2335	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	411	A	N1-C6-N6	-8.32	113.61	118.60
32	BK	70	ARG	NE-CZ-NH1	8.32	124.46	120.30
53	BA	1608	A	N1-C6-N6	-8.32	113.61	118.60
53	BA	1672	A	C5-C6-N1	8.32	121.86	117.70
21	AA	1093	A	C5-C6-N1	8.32	121.86	117.70
21	AA	1280	A	N1-C6-N6	-8.32	113.61	118.60
53	BA	262	A	N1-C6-N6	-8.32	113.61	118.60
53	BA	2135	A	C5-C6-N1	8.32	121.86	117.70
53	BA	2145	C	N3-C2-O2	-8.31	116.08	121.90
21	AA	831	A	C5-C6-N1	8.31	121.86	117.70
53	BA	2311	A	N1-C6-N6	-8.31	113.61	118.60
9	AJ	68	ARG	NE-CZ-NH1	8.31	124.46	120.30
21	AA	1279	G	O4'-C1'-N9	8.31	114.85	108.20
53	BA	1328	A	N1-C6-N6	-8.31	113.61	118.60
26	BE	69	ARG	NE-CZ-NH1	8.31	124.45	120.30
53	BA	1453	A	O4'-C1'-N9	8.31	114.85	108.20
53	BA	2163	A	C5-C6-N1	8.31	121.86	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2309	A	C5-C6-N1	8.31	121.85	117.70
21	AA	1360	A	C5-C6-N1	8.31	121.85	117.70
53	BA	2164	C	N3-C2-O2	-8.31	116.09	121.90
11	AL	53	ARG	NE-CZ-NH1	8.30	124.45	120.30
35	BN	103	ARG	NE-CZ-NH1	8.30	124.45	120.30
53	BA	2711	A	C4-C5-C6	-8.30	112.85	117.00
21	AA	1413	A	N1-C6-N6	-8.30	113.62	118.60
53	BA	1953	A	N1-C6-N6	-8.30	113.62	118.60
53	BA	429	A	N1-C6-N6	-8.29	113.62	118.60
53	BA	2820	A	C5-C6-N1	8.29	121.85	117.70
21	AA	1339	A	N1-C6-N6	-8.29	113.63	118.60
53	BA	279	A	C4-C5-C6	-8.29	112.86	117.00
53	BA	324	A	N1-C6-N6	-8.29	113.63	118.60
53	BA	2517	C	N3-C2-O2	-8.29	116.10	121.90
21	AA	161	A	N1-C6-N6	-8.28	113.63	118.60
53	BA	1439	A	C5-C6-N1	8.28	121.84	117.70
53	BA	1597	A	N1-C6-N6	-8.29	113.63	118.60
21	AA	179	A	C4-C5-C6	-8.28	112.86	117.00
21	AA	196	A	N1-C6-N6	-8.28	113.63	118.60
21	AA	648	A	C4-C5-C6	-8.28	112.86	117.00
53	BA	412	A	C5-C6-N1	8.28	121.84	117.70
53	BA	979	A	N1-C6-N6	-8.28	113.63	118.60
53	BA	1327	A	N1-C6-N6	-8.28	113.63	118.60
53	BA	1496	A	C5-C6-N1	8.28	121.84	117.70
53	BA	199	A	C5-C6-N1	8.28	121.84	117.70
53	BA	526	A	C5-C6-N1	8.28	121.84	117.70
53	BA	1080	A	C4-C5-C6	-8.28	112.86	117.00
21	AA	845	A	C4-C5-C6	-8.27	112.86	117.00
21	AA	622	A	C5-C6-N1	8.27	121.83	117.70
53	BA	514	A	C5-C6-N1	8.27	121.83	117.70
21	AA	1431	A	N1-C6-N6	-8.27	113.64	118.60
53	BA	609	A	N1-C6-N6	-8.27	113.64	118.60
53	BA	1469	A	C4-C5-C6	-8.26	112.87	117.00
10	AK	68	ARG	NE-CZ-NH1	8.26	124.43	120.30
21	AA	1101	A	C5-C6-N1	8.26	121.83	117.70
53	BA	240	C	N3-C2-O2	-8.26	116.12	121.90
21	AA	345	C	N1-C2-O2	8.26	123.85	118.90
21	AA	579	A	N1-C6-N6	-8.26	113.65	118.60
53	BA	176	A	N1-C6-N6	-8.26	113.65	118.60
53	BA	2340	A	C5-C6-N1	8.26	121.83	117.70
21	AA	794	A	C4-C5-C6	-8.25	112.87	117.00
53	BA	216	A	N1-C6-N6	-8.25	113.65	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	907	A	C5-C6-N1	8.25	121.83	117.70
53	BA	204	A	C5-C6-N1	8.25	121.83	117.70
53	BA	1156	A	C5-C6-N1	8.25	121.83	117.70
53	BA	1565	C	O4'-C1'-N1	8.25	114.80	108.20
53	BA	1626	A	C5-C6-N1	8.25	121.82	117.70
21	AA	363	A	N1-C6-N6	-8.24	113.65	118.60
53	BA	2406	A	O4'-C1'-N9	8.24	114.80	108.20
53	BA	2452	C	N3-C2-O2	-8.24	116.13	121.90
53	BA	2154	A	N1-C6-N6	-8.24	113.66	118.60
53	BA	1126	A	N1-C6-N6	-8.24	113.66	118.60
53	BA	2376	A	C5-C6-N1	8.24	121.82	117.70
21	AA	1446	A	N1-C6-N6	-8.23	113.66	118.60
53	BA	1175	A	N1-C6-N6	-8.23	113.66	118.60
53	BA	2388	A	C5-C6-N1	8.23	121.81	117.70
53	BA	492	A	N1-C6-N6	-8.23	113.66	118.60
53	BA	2867	G	O4'-C1'-N9	8.23	114.78	108.20
21	AA	1037	C	N3-C2-O2	-8.22	116.14	121.90
53	BA	920	A	N1-C6-N6	-8.22	113.67	118.60
53	BA	1046	A	C5-C6-N1	8.22	121.81	117.70
53	BA	1553	A	N1-C6-N6	-8.22	113.67	118.60
53	BA	2872	A	N1-C6-N6	-8.22	113.67	118.60
53	BA	794	A	C5-C6-N1	8.22	121.81	117.70
24	BC	62	ARG	NE-CZ-NH1	8.22	124.41	120.30
53	BA	1809	A	N1-C6-N6	-8.21	113.67	118.60
53	BA	2412	A	N1-C6-N6	-8.21	113.67	118.60
21	AA	1447	A	C5-C6-N1	8.21	121.81	117.70
53	BA	265	A	N1-C6-N6	-8.21	113.67	118.60
53	BA	1084	A	N1-C6-N6	-8.21	113.67	118.60
53	BA	1077	A	N1-C6-N6	-8.21	113.67	118.60
21	AA	262	A	C4-C5-C6	-8.21	112.90	117.00
21	AA	1465	A	C5-C6-N1	8.21	121.81	117.70
53	BA	844	A	C5-C6-N1	8.21	121.81	117.70
21	AA	298	A	N1-C6-N6	-8.21	113.68	118.60
21	AA	673	A	N1-C6-N6	-8.21	113.68	118.60
53	BA	53	A	C5-C6-N1	8.21	121.80	117.70
53	BA	1508	A	C5-C6-N1	8.21	121.80	117.70
53	BA	1713	A	C4-C5-C6	-8.21	112.90	117.00
53	BA	2850	A	C4-C5-C6	-8.21	112.90	117.00
53	BA	599	A	N1-C6-N6	-8.21	113.68	118.60
21	AA	1109	C	N3-C2-O2	-8.20	116.16	121.90
21	AA	1378	C	N3-C2-O2	-8.20	116.16	121.90
53	BA	2764	A	N1-C6-N6	-8.20	113.68	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1048	A	C4-C5-C6	-8.20	112.90	117.00
53	BA	2117	A	O4'-C1'-N9	8.20	114.76	108.20
21	AA	1278	G	N3-C2-N2	-8.19	114.16	119.90
53	BA	749	A	N1-C6-N6	-8.19	113.68	118.60
53	BA	1534	U	O4'-C1'-N1	8.19	114.75	108.20
53	BA	2432	A	N1-C6-N6	-8.20	113.68	118.60
53	BA	2766	A	N1-C6-N6	-8.19	113.68	118.60
53	BA	2459	A	N1-C6-N6	-8.19	113.68	118.60
21	AA	1271	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	130	A	C5-C6-N1	8.19	121.80	117.70
53	BA	1039	A	C4-C5-C6	-8.19	112.91	117.00
21	AA	1441	A	C5-C6-N1	8.19	121.79	117.70
53	BA	1077	A	C4-C5-C6	-8.19	112.91	117.00
53	BA	1894	C	N3-C2-O2	-8.19	116.17	121.90
53	BA	2776	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	865	A	C4-C5-C6	-8.19	112.91	117.00
53	BA	1328	A	C5-C6-N1	8.19	121.79	117.70
21	AA	243	A	C4-C5-C6	-8.18	112.91	117.00
53	BA	721	A	C5-C6-N1	8.18	121.79	117.70
53	BA	1095	A	C5-C6-N1	8.18	121.79	117.70
53	BA	1580	A	C5-C6-N1	8.18	121.79	117.70
53	BA	1713	A	N1-C6-N6	-8.18	113.69	118.60
21	AA	228	A	N1-C6-N6	-8.18	113.69	118.60
37	BP	61	ARG	NE-CZ-NH1	8.18	124.39	120.30
53	BA	2670	A	N1-C6-N6	-8.17	113.70	118.60
3	AD	114	ARG	NE-CZ-NH1	8.17	124.39	120.30
9	AJ	9	ARG	NE-CZ-NH1	8.17	124.38	120.30
21	AA	621	A	C5-C6-N1	8.17	121.78	117.70
53	BA	1129	A	N1-C6-N6	-8.17	113.70	118.60
53	BA	2646	C	N3-C2-O2	-8.17	116.18	121.90
21	AA	1157	A	C5-C6-N1	8.16	121.78	117.70
53	BA	861	A	C5-C6-N1	8.16	121.78	117.70
54	BB	29	A	C4-C5-C6	-8.16	112.92	117.00
21	AA	1044	A	C5-C6-N1	8.16	121.78	117.70
21	AA	1246	A	C4-C5-C6	-8.16	112.92	117.00
53	BA	2173	A	N1-C6-N6	-8.16	113.70	118.60
53	BA	119	A	O4'-C1'-N9	8.16	114.73	108.20
53	BA	2217	G	O4'-C1'-N9	8.16	114.73	108.20
53	BA	817	C	N3-C2-O2	-8.16	116.19	121.90
53	BA	1378	A	C5-C6-N1	8.16	121.78	117.70
21	AA	913	A	C5-C6-N1	8.15	121.78	117.70
35	BN	22	ARG	NE-CZ-NH1	8.15	124.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1069	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	253	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	765	G	O4'-C1'-N9	8.15	114.72	108.20
21	AA	1227	A	C5-C6-N1	8.15	121.78	117.70
21	AA	1269	A	C5-C6-N1	8.15	121.77	117.70
53	BA	139	U	O4'-C1'-N1	8.15	114.72	108.20
53	BA	1570	A	N1-C6-N6	-8.15	113.71	118.60
53	BA	2868	A	C5-C6-N1	8.15	121.77	117.70
21	AA	1311	A	C4-C5-C6	-8.14	112.93	117.00
21	AA	1456	A	C5-C6-N1	8.14	121.77	117.70
53	BA	920	A	C5-C6-N1	8.14	121.77	117.70
21	AA	1014	A	N1-C6-N6	-8.14	113.72	118.60
53	BA	244	A	N1-C6-N6	-8.14	113.72	118.60
53	BA	572	A	C5-C6-N1	8.14	121.77	117.70
53	BA	2077	A	C5-C6-N1	8.14	121.77	117.70
53	BA	1393	A	C5-C6-N1	8.14	121.77	117.70
21	AA	313	A	N1-C6-N6	-8.13	113.72	118.60
53	BA	118	A	N1-C6-N6	-8.14	113.72	118.60
53	BA	1039	A	C5-C6-N1	8.14	121.77	117.70
53	BA	547	A	C4-C5-C6	-8.13	112.93	117.00
53	BA	1701	A	N1-C6-N6	-8.13	113.72	118.60
53	BA	2547	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	622	A	N1-C6-N6	-8.13	113.72	118.60
53	BA	320	A	N1-C6-N6	-8.13	113.72	118.60
53	BA	705	A	C5-C6-N1	8.13	121.77	117.70
10	AK	55	ARG	NE-CZ-NH2	8.13	124.37	120.30
22	A1	38	A	C4-C5-C6	-8.13	112.93	117.00
53	BA	1885	A	C5-C6-N1	8.13	121.77	117.70
53	BA	2169	A	C5-C6-N1	8.13	121.77	117.70
53	BA	2797	U	O4'-C1'-N1	8.13	114.71	108.20
53	BA	2823	A	N1-C6-N6	-8.13	113.72	118.60
53	BA	1815	A	C4-C5-C6	-8.13	112.94	117.00
53	BA	1639	C	N3-C2-O2	-8.12	116.21	121.90
53	BA	2211	A	C4-C5-C6	-8.12	112.94	117.00
6	AG	101	ARG	NE-CZ-NH1	8.12	124.36	120.30
53	BA	2573	C	N3-C2-O2	-8.12	116.22	121.90
53	BA	608	A	N1-C6-N6	-8.12	113.73	118.60
53	BA	2020	A	C5-C6-N1	8.12	121.76	117.70
53	BA	2090	A	N1-C6-N6	-8.12	113.73	118.60
53	BA	38	A	C5-C6-N1	8.12	121.76	117.70
53	BA	586	A	N1-C6-N6	-8.12	113.73	118.60
53	BA	2114	A	C5-C6-N1	8.12	121.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2266	A	C5-C6-N1	8.11	121.76	117.70
21	AA	935	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	1225	A	C5-C6-N1	8.11	121.76	117.70
53	BA	195	A	C4-C5-C6	-8.11	112.95	117.00
53	BA	541	A	C4-C5-C6	-8.11	112.95	117.00
21	AA	1246	A	C5-C6-N1	8.10	121.75	117.70
53	BA	1739	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	807	A	N1-C6-N6	-8.10	113.74	118.60
53	BA	1000	A	N1-C6-N6	-8.10	113.74	118.60
53	BA	1722	A	N1-C6-N6	-8.10	113.74	118.60
28	BG	151	ARG	NE-CZ-NH1	8.10	124.35	120.30
53	BA	265	A	C4-C5-C6	-8.10	112.95	117.00
53	BA	861	A	C4-C5-C6	-8.10	112.95	117.00
21	AA	197	A	C4-C5-C6	-8.09	112.95	117.00
21	AA	414	A	C5-C6-N1	8.09	121.75	117.70
21	AA	743	A	N1-C6-N6	-8.09	113.74	118.60
42	BU	81	ARG	NE-CZ-NH1	8.09	124.35	120.30
53	BA	2211	A	C5-C6-N1	8.09	121.75	117.70
53	BA	1044	C	N3-C2-O2	-8.09	116.24	121.90
53	BA	1451	C	N1-C2-O2	8.09	123.75	118.90
53	BA	2327	A	C5-C6-N1	8.09	121.74	117.70
21	AA	560	A	C5-C6-N1	8.09	121.74	117.70
53	BA	554	U	O4'-C1'-N1	8.09	114.67	108.20
53	BA	1503	A	N1-C6-N6	-8.09	113.75	118.60
53	BA	2483	C	N3-C2-O2	-8.08	116.24	121.90
53	BA	795	C	N3-C2-O2	-8.08	116.24	121.90
53	BA	2572	A	C5-C6-N1	8.08	121.74	117.70
53	BA	829	A	C5-C6-N1	8.08	121.74	117.70
53	BA	2214	C	N3-C2-O2	-8.08	116.24	121.90
53	BA	1728	C	N3-C2-O2	-8.08	116.25	121.90
53	BA	1912	A	C5-C6-N1	8.07	121.74	117.70
21	AA	1008	U	O4'-C1'-N1	8.07	114.66	108.20
53	BA	282	A	N1-C6-N6	-8.07	113.76	118.60
53	BA	1705	A	C5-C6-N1	8.07	121.74	117.70
15	AP	25	ARG	NE-CZ-NH2	8.07	124.33	120.30
21	AA	162	A	C5-C6-N1	8.07	121.74	117.70
21	AA	1005	A	C5-C6-N1	8.07	121.74	117.70
21	AA	65	A	C5-C6-N1	8.07	121.73	117.70
21	AA	119	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	702	A	N1-C6-N6	-8.07	113.76	118.60
53	BA	507	A	C5-C6-N1	8.07	121.73	117.70
53	BA	142	A	N1-C6-N6	-8.07	113.76	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BB	115	A	C5-C6-N1	8.07	121.73	117.70
53	BA	1029	A	C5-C6-N1	8.06	121.73	117.70
53	BA	2247	A	N1-C6-N6	-8.06	113.76	118.60
21	AA	1163	A	C5-C6-N1	8.06	121.73	117.70
21	AA	371	A	C5-C6-N1	8.06	121.73	117.70
53	BA	1046	A	O4'-C1'-N9	8.06	114.65	108.20
53	BA	1871	A	O4'-C1'-N9	8.06	114.65	108.20
54	BB	50	A	C5-C6-N1	8.06	121.73	117.70
21	AA	109	A	C5-C6-N1	8.05	121.73	117.70
53	BA	2541	A	C5-C6-N1	8.05	121.73	117.70
21	AA	478	A	N1-C6-N6	-8.05	113.77	118.60
53	BA	1204	A	O4'-C1'-N9	8.05	114.64	108.20
53	BA	1532	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	994	A	C5-C6-N1	8.05	121.72	117.70
21	AA	1352	C	N3-C2-O2	-8.05	116.27	121.90
21	AA	535	A	C5-C6-N1	8.05	121.72	117.70
53	BA	945	A	C4-C5-C6	-8.05	112.98	117.00
21	AA	546	A	C5-C6-N1	8.04	121.72	117.70
21	AA	649	A	N1-C6-N6	-8.04	113.78	118.60
53	BA	1678	A	N1-C6-N6	-8.04	113.78	118.60
53	BA	2191	A	C5-C6-N1	8.04	121.72	117.70
53	BA	1535	A	C5-C6-N1	8.04	121.72	117.70
31	BJ	27	ARG	NE-CZ-NH2	-8.04	116.28	120.30
53	BA	2613	U	O4'-C1'-N1	8.03	114.63	108.20
53	BA	2781	A	C5-C6-N1	8.03	121.72	117.70
54	BB	35	C	N3-C2-O2	-8.04	116.28	121.90
11	AL	30	ARG	NE-CZ-NH1	8.03	124.32	120.30
53	BA	219	A	C5-C6-N1	8.03	121.72	117.70
21	AA	815	A	C4-C5-C6	-8.03	112.99	117.00
21	AA	1213	A	C5-C6-N1	8.03	121.71	117.70
53	BA	1073	A	N1-C6-N6	-8.03	113.78	118.60
21	AA	1081	A	N1-C6-N6	-8.03	113.78	118.60
53	BA	466	A	C5-C6-N1	8.03	121.71	117.70
53	BA	2031	A	C5-C6-N1	8.03	121.71	117.70
53	BA	99	U	O4'-C1'-N1	8.02	114.62	108.20
53	BA	1077	A	C5-C6-N1	8.02	121.71	117.70
21	AA	907	A	N1-C6-N6	-8.02	113.79	118.60
46	BY	52	ARG	NE-CZ-NH1	8.02	124.31	120.30
53	BA	1502	A	C4-C5-C6	-8.02	112.99	117.00
53	BA	2060	A	N1-C6-N6	-8.02	113.79	118.60
53	BA	1205	A	C5-C6-N1	8.02	121.71	117.70
53	BA	1821	A	N1-C6-N6	-8.02	113.79	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2850	A	C5-C6-N1	8.02	121.71	117.70
15	AP	31	ARG	NE-CZ-NH1	8.01	124.31	120.30
21	AA	451	A	C5-C6-N1	8.01	121.71	117.70
36	BO	13	ARG	NE-CZ-NH1	8.01	124.31	120.30
52	B4	4	ARG	NE-CZ-NH1	8.01	124.31	120.30
53	BA	1534	U	N3-C2-O2	-8.01	116.59	122.20
13	AN	24	ARG	NE-CZ-NH1	8.01	124.30	120.30
21	AA	363	A	C4-C5-C6	-8.01	113.00	117.00
53	BA	2799	A	O4'-C1'-N9	8.01	114.61	108.20
53	BA	1739	A	C5-C6-N1	8.01	121.70	117.70
21	AA	315	A	N1-C6-N6	-8.01	113.80	118.60
53	BA	1966	A	C5-C6-N1	8.01	121.70	117.70
53	BA	2813	A	C5-C6-N1	8.00	121.70	117.70
53	BA	1147	A	C5-C6-N1	8.00	121.70	117.70
53	BA	1596	A	C5-C6-N1	8.00	121.70	117.70
53	BA	371	A	N1-C6-N6	-7.99	113.80	118.60
53	BA	2422	C	N3-C2-O2	-7.99	116.30	121.90
21	AA	493	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	1518	A	C4-C5-C6	-7.99	113.00	117.00
53	BA	460	A	C5-C6-N1	7.99	121.69	117.70
53	BA	1194	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	415	A	O4'-C1'-N9	7.99	114.59	108.20
21	AA	1336	C	O4'-C1'-N1	7.99	114.59	108.20
21	AA	1503	A	C5-C6-N1	7.99	121.69	117.70
48	B0	12	ARG	NE-CZ-NH2	7.99	124.29	120.30
53	BA	936	A	C5-C6-N1	7.99	121.69	117.70
53	BA	1755	A	C5-C6-N1	7.99	121.69	117.70
7	AH	76	ARG	NE-CZ-NH1	7.99	124.29	120.30
53	BA	265	A	C5-C6-N1	7.99	121.69	117.70
2	AC	53	ARG	NE-CZ-NH1	7.98	124.29	120.30
21	AA	892	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	768	A	C5-C6-N1	7.98	121.69	117.70
53	BA	2281	A	N1-C6-N6	-7.98	113.81	118.60
53	BA	2758	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	1285	A	C4-C5-C6	-7.98	113.01	117.00
53	BA	155	A	N1-C6-N6	-7.98	113.81	118.60
53	BA	2534	A	N1-C6-N6	-7.98	113.81	118.60
53	BA	1899	A	C5-C6-N1	7.98	121.69	117.70
21	AA	131	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	1476	A	N1-C6-N6	-7.97	113.82	118.60
53	BA	2439	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	845	A	C5-C6-N1	7.97	121.68	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1402	C	N3-C2-O2	-7.97	116.32	121.90
24	BC	51	ARG	NE-CZ-NH2	7.97	124.28	120.30
53	BA	531	C	O4'-C1'-N1	7.97	114.57	108.20
21	AA	303	A	C5-C6-N1	7.96	121.68	117.70
21	AA	913	A	C4-C5-C6	-7.96	113.02	117.00
53	BA	28	A	C5-C6-N1	7.96	121.68	117.70
53	BA	1650	A	C5-C6-N1	7.96	121.68	117.70
53	BA	251	A	N1-C6-N6	-7.96	113.82	118.60
13	AN	85	ARG	NE-CZ-NH1	7.96	124.28	120.30
21	AA	7	A	N1-C6-N6	-7.96	113.82	118.60
21	AA	958	A	C4-C5-C6	-7.96	113.02	117.00
53	BA	1304	A	N1-C6-N6	-7.96	113.82	118.60
53	BA	1808	A	N1-C6-N6	-7.96	113.82	118.60
53	BA	2682	A	N1-C6-N6	-7.96	113.82	118.60
53	BA	1395	A	C5-C6-N1	7.96	121.68	117.70
21	AA	303	A	C4-C5-C6	-7.96	113.02	117.00
21	AA	983	A	C4-C5-C6	-7.96	113.02	117.00
53	BA	428	A	C5-C6-N1	7.96	121.68	117.70
53	BA	941	A	C5-C6-N1	7.96	121.68	117.70
53	BA	2051	A	C5-C6-N1	7.96	121.68	117.70
53	BA	2411	A	N1-C6-N6	-7.96	113.83	118.60
53	BA	2851	A	N1-C6-N6	-7.96	113.83	118.60
53	BA	2823	A	C5-C6-N1	7.96	121.68	117.70
53	BA	1927	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	1340	A	N1-C6-N6	-7.95	113.83	118.60
53	BA	2274	A	C4-C5-C6	-7.95	113.03	117.00
53	BA	1899	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	1236	A	C4-C5-C6	-7.95	113.03	117.00
53	BA	311	A	C5-C6-N1	7.95	121.67	117.70
53	BA	505	A	N1-C6-N6	-7.95	113.83	118.60
53	BA	544	C	N3-C2-O2	-7.95	116.34	121.90
53	BA	347	A	N1-C6-N6	-7.94	113.83	118.60
53	BA	299	A	N1-C6-N6	-7.94	113.83	118.60
53	BA	1877	A	N1-C6-N6	-7.94	113.83	118.60
21	AA	1042	A	C5-C6-N1	7.94	121.67	117.70
22	A1	38	A	C5-C6-N1	7.94	121.67	117.70
52	B4	12	ARG	NE-CZ-NH2	7.94	124.27	120.30
53	BA	176	A	C4-C5-C6	-7.94	113.03	117.00
21	AA	937	A	C5-C6-N1	7.94	121.67	117.70
21	AA	1214	C	O4'-C1'-N1	7.94	114.55	108.20
53	BA	866	A	C4-C5-C6	-7.94	113.03	117.00
53	BA	854	C	N3-C2-O2	-7.94	116.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BB	91	C	O4'-C1'-N1	7.94	114.55	108.20
21	AA	1170	A	N1-C6-N6	-7.93	113.84	118.60
53	BA	481	G	O4'-C1'-N9	7.93	114.55	108.20
53	BA	1626	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	1197	A	N1-C6-N6	-7.93	113.84	118.60
33	BL	48	ARG	NE-CZ-NH1	7.93	124.27	120.30
53	BA	710	U	O4'-C1'-N1	7.93	114.54	108.20
53	BA	844	A	N1-C6-N6	-7.93	113.84	118.60
53	BA	1602	U	O4'-C1'-N1	7.93	114.54	108.20
53	BA	382	A	C4-C5-C6	-7.93	113.04	117.00
53	BA	2119	A	C4-C5-C6	-7.93	113.04	117.00
53	BA	95	A	N1-C6-N6	-7.93	113.84	118.60
19	AT	24	ARG	NE-CZ-NH1	7.92	124.26	120.30
21	AA	1492	A	C5-C6-N1	7.92	121.66	117.70
22	A1	76	A	C5-C6-N1	7.92	121.66	117.70
53	BA	2114	A	C4-C5-C6	-7.92	113.04	117.00
21	AA	59	A	C5-C6-N1	7.92	121.66	117.70
21	AA	607	A	C5-C6-N1	7.92	121.66	117.70
21	AA	1299	A	N1-C6-N6	-7.92	113.85	118.60
21	AA	196	A	C5-C6-N1	7.92	121.66	117.70
53	BA	2501	C	N3-C2-O2	-7.92	116.36	121.90
54	BB	108	A	N1-C6-N6	-7.92	113.85	118.60
24	BC	79	ARG	NE-CZ-NH1	7.92	124.26	120.30
53	BA	1815	A	C5-C6-N1	7.92	121.66	117.70
53	BA	2171	A	N1-C6-N6	-7.92	113.85	118.60
53	BA	1143	A	C4-C5-C6	-7.91	113.04	117.00
53	BA	44	A	C4-C5-C6	-7.91	113.05	117.00
53	BA	1978	A	C5-C6-N1	7.91	121.66	117.70
21	AA	19	A	C5-C6-N1	7.91	121.66	117.70
21	AA	325	A	N1-C6-N6	-7.91	113.86	118.60
53	BA	804	A	C4-C5-C6	-7.91	113.05	117.00
53	BA	2082	A	N1-C6-N6	-7.91	113.86	118.60
21	AA	161	A	C5-C6-N1	7.91	121.65	117.70
53	BA	423	A	N1-C6-N6	-7.90	113.86	118.60
53	BA	1428	C	N3-C2-O2	-7.90	116.37	121.90
21	AA	1019	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1158	C	N1-C2-O2	7.90	123.64	118.90
53	BA	2778	A	N1-C6-N6	-7.90	113.86	118.60
53	BA	1135	C	N3-C2-O2	-7.90	116.37	121.90
55	B5	7	ARG	NE-CZ-NH1	7.90	124.25	120.30
21	AA	572	A	C5-C6-N1	7.89	121.65	117.70
53	BA	1230	A	C5-C6-N1	7.89	121.65	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1634	A	N1-C6-N6	-7.89	113.86	118.60
21	AA	726	C	N3-C2-O2	-7.89	116.38	121.90
53	BA	644	A	N1-C6-N6	-7.89	113.87	118.60
53	BA	1304	A	C4-C5-C6	-7.89	113.06	117.00
21	AA	1394	A	C5-C6-N1	7.89	121.64	117.70
21	AA	1117	A	N1-C6-N6	-7.88	113.87	118.60
53	BA	332	A	C5-C6-N1	7.88	121.64	117.70
53	BA	1226	A	N1-C6-N6	-7.88	113.87	118.60
53	BA	574	A	C5-C6-N1	7.88	121.64	117.70
53	BA	761	A	N1-C6-N6	-7.88	113.87	118.60
53	BA	1488	C	N3-C2-O2	-7.88	116.39	121.90
21	AA	777	A	C5-C6-N1	7.88	121.64	117.70
53	BA	2893	A	C5-C6-N1	7.88	121.64	117.70
21	AA	487	A	N1-C6-N6	-7.88	113.88	118.60
53	BA	2887	A	N1-C6-N6	-7.88	113.88	118.60
27	BF	101	ARG	NE-CZ-NH1	7.87	124.24	120.30
53	BA	1155	A	N1-C6-N6	-7.87	113.88	118.60
53	BA	2888	C	O4'-C1'-N1	7.87	114.50	108.20
53	BA	973	A	C4-C5-C6	-7.87	113.06	117.00
21	AA	749	A	C4-C5-C6	-7.87	113.06	117.00
53	BA	207	A	C5-C6-N1	7.87	121.64	117.70
21	AA	781	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	1082	A	N1-C6-N6	-7.87	113.88	118.60
53	BA	391	A	C5-C6-N1	7.87	121.63	117.70
53	BA	877	A	C4-C5-C6	-7.87	113.07	117.00
3	AD	61	ARG	NE-CZ-NH1	7.86	124.23	120.30
53	BA	249	C	N3-C2-O2	-7.86	116.40	121.90
53	BA	1470	A	C5-C6-N1	7.86	121.63	117.70
53	BA	1794	A	C5-C6-N1	7.86	121.63	117.70
21	AA	583	A	C4-C5-C6	-7.86	113.07	117.00
53	BA	342	A	N1-C6-N6	-7.86	113.88	118.60
53	BA	1069	A	O4'-C1'-N9	7.86	114.49	108.20
53	BA	2804	U	O4'-C1'-N1	7.86	114.49	108.20
21	AA	274	A	C5-C6-N1	7.86	121.63	117.70
53	BA	480	A	N1-C6-N6	-7.86	113.88	118.60
21	AA	316	C	N3-C2-O2	-7.86	116.40	121.90
21	AA	595	A	N1-C6-N6	-7.86	113.89	118.60
53	BA	101	A	O4'-C1'-N9	7.85	114.48	108.20
53	BA	361	G	O4'-C1'-N9	7.85	114.48	108.20
54	BB	50	A	C4-C5-C6	-7.85	113.07	117.00
47	BZ	30	ARG	NE-CZ-NH1	7.85	124.23	120.30
53	BA	819	A	N1-C6-N6	-7.85	113.89	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2062	A	N1-C6-N6	-7.85	113.89	118.60
53	BA	2062	A	C4-C5-C6	-7.85	113.07	117.00
54	BB	53	A	C5-C6-N1	7.85	121.63	117.70
12	AM	70	ARG	NE-CZ-NH2	7.85	124.22	120.30
55	B5	162	ARG	NE-CZ-NH1	7.85	124.22	120.30
53	BA	2418	A	C5-C6-N1	7.85	121.62	117.70
53	BA	2281	A	C4-C5-C6	-7.84	113.08	117.00
53	BA	2328	A	C5-C6-N1	7.84	121.62	117.70
53	BA	2417	C	N3-C2-O2	-7.84	116.41	121.90
53	BA	165	A	C4-C5-C6	-7.84	113.08	117.00
21	AA	756	C	N3-C2-O2	-7.84	116.41	121.90
21	AA	1493	A	N1-C6-N6	-7.84	113.89	118.60
53	BA	878	A	C5-C6-N1	7.84	121.62	117.70
53	BA	2273	A	C5-C6-N1	7.84	121.62	117.70
53	BA	34	U	O4'-C1'-N1	7.84	114.47	108.20
21	AA	1395	C	N3-C2-O2	-7.84	116.41	121.90
24	BC	166	ARG	NE-CZ-NH1	7.84	124.22	120.30
38	BQ	57	ARG	NE-CZ-NH1	7.84	124.22	120.30
53	BA	1626	A	C4-C5-C6	-7.84	113.08	117.00
21	AA	250	A	C5-C6-N1	7.83	121.62	117.70
21	AA	327	A	C5-C6-N1	7.83	121.62	117.70
53	BA	362	A	N1-C6-N6	-7.83	113.90	118.60
53	BA	2297	A	N1-C6-N6	-7.83	113.90	118.60
53	BA	2440	C	N3-C2-O2	-7.83	116.42	121.90
21	AA	549	C	N3-C2-O2	-7.83	116.42	121.90
21	AA	635	A	C5-C6-N1	7.83	121.61	117.70
21	AA	1333	A	C5-C6-N1	7.83	121.61	117.70
21	AA	238	A	C5-C6-N1	7.83	121.61	117.70
9	AJ	5	ARG	NE-CZ-NH1	7.82	124.21	120.30
53	BA	2781	A	N1-C6-N6	-7.82	113.91	118.60
24	BC	155	ARG	NE-CZ-NH1	7.82	124.21	120.30
53	BA	1243	C	N3-C2-O2	-7.82	116.43	121.90
53	BA	2058	A	C5-C6-N1	7.82	121.61	117.70
55	B5	53	ARG	NE-CZ-NH2	-7.82	116.39	120.30
53	BA	1073	A	C4-C5-C6	-7.82	113.09	117.00
21	AA	1350	A	N1-C6-N6	-7.82	113.91	118.60
53	BA	673	C	N3-C2-O2	-7.81	116.43	121.90
53	BA	1593	A	N1-C6-N6	-7.81	113.91	118.60
21	AA	975	A	C5-C6-N1	7.81	121.61	117.70
53	BA	2241	A	N1-C6-N6	-7.81	113.91	118.60
53	BA	912	C	N3-C2-O2	-7.81	116.43	121.90
53	BA	64	A	N1-C6-N6	-7.81	113.91	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	340	A	C4-C5-C6	-7.81	113.09	117.00
53	BA	1365	A	C5-C6-N1	7.81	121.61	117.70
53	BA	1570	A	C5-C6-N1	7.81	121.61	117.70
53	BA	1606	C	O4'-C1'-N1	7.81	114.45	108.20
53	BA	715	A	N1-C6-N6	-7.81	113.92	118.60
53	BA	1475	G	O4'-C1'-N9	7.81	114.45	108.20
21	AA	600	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	890	G	O4'-C1'-N9	7.80	114.44	108.20
53	BA	2497	A	N1-C6-N6	-7.80	113.92	118.60
54	BB	109	A	C5-C6-N1	7.80	121.60	117.70
53	BA	678	C	N3-C2-O2	-7.80	116.44	121.90
53	BA	1566	A	N1-C6-N6	-7.80	113.92	118.60
53	BA	722	A	N1-C6-N6	-7.80	113.92	118.60
53	BA	2651	C	N3-C2-O2	-7.80	116.44	121.90
53	BA	1900	A	C4-C5-C6	-7.80	113.10	117.00
53	BA	1785	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	1219	A	C5-C6-N1	7.80	121.60	117.70
53	BA	1522	A	C5-C6-N1	7.80	121.60	117.70
53	BA	1899	A	C4-C5-C6	-7.80	113.10	117.00
21	AA	1349	A	N1-C6-N6	-7.79	113.92	118.60
53	BA	2634	A	C4-C5-C6	-7.79	113.10	117.00
21	AA	315	A	C5-C6-N1	7.79	121.60	117.70
53	BA	119	A	C5-C6-N1	7.79	121.60	117.70
53	BA	1558	C	N3-C2-O2	-7.79	116.45	121.90
53	BA	216	A	C5-C6-N1	7.79	121.59	117.70
21	AA	973	G	O4'-C1'-N9	7.79	114.43	108.20
24	BC	237	ARG	NE-CZ-NH2	-7.79	116.41	120.30
53	BA	2761	A	C5-C6-N1	7.79	121.59	117.70
53	BA	1027	A	C5-C6-N1	7.79	121.59	117.70
53	BA	1098	A	N1-C6-N6	-7.79	113.93	118.60
53	BA	1749	A	C5-C6-N1	7.79	121.59	117.70
53	BA	196	A	O4'-C1'-N9	7.78	114.43	108.20
53	BA	925	A	C4-C5-C6	-7.78	113.11	117.00
53	BA	1000	A	C4-C5-C6	-7.78	113.11	117.00
53	BA	1690	A	C5-C6-N1	7.78	121.59	117.70
53	BA	507	A	C4-C5-C6	-7.78	113.11	117.00
53	BA	1433	A	C5-C6-N1	7.78	121.59	117.70
53	BA	2037	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	1338	G	N3-C2-N2	-7.78	114.46	119.90
53	BA	104	A	C5-C6-N1	7.78	121.59	117.70
53	BA	2734	A	C5-C6-N1	7.78	121.59	117.70
53	BA	1454	C	N1-C2-O2	7.78	123.57	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1144	A	N1-C6-N6	-7.77	113.94	118.60
53	BA	1597	A	C5-C6-N1	7.77	121.59	117.70
53	BA	1237	A	N1-C6-N6	-7.77	113.94	118.60
21	AA	1157	A	C4-C5-C6	-7.77	113.11	117.00
29	BH	97	ARG	NE-CZ-NH1	7.77	124.18	120.30
53	BA	1347	A	C5-C6-N1	7.77	121.58	117.70
53	BA	2313	C	N3-C2-O2	-7.77	116.46	121.90
53	BA	2577	A	C5-C6-N1	7.77	121.58	117.70
21	AA	1285	A	C5-C6-N1	7.76	121.58	117.70
21	AA	994	A	C4-C5-C6	-7.76	113.12	117.00
53	BA	1298	C	N3-C2-O2	-7.76	116.47	121.90
21	AA	523	A	N1-C6-N6	-7.76	113.94	118.60
53	BA	324	A	C4-C5-C6	-7.76	113.12	117.00
53	BA	556	A	C5-C6-N1	7.76	121.58	117.70
53	BA	673	C	O4'-C1'-N1	7.76	114.41	108.20
53	BA	2434	A	N1-C6-N6	-7.76	113.94	118.60
21	AA	841	C	N3-C2-O2	-7.76	116.47	121.90
21	AA	1117	A	C5-C6-N1	7.76	121.58	117.70
53	BA	1365	A	N1-C6-N6	-7.76	113.94	118.60
21	AA	767	A	C4-C5-C6	-7.76	113.12	117.00
21	AA	1339	A	C5-C6-N1	7.76	121.58	117.70
21	AA	1501	C	N3-C2-O2	-7.76	116.47	121.90
53	BA	63	A	C5-C6-N1	7.76	121.58	117.70
53	BA	2088	A	C4-C5-C6	-7.76	113.12	117.00
53	BA	384	A	C5-C6-N1	7.75	121.58	117.70
53	BA	1638	C	N3-C2-O2	-7.75	116.47	121.90
21	AA	1111	A	C4-C5-C6	-7.75	113.12	117.00
53	BA	2020	A	N1-C6-N6	-7.75	113.95	118.60
53	BA	2232	C	O4'-C1'-N1	7.75	114.40	108.20
21	AA	1038	C	N3-C2-O2	-7.75	116.47	121.90
53	BA	191	A	C5-C6-N1	7.75	121.58	117.70
53	BA	1705	A	N1-C6-N6	-7.75	113.95	118.60
53	BA	750	A	C5-C6-N1	7.75	121.57	117.70
53	BA	1168	G	N1-C6-O6	-7.75	115.25	119.90
53	BA	2339	C	O4'-C1'-N1	7.75	114.40	108.20
53	BA	160	A	C4-C5-C6	-7.75	113.13	117.00
53	BA	2634	A	C5-C6-N1	7.75	121.57	117.70
53	BA	205	G	O4'-C1'-N9	7.74	114.39	108.20
53	BA	2426	A	C4-C5-C6	-7.74	113.13	117.00
40	BS	18	ARG	NE-CZ-NH1	7.74	124.17	120.30
53	BA	965	C	N3-C2-O2	-7.74	116.48	121.90
21	AA	695	A	C4-C5-C6	-7.74	113.13	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	44	A	N1-C6-N6	-7.74	113.96	118.60
21	AA	1374	A	C5-C6-N1	7.74	121.57	117.70
53	BA	1607	C	N3-C2-O2	-7.74	116.48	121.90
22	A1	41	A	C5-C6-N1	7.74	121.57	117.70
53	BA	165	A	C5-C6-N1	7.74	121.57	117.70
53	BA	590	A	N1-C6-N6	-7.74	113.96	118.60
53	BA	1117	C	N3-C2-O2	-7.74	116.48	121.90
22	A1	76	A	C4-C5-C6	-7.73	113.13	117.00
53	BA	592	A	C5-C6-N1	7.73	121.57	117.70
21	AA	878	A	C5-C6-N1	7.73	121.57	117.70
53	BA	2711	A	C5-C6-N1	7.73	121.57	117.70
21	AA	1430	A	C4-C5-C6	-7.73	113.14	117.00
53	BA	2134	A	C5-C6-N1	7.73	121.56	117.70
53	BA	2147	A	C4-C5-C6	-7.73	113.13	117.00
53	BA	990	A	N1-C6-N6	-7.73	113.96	118.60
53	BA	1262	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	1227	A	O4'-C1'-N9	7.73	114.38	108.20
22	A1	58	A	C5-C6-N1	7.73	121.56	117.70
53	BA	2183	A	C4-C5-C6	-7.73	113.14	117.00
53	BA	706	A	C4-C5-C6	-7.72	113.14	117.00
21	AA	1252	A	N1-C6-N6	-7.72	113.97	118.60
53	BA	382	A	C5-C6-N1	7.72	121.56	117.70
53	BA	2378	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	353	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	883	C	N3-C2-O2	-7.72	116.50	121.90
21	AA	967	C	N3-C2-O2	-7.72	116.50	121.90
53	BA	863	A	N1-C6-N6	-7.72	113.97	118.60
53	BA	19	A	N1-C6-N6	-7.72	113.97	118.60
53	BA	529	A	N1-C6-N6	-7.72	113.97	118.60
53	BA	2176	A	C4-C5-C6	-7.72	113.14	117.00
53	BA	1129	A	C5-C6-N1	7.71	121.56	117.70
53	BA	1803	A	N1-C6-N6	-7.71	113.97	118.60
53	BA	947	A	C5-C6-N1	7.71	121.56	117.70
53	BA	218	A	N1-C6-N6	-7.71	113.97	118.60
20	AU	16	ARG	NE-CZ-NH1	7.71	124.15	120.30
21	AA	1179	A	N1-C6-N6	-7.71	113.97	118.60
53	BA	1977	A	C5-C6-N1	7.71	121.55	117.70
21	AA	608	A	C5-C6-N1	7.71	121.55	117.70
53	BA	1342	A	C5-C6-N1	7.71	121.55	117.70
53	BA	294	A	C5-C6-N1	7.71	121.55	117.70
24	BC	216	ARG	NE-CZ-NH1	7.70	124.15	120.30
53	BA	1156	A	C4-C5-C6	-7.70	113.15	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2377	A	C5-C6-N1	7.70	121.55	117.70
21	AA	532	A	C5-C6-N1	7.70	121.55	117.70
53	BA	654	A	C5-C6-N1	7.70	121.55	117.70
21	AA	675	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	949	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	1000	A	N1-C6-N6	-7.70	113.98	118.60
20	AU	46	ARG	NE-CZ-NH1	7.70	124.15	120.30
21	AA	1111	A	C5-C6-N1	7.70	121.55	117.70
40	BS	95	ARG	NE-CZ-NH1	7.70	124.15	120.30
53	BA	1711	A	C4-C5-C6	-7.70	113.15	117.00
53	BA	2173	A	C5-C6-N1	7.70	121.55	117.70
53	BA	2453	A	C5-C6-N1	7.70	121.55	117.70
35	BN	30	ARG	NE-CZ-NH1	7.69	124.15	120.30
53	BA	10	A	C4-C5-C6	-7.69	113.15	117.00
53	BA	1708	C	N3-C2-O2	-7.69	116.52	121.90
21	AA	1502	A	O4'-C1'-N9	7.69	114.35	108.20
22	A1	69	A	N1-C6-N6	-7.69	113.98	118.60
53	BA	161	A	N1-C6-N6	-7.69	113.99	118.60
12	AM	112	ARG	NE-CZ-NH1	7.69	124.14	120.30
53	BA	863	A	C5-C6-N1	7.69	121.54	117.70
53	BA	2054	A	N1-C6-N6	-7.69	113.99	118.60
21	AA	1130	A	N1-C6-N6	-7.68	113.99	118.60
53	BA	1050	A	C5-C6-N1	7.68	121.54	117.70
53	BA	1810	A	C5-C6-N1	7.68	121.54	117.70
53	BA	2450	A	N1-C6-N6	-7.68	113.99	118.60
53	BA	449	A	C4-C5-C6	-7.68	113.16	117.00
53	BA	2359	C	N3-C2-O2	-7.68	116.52	121.90
21	AA	263	A	N1-C6-N6	-7.68	113.99	118.60
53	BA	2589	A	C5-C6-N1	7.68	121.54	117.70
21	AA	768	A	C4-C5-C6	-7.68	113.16	117.00
53	BA	2792	A	C5-C6-N1	7.68	121.54	117.70
53	BA	152	A	C5-C6-N1	7.68	121.54	117.70
21	AA	546	A	C4-C5-C6	-7.67	113.16	117.00
21	AA	878	A	C4-C5-C6	-7.67	113.16	117.00
53	BA	1327	A	C5-C6-N1	7.67	121.54	117.70
53	BA	1953	A	C5-C6-N1	7.67	121.54	117.70
21	AA	83	C	N3-C2-O2	-7.67	116.53	121.90
53	BA	876	C	N3-C2-O2	-7.67	116.53	121.90
53	BA	1103	A	C5-C6-N1	7.67	121.53	117.70
21	AA	309	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	1319	A	N1-C6-N6	-7.67	114.00	118.60
53	BA	2670	A	C5-C6-N1	7.67	121.53	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1871	A	C5-C6-N1	7.67	121.53	117.70
53	BA	2771	C	N3-C2-O2	-7.67	116.53	121.90
21	AA	67	C	N1-C2-O2	7.66	123.50	118.90
21	AA	1456	A	N1-C6-N6	-7.66	114.00	118.60
21	AA	915	A	C5-C6-N1	7.66	121.53	117.70
21	AA	363	A	C5-C6-N1	7.66	121.53	117.70
53	BA	547	A	C5-C6-N1	7.66	121.53	117.70
53	BA	1570	A	C4-C5-C6	-7.66	113.17	117.00
53	BA	1728	C	N1-C2-O2	7.66	123.50	118.90
53	BA	1872	A	N1-C6-N6	-7.66	114.00	118.60
53	BA	2536	G	O4'-C1'-N9	7.66	114.33	108.20
53	BA	1009	A	N1-C6-N6	-7.66	114.01	118.60
53	BA	2478	A	C5-C6-N1	7.66	121.53	117.70
53	BA	2062	A	O4'-C1'-N9	7.66	114.32	108.20
53	BA	2314	A	C5-C6-N1	7.66	121.53	117.70
21	AA	162	A	N1-C6-N6	-7.65	114.01	118.60
53	BA	257	C	O4'-C1'-N1	7.65	114.32	108.20
21	AA	918	A	N1-C6-N6	-7.65	114.01	118.60
53	BA	1952	A	C5-C6-N1	7.65	121.53	117.70
53	BA	149	A	N1-C6-N6	-7.65	114.01	118.60
53	BA	1090	A	N1-C6-N6	-7.65	114.01	118.60
53	BA	1236	G	O4'-C1'-N9	7.65	114.32	108.20
21	AA	306	A	C5-C6-N1	7.65	121.52	117.70
33	BL	60	ARG	NE-CZ-NH1	7.65	124.12	120.30
53	BA	644	A	C5-C6-N1	7.65	121.52	117.70
53	BA	988	A	C5-C6-N1	7.64	121.52	117.70
21	AA	694	A	N1-C6-N6	-7.64	114.02	118.60
53	BA	126	A	N1-C6-N6	-7.64	114.02	118.60
21	AA	412	A	C5-C6-N1	7.64	121.52	117.70
21	AA	640	A	N1-C6-N6	-7.64	114.02	118.60
21	AA	1306	A	C5-C6-N1	7.64	121.52	117.70
53	BA	118	A	C5-C6-N1	7.64	121.52	117.70
53	BA	722	A	C5-C6-N1	7.64	121.52	117.70
53	BA	2860	A	C5-C6-N1	7.64	121.52	117.70
53	BA	2326	C	N3-C2-O2	-7.64	116.55	121.90
53	BA	346	A	C5-C6-N1	7.64	121.52	117.70
53	BA	1274	A	C5-C6-N1	7.64	121.52	117.70
21	AA	918	A	C5-C6-N1	7.63	121.52	117.70
48	B0	9	ARG	NE-CZ-NH2	7.63	124.12	120.30
53	BA	515	A	C5-C6-N1	7.63	121.52	117.70
53	BA	2498	C	O4'-C1'-N1	7.63	114.31	108.20
53	BA	1879	C	N3-C2-O2	-7.63	116.56	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	586	A	C5-C6-N1	7.63	121.52	117.70
53	BA	960	A	C5-C6-N1	7.63	121.52	117.70
53	BA	1403	A	N1-C6-N6	-7.63	114.02	118.60
53	BA	1745	A	N1-C6-N6	-7.63	114.02	118.60
53	BA	2476	A	C5-C6-N1	7.63	121.51	117.70
21	AA	825	A	C5-C6-N1	7.63	121.51	117.70
54	BB	46	A	C5-C6-N1	7.63	121.51	117.70
21	AA	629	A	C5-C6-N1	7.62	121.51	117.70
21	AA	816	A	C5-C6-N1	7.62	121.51	117.70
53	BA	1213	A	C4-C5-C6	-7.62	113.19	117.00
53	BA	1656	C	N3-C2-O2	-7.62	116.56	121.90
21	AA	1054	C	O4'-C1'-N1	7.62	114.30	108.20
53	BA	1143	A	C5-C6-N1	7.62	121.51	117.70
21	AA	432	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	1031	C	N1-C2-O2	7.62	123.47	118.90
53	BA	897	C	N3-C2-O2	-7.62	116.57	121.90
53	BA	2755	C	N3-C2-O2	-7.62	116.57	121.90
21	AA	28	A	C5-C6-N1	7.62	121.51	117.70
21	AA	468	A	C5-C6-N1	7.62	121.51	117.70
53	BA	888	C	N3-C2-O2	-7.62	116.57	121.90
21	AA	182	A	C5-C6-N1	7.62	121.51	117.70
53	BA	1434	A	C5-C6-N1	7.62	121.51	117.70
53	BA	2205	A	C5-C6-N1	7.62	121.51	117.70
21	AA	502	A	N1-C6-N6	-7.61	114.03	118.60
21	AA	1510	C	N3-C2-O2	-7.61	116.57	121.90
53	BA	454	A	N1-C6-N6	-7.61	114.03	118.60
53	BA	2565	A	N1-C6-N6	-7.61	114.03	118.60
53	BA	1953	A	C4-C5-C6	-7.61	113.19	117.00
21	AA	1433	A	C5-C6-N1	7.61	121.51	117.70
53	BA	563	A	C5-C6-N1	7.61	121.50	117.70
53	BA	626	A	C5-C6-N1	7.61	121.50	117.70
34	BM	50	ARG	NE-CZ-NH1	7.61	124.10	120.30
53	BA	2287	A	N1-C6-N6	-7.61	114.03	118.60
50	B2	14	ARG	NE-CZ-NH1	7.61	124.10	120.30
53	BA	1315	C	N3-C2-O2	-7.61	116.57	121.90
53	BA	2248	C	N3-C2-O2	-7.61	116.58	121.90
21	AA	1327	C	N3-C2-O2	-7.61	116.58	121.90
53	BA	1233	C	N3-C2-O2	-7.61	116.58	121.90
53	BA	1287	A	C4-C5-C6	-7.61	113.20	117.00
53	BA	2430	A	C5-C6-N1	7.60	121.50	117.70
21	AA	188	C	N3-C2-O2	-7.60	116.58	121.90
21	AA	496	A	C5-C6-N1	7.60	121.50	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1876	A	N1-C6-N6	-7.60	114.04	118.60
25	BD	83	ARG	NE-CZ-NH1	7.60	124.10	120.30
53	BA	517	C	O4'-C1'-N1	7.60	114.28	108.20
21	AA	1336	C	N1-C2-O2	7.60	123.46	118.90
54	BB	57	A	C5-C6-N1	7.60	121.50	117.70
53	BA	1090	A	C4-C5-C6	-7.60	113.20	117.00
53	BA	1701	A	C5-C6-N1	7.60	121.50	117.70
21	AA	547	A	C4-C5-C6	-7.59	113.20	117.00
53	BA	634	C	N3-C2-O2	-7.59	116.58	121.90
53	BA	1916	A	C5-C6-N1	7.59	121.50	117.70
21	AA	171	A	C4-C5-C6	-7.59	113.20	117.00
21	AA	1145	A	C5-C6-N1	7.59	121.50	117.70
31	BJ	96	ARG	NE-CZ-NH2	7.59	124.09	120.30
53	BA	2900	A	N1-C6-N6	-7.59	114.05	118.60
21	AA	334	C	N3-C2-O2	-7.59	116.59	121.90
35	BN	86	ARG	NE-CZ-NH1	7.59	124.09	120.30
5	AF	44	ARG	NE-CZ-NH1	7.58	124.09	120.30
21	AA	1096	C	N3-C2-O2	-7.58	116.59	121.90
53	BA	2497	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1000	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1132	C	N3-C2-O2	-7.58	116.59	121.90
21	AA	547	A	C5-C6-N1	7.58	121.49	117.70
40	BS	110	ARG	NE-CZ-NH2	7.58	124.09	120.30
21	AA	1245	C	N3-C2-O2	-7.58	116.60	121.90
53	BA	1566	A	C5-C6-N1	7.58	121.49	117.70
25	BD	124	ARG	NE-CZ-NH1	7.57	124.09	120.30
53	BA	793	A	C5-C6-N1	7.57	121.49	117.70
53	BA	1264	A	C5-C6-N1	7.57	121.49	117.70
53	BA	788	A	N1-C6-N6	-7.57	114.06	118.60
53	BA	791	C	N3-C2-O2	-7.57	116.60	121.90
6	AG	118	ARG	NE-CZ-NH1	7.57	124.08	120.30
21	AA	195	A	C4-C5-C6	-7.57	113.22	117.00
21	AA	478	A	C5-C6-N1	7.57	121.48	117.70
53	BA	1384	A	C4-C5-C6	-7.57	113.22	117.00
53	BA	2015	A	C5-C6-N1	7.57	121.48	117.70
53	BA	182	A	N1-C6-N6	-7.56	114.06	118.60
21	AA	1283	U	N3-C2-O2	-7.56	116.91	122.20
53	BA	161	A	C5-C6-N1	7.56	121.48	117.70
21	AA	8	A	C5-C6-N1	7.56	121.48	117.70
21	AA	414	A	N1-C6-N6	-7.56	114.06	118.60
21	AA	1534	A	C5-C6-N1	7.56	121.48	117.70
53	BA	925	A	C5-C6-N1	7.56	121.48	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1802	A	C5-C6-N1	7.56	121.48	117.70
53	BA	2425	A	C4-C5-C6	-7.56	113.22	117.00
21	AA	1151	A	N1-C6-N6	-7.56	114.06	118.60
53	BA	1260	A	N1-C6-N6	-7.56	114.06	118.60
21	AA	1374	A	C4-C5-C6	-7.55	113.22	117.00
53	BA	10	A	C5-C6-N1	7.55	121.47	117.70
53	BA	1140	C	O4'-C1'-N1	7.55	114.24	108.20
21	AA	1274	A	C5-C6-N1	7.55	121.47	117.70
53	BA	2666	C	N3-C2-O2	-7.55	116.61	121.90
53	BA	61	C	N3-C2-O2	-7.55	116.62	121.90
53	BA	2590	A	C4-C5-C6	-7.55	113.23	117.00
53	BA	505	A	C5-C6-N1	7.54	121.47	117.70
21	AA	431	A	N1-C6-N6	-7.54	114.07	118.60
22	A1	66	A	C5-C6-N1	7.54	121.47	117.70
53	BA	2606	C	N3-C2-O2	-7.54	116.62	121.90
21	AA	321	A	C5-C6-N1	7.54	121.47	117.70
53	BA	1109	C	N3-C2-O2	-7.54	116.62	121.90
53	BA	2374	C	N3-C2-O2	-7.54	116.62	121.90
53	BA	2577	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	802	A	C5-C6-N1	7.54	121.47	117.70
53	BA	1761	C	N1-C2-O2	7.54	123.42	118.90
53	BA	105	C	O4'-C1'-N1	7.54	114.23	108.20
53	BA	1152	C	N3-C2-O2	-7.54	116.62	121.90
53	BA	735	A	N1-C6-N6	-7.54	114.08	118.60
53	BA	1096	A	C5-C6-N1	7.54	121.47	117.70
21	AA	129	A	C5-C6-N1	7.54	121.47	117.70
53	BA	415	A	C5-C6-N1	7.54	121.47	117.70
21	AA	309	A	C5-C6-N1	7.53	121.47	117.70
53	BA	2082	A	C5-C6-N1	7.53	121.47	117.70
53	BA	672	C	N3-C2-O2	-7.53	116.63	121.90
53	BA	1378	A	C4-C5-C6	-7.53	113.23	117.00
3	AD	103	ARG	NE-CZ-NH2	-7.53	116.53	120.30
21	AA	1408	A	C5-C6-N1	7.53	121.47	117.70
53	BA	2792	A	N1-C6-N6	-7.53	114.08	118.60
21	AA	1499	A	C5-C6-N1	7.53	121.47	117.70
54	BB	12	C	N3-C2-O2	-7.53	116.63	121.90
53	BA	2469	A	C5-C6-N1	7.53	121.46	117.70
53	BA	1791	A	C5-C6-N1	7.52	121.46	117.70
53	BA	515	A	C4-C5-C6	-7.52	113.24	117.00
53	BA	1010	A	C5-C6-N1	7.52	121.46	117.70
53	BA	1894	C	N1-C2-O2	7.52	123.41	118.90
21	AA	749	A	C5-C6-N1	7.52	121.46	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	227	A	C5-C6-N1	7.52	121.46	117.70
53	BA	1264	A	N1-C6-N6	-7.52	114.09	118.60
53	BA	1677	A	C5-C6-N1	7.52	121.46	117.70
53	BA	2103	C	O4'-C1'-N1	7.52	114.21	108.20
53	BA	643	A	N1-C6-N6	-7.52	114.09	118.60
53	BA	892	A	C5-C6-N1	7.52	121.46	117.70
53	BA	401	A	C5-C6-N1	7.51	121.46	117.70
53	BA	1762	A	C5-C6-N1	7.51	121.46	117.70
53	BA	655	A	C5-C6-N1	7.51	121.46	117.70
53	BA	936	A	N1-C6-N6	-7.51	114.09	118.60
53	BA	1603	A	C4-C5-C6	-7.51	113.24	117.00
53	BA	2369	A	C4-C5-C6	-7.51	113.24	117.00
21	AA	167	A	C5-C6-N1	7.51	121.45	117.70
53	BA	435	C	N3-C2-O2	-7.51	116.64	121.90
21	AA	16	A	C5-C6-N1	7.51	121.45	117.70
21	AA	1230	C	N3-C2-O2	-7.51	116.65	121.90
53	BA	2031	A	N1-C6-N6	-7.51	114.10	118.60
53	BA	2184	A	N1-C6-N6	-7.51	114.10	118.60
21	AA	873	A	C4-C5-C6	-7.50	113.25	117.00
21	AA	1289	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1376	U	O4'-C1'-N1	7.50	114.20	108.20
53	BA	671	C	N3-C2-O2	-7.50	116.65	121.90
54	BB	36	C	O4'-C1'-N1	7.50	114.20	108.20
21	AA	807	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1105	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	286	C	N3-C2-O2	-7.50	116.65	121.90
21	AA	155	A	C5-C6-N1	7.50	121.45	117.70
21	AA	499	A	C4-C5-C6	-7.50	113.25	117.00
21	AA	1344	C	N3-C2-O2	-7.50	116.65	121.90
53	BA	121	G	O4'-C1'-N9	7.50	114.20	108.20
21	AA	1044	A	C4-C5-C6	-7.50	113.25	117.00
34	BM	59	ARG	NE-CZ-NH1	7.50	124.05	120.30
53	BA	423	A	C4-C5-C6	-7.49	113.25	117.00
53	BA	430	A	N1-C6-N6	-7.49	114.10	118.60
21	AA	819	A	C4-C5-C6	-7.49	113.25	117.00
53	BA	2005	A	C4-C5-C6	-7.49	113.25	117.00
21	AA	546	A	N1-C6-N6	-7.49	114.11	118.60
53	BA	801	G	N3-C2-N2	-7.49	114.66	119.90
53	BA	2741	A	C5-C6-N1	7.49	121.44	117.70
53	BA	1311	G	N3-C2-N2	-7.49	114.66	119.90
21	AA	583	A	N1-C6-N6	-7.49	114.11	118.60
53	BA	804	A	C5-C6-N1	7.49	121.44	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1987	A	N1-C6-N6	-7.49	114.11	118.60
53	BA	57	C	N3-C2-O2	-7.48	116.66	121.90
53	BA	607	U	O4'-C1'-N1	7.48	114.18	108.20
53	BA	2835	A	C4-C5-C6	-7.48	113.26	117.00
8	AI	48	ARG	NE-CZ-NH1	7.48	124.04	120.30
53	BA	2888	C	N3-C2-O2	-7.48	116.67	121.90
21	AA	1136	C	N3-C2-O2	-7.48	116.67	121.90
53	BA	2667	C	N3-C2-O2	-7.48	116.67	121.90
21	AA	336	A	N1-C6-N6	-7.48	114.11	118.60
21	AA	974	A	C4-C5-C6	-7.48	113.26	117.00
53	BA	56	A	C5-C6-N1	7.48	121.44	117.70
21	AA	1167	A	N1-C6-N6	-7.47	114.12	118.60
35	BN	63	ARG	NE-CZ-NH1	7.47	124.04	120.30
53	BA	2468	A	C4-C5-C6	-7.47	113.26	117.00
21	AA	1349	A	C5-C6-N1	7.47	121.44	117.70
53	BA	1244	A	C4-C5-C6	-7.47	113.26	117.00
53	BA	2585	U	O4'-C1'-N1	7.47	114.18	108.20
54	BB	97	C	N3-C2-O2	-7.47	116.67	121.90
53	BA	992	C	O4'-C1'-N1	7.47	114.18	108.20
53	BA	2628	C	N1-C2-O2	7.47	123.38	118.90
21	AA	80	A	C5-C6-N1	7.47	121.44	117.70
53	BA	1993	U	O4'-C1'-N1	7.47	114.17	108.20
53	BA	2275	C	N3-C2-O2	-7.47	116.67	121.90
53	BA	2291	U	O4'-C1'-N1	7.47	114.17	108.20
21	AA	649	A	C4-C5-C6	-7.47	113.27	117.00
41	BT	12	ARG	NE-CZ-NH1	7.47	124.03	120.30
21	AA	193	C	N3-C2-O2	-7.46	116.67	121.90
21	AA	998	C	N3-C2-O2	-7.46	116.67	121.90
53	BA	1591	A	C4-C5-C6	-7.46	113.27	117.00
21	AA	906	A	C5-C6-N1	7.46	121.43	117.70
21	AA	647	C	N3-C2-O2	-7.46	116.68	121.90
53	BA	2600	A	C5-C6-N1	7.46	121.43	117.70
21	AA	696	A	N1-C6-N6	-7.46	114.13	118.60
53	BA	1630	A	C4-C5-C6	-7.46	113.27	117.00
53	BA	2142	A	N1-C6-N6	-7.46	114.13	118.60
54	BB	88	C	N3-C2-O2	-7.46	116.68	121.90
53	BA	1610	A	N1-C6-N6	-7.45	114.13	118.60
53	BA	1679	A	C4-C5-C6	-7.45	113.27	117.00
53	BA	89	A	C4-C5-C6	-7.45	113.28	117.00
53	BA	1095	A	C4-C5-C6	-7.45	113.27	117.00
53	BA	788	A	O4'-C1'-N9	7.45	114.16	108.20
53	BA	1787	A	C4-C5-C6	-7.45	113.28	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	756	A	C4-C5-C6	-7.45	113.28	117.00
21	AA	320	A	C5-C6-N1	7.45	121.42	117.70
22	A1	16	C	N1-C2-O2	7.45	123.37	118.90
53	BA	699	A	C5-C6-N1	7.45	121.42	117.70
53	BA	1118	C	N3-C2-O2	-7.45	116.69	121.90
53	BA	2736	A	N1-C6-N6	-7.45	114.13	118.60
53	BA	2142	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	995	C	N1-C2-O2	7.44	123.36	118.90
21	AA	1451	U	O4'-C1'-N1	7.44	114.15	108.20
53	BA	374	A	N1-C6-N6	-7.44	114.13	118.60
53	BA	1787	A	C5-C6-N1	7.44	121.42	117.70
3	AD	55	ARG	NE-CZ-NH1	7.44	124.02	120.30
53	BA	262	A	C5-C6-N1	7.44	121.42	117.70
53	BA	2639	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	196	A	C4-C5-C6	-7.44	113.28	117.00
53	BA	2566	A	C5-C6-N1	7.43	121.42	117.70
21	AA	463	U	O4'-C1'-N1	7.43	114.15	108.20
53	BA	1304	A	C5-C6-N1	7.43	121.42	117.70
53	BA	2654	A	C5-C6-N1	7.43	121.42	117.70
21	AA	397	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	855	U	O4'-C1'-N1	7.43	114.14	108.20
21	AA	1468	A	N1-C6-N6	-7.43	114.14	118.60
39	BR	68	ARG	NE-CZ-NH1	7.43	124.01	120.30
21	AA	931	C	O4'-C1'-N1	7.42	114.14	108.20
21	AA	959	A	C4-C5-C6	-7.42	113.29	117.00
53	BA	1795	C	N3-C2-O2	-7.42	116.71	121.90
1	AB	138	ARG	NE-CZ-NH1	7.42	124.01	120.30
21	AA	116	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	270	A	C5-C6-N1	7.42	121.41	117.70
21	AA	812	G	O4'-C1'-N9	7.42	114.13	108.20
53	BA	1774	C	N3-C2-O2	-7.42	116.71	121.90
53	BA	2039	U	O4'-C1'-N1	7.42	114.13	108.20
53	BA	2080	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	1346	A	O4'-C1'-N9	7.41	114.13	108.20
53	BA	1286	A	C5-C6-N1	7.41	121.41	117.70
53	BA	2761	A	C4-C5-C6	-7.41	113.29	117.00
53	BA	89	A	C5-C6-N1	7.41	121.41	117.70
53	BA	1694	C	N3-C2-O2	-7.41	116.71	121.90
53	BA	2720	U	O4'-C1'-N1	7.41	114.13	108.20
21	AA	937	A	C4-C5-C6	-7.41	113.30	117.00
53	BA	523	C	N3-C2-O2	-7.41	116.71	121.90
53	BA	627	A	C4-C5-C6	-7.41	113.30	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	675	A	C5-C6-N1	7.41	121.40	117.70
53	BA	730	A	N1-C6-N6	-7.41	114.16	118.60
53	BA	2886	A	C4-C5-C6	-7.41	113.30	117.00
21	AA	329	A	C4-C5-C6	-7.41	113.30	117.00
53	BA	131	A	C5-C6-N1	7.41	121.40	117.70
21	AA	718	A	C5-C6-N1	7.41	121.40	117.70
53	BA	2471	A	N1-C6-N6	-7.41	114.16	118.60
53	BA	2031	A	C4-C5-C6	-7.40	113.30	117.00
21	AA	1225	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	1418	A	N1-C6-N6	-7.40	114.16	118.60
29	BH	27	ARG	NE-CZ-NH1	7.40	124.00	120.30
53	BA	2462	C	N3-C2-O2	-7.40	116.72	121.90
4	AE	53	ARG	NE-CZ-NH2	7.40	124.00	120.30
21	AA	1363	A	C5-C6-N1	7.40	121.40	117.70
35	BN	90	ARG	NE-CZ-NH1	7.40	124.00	120.30
53	BA	1847	A	N1-C6-N6	-7.40	114.16	118.60
53	BA	2809	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	55	A	N1-C6-N6	-7.40	114.16	118.60
53	BA	231	A	C5-C6-N1	7.40	121.40	117.70
53	BA	384	A	C4-C5-C6	-7.40	113.30	117.00
53	BA	2806	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	631	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	1151	A	C5-C6-N1	7.40	121.40	117.70
53	BA	402	A	C4-C5-C6	-7.40	113.30	117.00
53	BA	743	A	C5-C6-N1	7.40	121.40	117.70
53	BA	1551	A	C5-C6-N1	7.40	121.40	117.70
53	BA	2800	A	C4-C5-C6	-7.40	113.30	117.00
53	BA	2835	A	C5-C6-N1	7.40	121.40	117.70
21	AA	738	C	N3-C2-O2	-7.40	116.72	121.90
20	AU	20	ARG	NE-CZ-NH1	7.39	124.00	120.30
33	BL	69	ARG	NE-CZ-NH1	7.39	124.00	120.30
53	BA	91	A	C5-C6-N1	7.39	121.40	117.70
21	AA	1055	A	C5-C6-N1	7.39	121.40	117.70
53	BA	1396	U	O4'-C1'-N1	7.39	114.11	108.20
53	BA	1586	A	C5-C6-N1	7.39	121.40	117.70
53	BA	1650	A	N1-C6-N6	-7.39	114.16	118.60
53	BA	517	C	N3-C2-O2	-7.39	116.73	121.90
53	BA	1582	C	N3-C2-O2	-7.39	116.73	121.90
21	AA	1274	A	C4-C5-C6	-7.39	113.31	117.00
53	BA	244	A	C4-C5-C6	-7.39	113.31	117.00
53	BA	1151	A	N1-C6-N6	-7.39	114.17	118.60
22	A1	25	C	N3-C2-O2	-7.39	116.73	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	735	A	C5-C6-N1	7.39	121.39	117.70
53	BA	1090	A	C5-C6-N1	7.39	121.39	117.70
53	BA	1508	A	O4'-C1'-N9	7.39	114.11	108.20
53	BA	1387	A	C5-C6-N1	7.39	121.39	117.70
53	BA	1676	A	N1-C6-N6	-7.39	114.17	118.60
53	BA	2014	A	N1-C6-N6	-7.39	114.17	118.60
21	AA	919	A	C5-C6-N1	7.38	121.39	117.70
50	B2	39	ARG	NE-CZ-NH1	7.38	123.99	120.30
53	BA	718	A	N1-C6-N6	-7.38	114.17	118.60
53	BA	1096	A	C4-C5-C6	-7.38	113.31	117.00
53	BA	2632	A	C5-C6-N1	7.38	121.39	117.70
21	AA	10	A	C4-C5-C6	-7.38	113.31	117.00
21	AA	649	A	C5-C6-N1	7.38	121.39	117.70
53	BA	480	A	C5-C6-N1	7.38	121.39	117.70
53	BA	749	A	C5-C6-N1	7.38	121.39	117.70
53	BA	1196	C	N3-C2-O2	-7.38	116.73	121.90
21	AA	1267	C	N1-C2-O2	7.38	123.33	118.90
53	BA	734	A	C5-C6-N1	7.38	121.39	117.70
53	BA	62	U	O4'-C1'-N1	7.38	114.10	108.20
53	BA	71	A	O4'-C1'-N9	7.38	114.10	108.20
53	BA	1413	A	C4-C5-C6	-7.38	113.31	117.00
54	BB	34	A	C5-C6-N1	7.38	121.39	117.70
8	AI	122	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	622	A	C4-C5-C6	-7.38	113.31	117.00
53	BA	1705	A	C4-C5-C6	-7.38	113.31	117.00
21	AA	728	A	C5-C6-N1	7.37	121.39	117.70
53	BA	404	A	C4-C5-C6	-7.37	113.31	117.00
53	BA	666	A	C5-C6-N1	7.37	121.39	117.70
53	BA	1871	A	N1-C6-N6	-7.37	114.18	118.60
53	BA	2628	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	663	A	C4-C5-C6	-7.37	113.32	117.00
21	AA	814	A	C5-C6-N1	7.37	121.38	117.70
21	AA	1059	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	1369	C	N3-C2-O2	-7.37	116.74	121.90
53	BA	908	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	67	C	N3-C2-O2	-7.37	116.74	121.90
53	BA	1962	C	N3-C2-O2	-7.37	116.74	121.90
14	AO	52	ARG	NE-CZ-NH1	7.36	123.98	120.30
21	AA	969	A	C5-C6-N1	7.36	121.38	117.70
53	BA	323	C	N1-C2-O2	7.36	123.32	118.90
53	BA	1978	A	C4-C5-C6	-7.36	113.32	117.00
53	BA	2261	C	N3-C2-O2	-7.36	116.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1434	A	C5-C6-N1	7.36	121.38	117.70
53	BA	2706	A	N1-C6-N6	-7.36	114.18	118.60
22	A1	38	A	N1-C6-N6	-7.36	114.18	118.60
53	BA	1321	A	C5-C6-N1	7.36	121.38	117.70
53	BA	1591	A	C5-C6-N1	7.36	121.38	117.70
21	AA	77	A	N1-C6-N6	-7.36	114.19	118.60
21	AA	393	A	N1-C6-N6	-7.36	114.19	118.60
21	AA	1234	C	N3-C2-O2	-7.36	116.75	121.90
53	BA	889	C	N3-C2-O2	-7.36	116.75	121.90
53	BA	1029	A	C4-C5-C6	-7.36	113.32	117.00
53	BA	2161	C	N3-C2-O2	-7.35	116.75	121.90
53	BA	816	C	N3-C2-O2	-7.35	116.75	121.90
21	AA	1519	A	N1-C6-N6	-7.35	114.19	118.60
53	BA	1836	C	N3-C2-O2	-7.35	116.75	121.90
21	AA	5	U	O4'-C1'-N1	7.35	114.08	108.20
21	AA	381	C	N3-C2-O2	-7.35	116.75	121.90
21	AA	792	A	N1-C6-N6	-7.35	114.19	118.60
53	BA	1158	C	N3-C2-O2	-7.35	116.76	121.90
53	BA	1689	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	1302	C	N3-C2-O2	-7.35	116.76	121.90
53	BA	1764	C	N3-C2-O2	-7.35	116.76	121.90
53	BA	2169	A	O4'-C1'-N9	7.35	114.08	108.20
54	BB	78	A	C5-C6-N1	7.35	121.37	117.70
53	BA	1040	A	C5-C6-N1	7.35	121.37	117.70
53	BA	2381	A	C5-C6-N1	7.35	121.37	117.70
6	AG	108	ARG	NE-CZ-NH1	7.34	123.97	120.30
53	BA	354	A	N1-C6-N6	-7.34	114.19	118.60
21	AA	415	A	C5-C6-N1	7.34	121.37	117.70
21	AA	680	C	N3-C2-O2	-7.34	116.76	121.90
53	BA	1672	A	C4-C5-C6	-7.34	113.33	117.00
12	AM	2	ARG	NE-CZ-NH1	7.34	123.97	120.30
21	AA	279	A	C5-C6-N1	7.34	121.37	117.70
21	AA	971	G	O4'-C1'-N9	7.34	114.07	108.20
21	AA	1465	A	C4-C5-C6	-7.34	113.33	117.00
53	BA	268	C	N3-C2-O2	-7.34	116.76	121.90
53	BA	1799	G	C8-N9-C4	-7.34	103.46	106.40
21	AA	177	G	O4'-C1'-N9	7.34	114.07	108.20
53	BA	737	C	O4'-C1'-N1	7.34	114.07	108.20
53	BA	1027	A	C4-C5-C6	-7.34	113.33	117.00
53	BA	270	A	C4-C5-C6	-7.33	113.33	117.00
53	BA	2199	A	N1-C6-N6	-7.33	114.20	118.60
53	BA	2750	A	C5-C6-N1	7.33	121.37	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1272	A	O4'-C1'-N9	7.33	114.07	108.20
53	BA	1505	A	C5-C6-N1	7.33	121.37	117.70
53	BA	509	C	N3-C2-O2	-7.33	116.77	121.90
53	BA	2426	A	C5-C6-N1	7.33	121.36	117.70
21	AA	124	C	N3-C2-O2	-7.33	116.77	121.90
53	BA	1092	C	O4'-C1'-N1	7.33	114.06	108.20
53	BA	2705	A	C5-C6-N1	7.33	121.36	117.70
53	BA	843	G	O4'-C1'-N9	7.33	114.06	108.20
21	AA	271	C	O4'-C1'-N1	7.32	114.06	108.20
53	BA	83	A	C5-C6-N1	7.32	121.36	117.70
53	BA	927	A	N1-C6-N6	-7.32	114.21	118.60
54	BB	73	A	C5-C6-N1	7.32	121.36	117.70
53	BA	213	A	C5-C6-N1	7.32	121.36	117.70
53	BA	391	A	C4-C5-C6	-7.32	113.34	117.00
53	BA	1706	C	N3-C2-O2	-7.32	116.78	121.90
53	BA	1905	C	N3-C2-O2	-7.32	116.78	121.90
53	BA	2126	A	C5-C6-N1	7.32	121.36	117.70
53	BA	125	A	C4-C5-C6	-7.32	113.34	117.00
21	AA	262	A	C5-C6-N1	7.32	121.36	117.70
53	BA	2392	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	1350	A	N7-C8-N9	7.31	117.46	113.80
53	BA	2072	C	N3-C2-O2	-7.31	116.78	121.90
53	BA	2840	C	N3-C2-O2	-7.31	116.78	121.90
21	AA	780	A	C5-C6-N1	7.31	121.36	117.70
23	A2	91	A	C5-C6-N1	7.31	121.36	117.70
53	BA	1237	A	C5-C6-N1	7.31	121.36	117.70
21	AA	658	C	N3-C2-O2	-7.31	116.78	121.90
21	AA	1130	A	C5-C6-N1	7.31	121.36	117.70
53	BA	2000	C	N3-C2-O2	-7.31	116.78	121.90
21	AA	108	G	O4'-C1'-N9	7.31	114.05	108.20
21	AA	825	A	C4-C5-C6	-7.31	113.34	117.00
53	BA	689	A	C5-C6-N1	7.31	121.36	117.70
53	BA	1932	A	C4-C5-C6	-7.31	113.34	117.00
53	BA	2467	C	N3-C2-O2	-7.31	116.78	121.90
21	AA	1453	G	O4'-C1'-N9	7.31	114.05	108.20
22	A1	60	C	N1-C2-O2	7.31	123.28	118.90
53	BA	479	A	C5-C6-N1	7.31	121.35	117.70
53	BA	1535	A	C4-C5-C6	-7.31	113.35	117.00
53	BA	1669	A	C4-C5-C6	-7.31	113.35	117.00
53	BA	1786	A	N1-C6-N6	-7.31	114.22	118.60
53	BA	2601	C	N3-C2-O2	-7.31	116.78	121.90
21	AA	1430	A	C5-C6-N1	7.30	121.35	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1134	A	C4-C5-C6	-7.30	113.35	117.00
53	BA	172	A	N1-C6-N6	-7.30	114.22	118.60
53	BA	2727	A	C5-C6-N1	7.30	121.35	117.70
3	AD	2	ARG	NE-CZ-NH1	7.30	123.95	120.30
21	AA	579	A	C5-C6-N1	7.30	121.35	117.70
53	BA	896	A	C5-C6-N1	7.30	121.35	117.70
54	BB	36	C	N1-C2-O2	7.30	123.28	118.90
21	AA	596	A	N1-C6-N6	-7.30	114.22	118.60
53	BA	635	C	N3-C2-O2	-7.30	116.79	121.90
54	BB	62	C	N3-C2-O2	-7.30	116.79	121.90
21	AA	554	A	C5-C6-N1	7.29	121.35	117.70
21	AA	787	A	C4-C5-C6	-7.29	113.35	117.00
53	BA	236	C	N3-C2-O2	-7.29	116.80	121.90
53	BA	1918	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	71	A	C5-C6-N1	7.29	121.35	117.70
21	AA	253	A	C5-C6-N1	7.29	121.35	117.70
53	BA	2019	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	1169	A	C5-C6-N1	7.29	121.34	117.70
21	AA	98	A	C4-C5-C6	-7.29	113.36	117.00
21	AA	243	A	C5-C6-N1	7.29	121.34	117.70
21	AA	1000	A	C4-C5-C6	-7.29	113.36	117.00
53	BA	1393	A	N1-C6-N6	-7.29	114.23	118.60
53	BA	1020	A	N1-C6-N6	-7.29	114.23	118.60
53	BA	1802	A	C4-C5-C6	-7.29	113.36	117.00
53	BA	2117	A	C4-C5-C6	-7.28	113.36	117.00
21	AA	1431	A	C5-C6-N1	7.28	121.34	117.70
53	BA	718	A	C5-C6-N1	7.28	121.34	117.70
53	BA	722	A	C4-C5-C6	-7.28	113.36	117.00
21	AA	460	A	C5-C6-N1	7.28	121.34	117.70
53	BA	1632	A	N1-C6-N6	-7.28	114.23	118.60
21	AA	712	A	C4-C5-C6	-7.28	113.36	117.00
53	BA	433	C	N3-C2-O2	-7.28	116.81	121.90
53	BA	2733	A	C5-C6-N1	7.28	121.34	117.70
53	BA	1574	C	N3-C2-O2	-7.27	116.81	121.90
53	BA	2322	A	N1-C6-N6	-7.27	114.24	118.60
53	BA	730	A	C5-C6-N1	7.27	121.33	117.70
53	BA	823	C	N3-C2-O2	-7.27	116.81	121.90
4	AE	92	ARG	NE-CZ-NH1	7.27	123.94	120.30
21	AA	1201	A	P-O3'-C3'	7.27	128.42	119.70
53	BA	936	A	C4-C5-C6	-7.27	113.36	117.00
21	AA	236	A	C5-C6-N1	7.27	121.33	117.70
21	AA	871	U	O4'-C1'-N1	7.27	114.01	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1961	C	N3-C2-O2	-7.27	116.81	121.90
53	BA	2456	C	N3-C2-O2	-7.27	116.81	121.90
21	AA	729	A	C5-C6-N1	7.26	121.33	117.70
30	BI	126	ARG	NE-CZ-NH1	7.26	123.93	120.30
53	BA	63	A	C4-C5-C6	-7.26	113.37	117.00
53	BA	1121	C	N3-C2-O2	-7.26	116.81	121.90
53	BA	1387	A	O4'-C1'-N9	7.26	114.01	108.20
53	BA	2721	A	C5-C6-N1	7.26	121.33	117.70
21	AA	325	A	C5-C6-N1	7.26	121.33	117.70
53	BA	802	A	C5-C6-N1	7.26	121.33	117.70
53	BA	849	A	C4-C5-C6	-7.26	113.37	117.00
15	AP	28	ARG	NE-CZ-NH1	7.26	123.93	120.30
21	AA	602	A	C5-C6-N1	7.26	121.33	117.70
52	B4	24	ARG	NE-CZ-NH1	7.25	123.93	120.30
53	BA	1731	G	O4'-C1'-N9	7.25	114.00	108.20
21	AA	938	A	C5-C6-N1	7.25	121.33	117.70
23	A2	91	A	C4-C5-C6	-7.25	113.37	117.00
53	BA	1127	A	C5-C6-N1	7.25	121.33	117.70
53	BA	2853	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	1520	C	N3-C2-O2	-7.25	116.82	121.90
53	BA	1293	C	N3-C2-O2	-7.25	116.83	121.90
21	AA	502	A	C5-C6-N1	7.25	121.33	117.70
21	AA	1447	A	C4-C5-C6	-7.25	113.38	117.00
53	BA	899	A	N1-C6-N6	-7.25	114.25	118.60
53	BA	1487	U	O4'-C1'-N1	7.25	114.00	108.20
53	BA	2078	C	N3-C4-C5	7.25	124.80	121.90
21	AA	530	G	O4'-C1'-N9	7.25	114.00	108.20
22	A1	72	C	O4'-C1'-N1	7.25	114.00	108.20
53	BA	2530	A	C5-C6-N1	7.25	121.32	117.70
5	AF	24	ARG	NE-CZ-NH1	7.24	123.92	120.30
6	AG	3	ARG	NE-CZ-NH1	7.24	123.92	120.30
21	AA	706	A	C5-C6-N1	7.24	121.32	117.70
53	BA	2009	A	C4-C5-C6	-7.24	113.38	117.00
9	AJ	45	ARG	NE-CZ-NH1	7.24	123.92	120.30
53	BA	1612	C	N3-C2-O2	-7.24	116.83	121.90
53	BA	1877	A	C5-C6-N1	7.24	121.32	117.70
21	AA	1502	A	C4-C5-C6	-7.24	113.38	117.00
53	BA	804	A	N1-C6-N6	-7.24	114.26	118.60
53	BA	2267	A	C5-C6-N1	7.24	121.32	117.70
21	AA	148	G	N3-C2-N2	-7.24	114.83	119.90
53	BA	1553	A	C5-C6-N1	7.24	121.32	117.70
21	AA	878	A	N1-C6-N6	-7.24	114.26	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	206	C	N3-C2-O2	-7.23	116.84	121.90
21	AA	1524	C	N3-C2-O2	-7.23	116.84	121.90
53	BA	677	A	C5-C6-N1	7.23	121.32	117.70
53	BA	1070	A	C4-C5-C6	-7.23	113.38	117.00
53	BA	1515	A	C5-C6-N1	7.23	121.32	117.70
53	BA	1548	A	N1-C6-N6	-7.23	114.26	118.60
53	BA	1801	A	C5-C6-N1	7.23	121.32	117.70
53	BA	2205	A	N1-C6-N6	-7.23	114.26	118.60
53	BA	1027	A	N1-C6-N6	-7.23	114.26	118.60
53	BA	1609	A	C4-C5-C6	-7.23	113.39	117.00
53	BA	853	C	N3-C2-O2	-7.23	116.84	121.90
53	BA	1746	A	N1-C6-N6	-7.23	114.26	118.60
21	AA	784	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1518	A	N1-C6-N6	-7.22	114.27	118.60
33	BL	132	ARG	NE-CZ-NH1	7.22	123.91	120.30
53	BA	1032	A	C5-C6-N1	7.22	121.31	117.70
53	BA	1314	C	N3-C2-O2	-7.22	116.84	121.90
53	BA	1420	A	N1-C6-N6	-7.22	114.27	118.60
53	BA	103	A	C4-C5-C6	-7.22	113.39	117.00
53	BA	522	A	N1-C6-N6	-7.22	114.27	118.60
36	BO	15	ARG	NE-CZ-NH1	7.22	123.91	120.30
53	BA	1005	C	N3-C2-O2	-7.22	116.85	121.90
21	AA	495	A	C5-C6-N1	7.22	121.31	117.70
53	BA	472	A	C5-C6-N1	7.22	121.31	117.70
44	BW	19	ARG	NE-CZ-NH1	7.22	123.91	120.30
21	AA	624	C	N3-C2-O2	-7.21	116.85	121.90
21	AA	675	A	C5-C6-N1	7.21	121.31	117.70
53	BA	320	A	C5-C6-N1	7.21	121.31	117.70
53	BA	911	A	C4-C5-C6	-7.21	113.39	117.00
53	BA	1040	A	C4-C5-C6	-7.21	113.39	117.00
53	BA	1155	A	C4-C5-C6	-7.21	113.39	117.00
53	BA	2094	A	N1-C6-N6	-7.21	114.27	118.60
53	BA	2723	C	N3-C2-O2	-7.21	116.85	121.90
43	BV	79	ARG	NE-CZ-NH1	7.21	123.91	120.30
53	BA	1603	A	C5-C6-N1	7.21	121.31	117.70
54	BB	11	C	N3-C2-O2	-7.21	116.85	121.90
53	BA	540	C	N3-C2-O2	-7.21	116.85	121.90
54	BB	116	G	O4'-C1'-N9	7.21	113.97	108.20
21	AA	643	C	N3-C2-O2	-7.21	116.85	121.90
21	AA	1080	A	C5-C6-N1	7.21	121.30	117.70
21	AA	1188	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1500	A	C4-C5-C6	-7.21	113.40	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	330	A	C5-C6-N1	7.21	121.30	117.70
53	BA	1847	A	C5-C6-N1	7.21	121.30	117.70
3	AD	13	ARG	NE-CZ-NH1	7.21	123.90	120.30
53	BA	1204	A	C5-C6-N1	7.21	121.30	117.70
53	BA	2837	A	N1-C6-N6	-7.21	114.28	118.60
21	AA	1163	A	C4-C5-C6	-7.21	113.40	117.00
21	AA	1447	A	N1-C6-N6	-7.21	114.28	118.60
53	BA	278	A	C5-C6-N1	7.21	121.30	117.70
53	BA	394	C	N3-C2-O2	-7.21	116.86	121.90
2	AC	106	ARG	NE-CZ-NH1	7.20	123.90	120.30
21	AA	1054	C	N3-C2-O2	-7.20	116.86	121.90
53	BA	1578	U	O4'-C1'-N1	7.20	113.96	108.20
53	BA	1843	C	N3-C2-O2	-7.20	116.86	121.90
10	AK	126	ARG	NE-CZ-NH2	7.20	123.90	120.30
21	AA	349	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	790	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1396	A	C4-C5-C6	-7.20	113.40	117.00
53	BA	1647	U	N3-C2-O2	-7.20	117.16	122.20
21	AA	712	A	C5-C6-N1	7.20	121.30	117.70
21	AA	787	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	1032	G	O4'-C1'-N9	7.20	113.96	108.20
21	AA	1200	C	C3'-C2'-C1'	7.20	107.26	101.50
21	AA	1329	A	C4-C5-C6	-7.20	113.40	117.00
53	BA	228	C	N3-C2-O2	-7.20	116.86	121.90
53	BA	2760	C	O4'-C1'-N1	7.20	113.96	108.20
21	AA	653	U	O4'-C1'-N1	7.20	113.96	108.20
53	BA	270	A	C5-C6-N1	7.20	121.30	117.70
53	BA	432	A	N1-C6-N6	-7.20	114.28	118.60
53	BA	693	A	C5-C6-N1	7.20	121.30	117.70
53	BA	2078	C	N3-C2-O2	-7.20	116.86	121.90
53	BA	2706	A	C5-C6-N1	7.20	121.30	117.70
53	BA	878	A	C4-C5-C6	-7.19	113.40	117.00
21	AA	1229	A	C5-C6-N1	7.19	121.30	117.70
21	AA	1349	A	C4-C5-C6	-7.19	113.40	117.00
53	BA	1913	A	C5-C6-N1	7.19	121.30	117.70
21	AA	1046	A	C5-C6-N1	7.19	121.29	117.70
53	BA	1265	A	C4-C5-C6	-7.19	113.41	117.00
21	AA	143	A	N1-C6-N6	-7.19	114.29	118.60
21	AA	513	C	O4'-C1'-N1	7.19	113.95	108.20
21	AA	1281	C	N3-C2-O2	-7.19	116.87	121.90
53	BA	602	A	C5-C6-N1	7.19	121.29	117.70
53	BA	1040	A	N1-C6-N6	-7.19	114.29	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2767	C	N3-C2-O2	-7.19	116.87	121.90
53	BA	2826	A	C5-C6-N1	7.19	121.29	117.70
21	AA	430	A	C5-C6-N1	7.19	121.29	117.70
21	AA	451	A	N1-C6-N6	-7.19	114.29	118.60
20	AU	17	ARG	NE-CZ-NH1	7.18	123.89	120.30
53	BA	101	A	C5-C6-N1	7.18	121.29	117.70
53	BA	789	A	C5-C6-N1	7.18	121.29	117.70
53	BA	1352	U	O4'-C1'-N1	7.18	113.95	108.20
21	AA	465	A	C5-C6-N1	7.18	121.29	117.70
21	AA	687	A	N1-C6-N6	-7.18	114.29	118.60
53	BA	10	A	N1-C6-N6	-7.18	114.29	118.60
53	BA	503	A	O4'-C1'-N9	7.18	113.94	108.20
21	AA	167	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	123	U	O4'-C1'-N1	7.18	113.94	108.20
21	AA	1219	A	C4-C5-C6	-7.18	113.41	117.00
53	BA	2176	A	C5-C6-N1	7.18	121.29	117.70
21	AA	309	A	C4-C5-C6	-7.17	113.41	117.00
35	BN	64	ARG	NE-CZ-NH1	7.17	123.89	120.30
53	BA	234	U	O4'-C1'-N1	7.17	113.94	108.20
24	BC	261	ARG	NE-CZ-NH1	7.17	123.89	120.30
45	BX	73	ARG	NE-CZ-NH1	7.17	123.89	120.30
53	BA	79	C	N3-C2-O2	-7.17	116.88	121.90
53	BA	183	C	N3-C2-O2	-7.17	116.88	121.90
22	A1	26	A	C5-C6-N1	7.17	121.28	117.70
23	A2	82	A	C4-C5-C6	-7.17	113.42	117.00
53	BA	2830	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	314	C	N3-C2-O2	-7.17	116.88	121.90
53	BA	219	A	C4-C5-C6	-7.17	113.42	117.00
53	BA	2309	A	C4-C5-C6	-7.17	113.42	117.00
21	AA	1170	A	C5-C6-N1	7.17	121.28	117.70
22	A1	16	C	C6-N1-C2	-7.17	117.43	120.30
53	BA	1153	C	N3-C2-O2	-7.17	116.89	121.90
21	AA	282	A	C4-C5-C6	-7.16	113.42	117.00
32	BK	98	ARG	NE-CZ-NH1	7.16	123.88	120.30
53	BA	157	C	N3-C2-O2	-7.16	116.89	121.90
53	BA	208	C	N3-C2-O2	-7.16	116.89	121.90
53	BA	650	C	N3-C2-O2	-7.16	116.89	121.90
53	BA	1664	A	N1-C6-N6	-7.16	114.30	118.60
53	BA	2450	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	1429	A	C4-C5-C6	-7.16	113.42	117.00
53	BA	1427	A	C4-C5-C6	-7.16	113.42	117.00
53	BA	1678	A	C5-C6-N1	7.16	121.28	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	116	A	C4-C5-C6	-7.16	113.42	117.00
53	BA	2263	C	N3-C2-O2	-7.16	116.89	121.90
53	BA	2902	C	N3-C2-O2	-7.16	116.89	121.90
54	BB	28	C	N3-C2-O2	-7.16	116.89	121.90
21	AA	618	C	N3-C2-O2	-7.16	116.89	121.90
53	BA	529	A	C5-C6-N1	7.16	121.28	117.70
53	BA	197	A	C4-C5-C6	-7.16	113.42	117.00
53	BA	460	A	N1-C6-N6	-7.16	114.31	118.60
53	BA	2288	A	C4-C5-C6	-7.16	113.42	117.00
53	BA	2461	A	C5-C6-N1	7.16	121.28	117.70
53	BA	244	A	C5-C6-N1	7.15	121.28	117.70
53	BA	1490	A	C5-C6-N1	7.15	121.28	117.70
53	BA	2424	C	N3-C2-O2	-7.15	116.89	121.90
21	AA	316	C	O4'-C1'-N1	7.15	113.92	108.20
21	AA	949	A	C5-C6-N1	7.15	121.27	117.70
34	BM	81	ARG	NE-CZ-NH2	7.15	123.87	120.30
53	BA	371	A	C4-C5-C6	-7.15	113.43	117.00
53	BA	2284	A	C5-C6-N1	7.15	121.27	117.70
21	AA	81	A	C5-C6-N1	7.15	121.27	117.70
53	BA	1098	A	C5-C6-N1	7.15	121.27	117.70
2	AC	135	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	AC	142	ARG	NE-CZ-NH1	7.14	123.87	120.30
3	AD	96	ARG	NE-CZ-NH1	7.14	123.87	120.30
21	AA	101	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	586	C	N3-C2-O2	-7.14	116.90	121.90
53	BA	265	A	O4'-C1'-N9	7.14	113.92	108.20
21	AA	120	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	482	A	C5-C6-N1	7.14	121.27	117.70
53	BA	878	A	N1-C6-N6	-7.14	114.31	118.60
53	BA	1404	C	O4'-C1'-N1	7.14	113.92	108.20
53	BA	2841	C	N3-C2-O2	-7.14	116.90	121.90
53	BA	639	U	O4'-C1'-N1	7.14	113.91	108.20
53	BA	2527	C	N3-C2-O2	-7.14	116.90	121.90
53	BA	911	A	C5-C6-N1	7.14	121.27	117.70
53	BA	2064	C	N3-C2-O2	-7.14	116.91	121.90
21	AA	253	A	C4-C5-C6	-7.13	113.43	117.00
21	AA	263	A	C5-C6-N1	7.13	121.27	117.70
53	BA	1866	A	C5-C6-N1	7.13	121.27	117.70
53	BA	1654	A	N1-C6-N6	-7.13	114.32	118.60
3	AD	153	ARG	NE-CZ-NH1	7.13	123.87	120.30
21	AA	642	A	C5-C6-N1	7.13	121.27	117.70
53	BA	2799	A	N1-C6-N6	-7.13	114.32	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	330	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	611	C	N3-C2-O2	-7.13	116.91	121.90
21	AA	1219	A	N1-C6-N6	-7.13	114.32	118.60
53	BA	2055	C	N3-C2-O2	-7.13	116.91	121.90
53	BA	2883	A	C5-C6-N1	7.13	121.26	117.70
22	A1	21	A	N1-C6-N6	-7.13	114.32	118.60
53	BA	1297	C	N3-C2-O2	-7.13	116.91	121.90
53	BA	1938	A	C5-C6-N1	7.13	121.26	117.70
53	BA	201	C	N3-C2-O2	-7.12	116.91	121.90
53	BA	1322	A	C4-C5-C6	-7.12	113.44	117.00
53	BA	1504	A	N1-C6-N6	-7.12	114.33	118.60
21	AA	102	G	C8-N9-C4	-7.12	103.55	106.40
21	AA	295	C	N3-C2-O2	-7.12	116.91	121.90
53	BA	2665	A	C5-C6-N1	7.12	121.26	117.70
21	AA	26	A	C5-C6-N1	7.12	121.26	117.70
53	BA	1413	A	C5-C6-N1	7.12	121.26	117.70
53	BA	1614	A	N1-C6-N6	-7.12	114.33	118.60
53	BA	2047	C	N3-C2-O2	-7.12	116.92	121.90
53	BA	1552	A	C5-C6-N1	7.12	121.26	117.70
53	BA	422	A	C5-C6-N1	7.12	121.26	117.70
53	BA	482	A	N1-C6-N6	-7.12	114.33	118.60
53	BA	1650	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	1429	A	C5-C6-N1	7.12	121.26	117.70
53	BA	2115	G	O4'-C1'-N9	7.12	113.89	108.20
21	AA	171	A	C5-C6-N1	7.11	121.26	117.70
53	BA	2156	G	N1-C6-O6	-7.11	115.63	119.90
21	AA	303	A	N1-C6-N6	-7.11	114.33	118.60
21	AA	1467	C	N3-C2-O2	-7.11	116.92	121.90
53	BA	1477	A	C5-C6-N1	7.11	121.26	117.70
53	BA	1608	A	C5-C6-N1	7.11	121.26	117.70
21	AA	621	A	C4-C5-C6	-7.11	113.44	117.00
53	BA	460	A	C4-C5-C6	-7.11	113.44	117.00
21	AA	712	A	N1-C6-N6	-7.11	114.33	118.60
53	BA	2225	A	C5-C6-N1	7.11	121.25	117.70
21	AA	189	A	C5-C6-N1	7.11	121.25	117.70
53	BA	2851	A	C5-C6-N1	7.11	121.25	117.70
53	BA	278	A	N1-C6-N6	-7.10	114.34	118.60
16	AQ	64	ARG	NE-CZ-NH2	7.10	123.85	120.30
21	AA	908	A	C5-C6-N1	7.10	121.25	117.70
23	A2	80	C	N3-C2-O2	-7.10	116.93	121.90
53	BA	2029	G	N3-C2-N2	-7.10	114.93	119.90
53	BA	2042	A	C4-C5-C6	-7.10	113.45	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BB	35	C	N1-C2-O2	7.10	123.16	118.90
21	AA	1411	C	O4'-C1'-N1	7.10	113.88	108.20
53	BA	538	A	N1-C6-N6	-7.10	114.34	118.60
21	AA	1314	C	O4'-C1'-N1	7.10	113.88	108.20
21	AA	411	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1251	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1518	A	C5-C6-N1	7.10	121.25	117.70
53	BA	251	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1067	A	C4-C5-C6	-7.10	113.45	117.00
53	BA	2036	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	681	A	C4-C5-C6	-7.09	113.45	117.00
53	BA	331	C	N3-C2-O2	-7.09	116.94	121.90
53	BA	685	A	C4-C5-C6	-7.09	113.45	117.00
21	AA	320	A	C4-C5-C6	-7.09	113.45	117.00
53	BA	2386	A	C5-C6-N1	7.09	121.25	117.70
2	AC	178	ARG	NE-CZ-NH1	7.09	123.85	120.30
14	AO	83	ARG	NE-CZ-NH1	7.09	123.85	120.30
21	AA	490	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	969	A	C4-C5-C6	-7.09	113.45	117.00
53	BA	452	G	C8-N9-C4	-7.09	103.56	106.40
53	BA	1936	A	N1-C6-N6	-7.09	114.35	118.60
53	BA	1254	A	N1-C6-N6	-7.09	114.35	118.60
21	AA	448	A	C5-C6-N1	7.09	121.24	117.70
36	BO	102	ARG	NE-CZ-NH1	7.08	123.84	120.30
16	AQ	61	ARG	NE-CZ-NH1	7.08	123.84	120.30
21	AA	344	A	C5-C6-N1	7.08	121.24	117.70
53	BA	853	C	O4'-C1'-N1	7.08	113.87	108.20
53	BA	1392	A	C1'-O4'-C4'	-7.08	104.23	109.90
53	BA	2059	A	N1-C6-N6	-7.08	114.35	118.60
53	BA	1914	C	N3-C2-O2	-7.08	116.94	121.90
53	BA	2033	A	C4-C5-C6	-7.08	113.46	117.00
53	BA	2566	A	N1-C6-N6	-7.08	114.35	118.60
53	BA	2078	C	N1-C2-O2	7.08	123.15	118.90
21	AA	155	A	C4-C5-C6	-7.08	113.46	117.00
51	B3	44	ARG	NE-CZ-NH2	-7.08	116.76	120.30
53	BA	1999	C	N3-C2-O2	-7.08	116.95	121.90
53	BA	2829	A	C5-C6-N1	7.08	121.24	117.70
21	AA	872	A	C5-C6-N1	7.07	121.24	117.70
21	AA	876	C	N3-C2-O2	-7.07	116.95	121.90
53	BA	2826	A	N1-C6-N6	-7.07	114.36	118.60
54	BB	59	A	C5-C6-N1	7.07	121.24	117.70
21	AA	397	A	C4-C5-C6	-7.07	113.46	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BF	177	ARG	NE-CZ-NH1	7.07	123.84	120.30
53	BA	599	A	C5-C6-N1	7.07	121.24	117.70
53	BA	959	A	N1-C6-N6	-7.07	114.36	118.60
53	BA	2810	A	N1-C6-N6	-7.07	114.36	118.60
53	BA	2814	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	1503	A	N1-C6-N6	-7.07	114.36	118.60
53	BA	1593	A	C5-C6-N1	7.07	121.24	117.70
53	BA	13	A	C5-C6-N1	7.07	121.23	117.70
21	AA	162	A	C4-C5-C6	-7.07	113.47	117.00
45	BX	26	ARG	NE-CZ-NH1	7.07	123.83	120.30
53	BA	1308	A	C5-C6-N1	7.07	121.23	117.70
53	BA	2741	A	N1-C6-N6	-7.07	114.36	118.60
53	BA	144	A	C5-C6-N1	7.07	121.23	117.70
53	BA	752	A	C1'-O4'-C4'	-7.07	104.25	109.90
53	BA	1165	A	C5-C6-N1	7.07	121.23	117.70
53	BA	2310	C	N3-C2-O2	-7.07	116.95	121.90
54	BB	63	C	N3-C2-O2	-7.06	116.95	121.90
21	AA	816	A	C4-C5-C6	-7.06	113.47	117.00
21	AA	959	A	C5-C6-N1	7.06	121.23	117.70
53	BA	1901	A	C5-C6-N1	7.06	121.23	117.70
53	BA	2757	A	N1-C6-N6	-7.06	114.36	118.60
54	BB	115	A	N1-C6-N6	-7.06	114.36	118.60
29	BH	123	ARG	NE-CZ-NH1	7.06	123.83	120.30
53	BA	526	A	C4-C5-C6	-7.06	113.47	117.00
21	AA	352	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	1063	C	N3-C2-O2	-7.06	116.96	121.90
53	BA	507	A	N1-C6-N6	-7.06	114.37	118.60
53	BA	602	A	C4-C5-C6	-7.06	113.47	117.00
53	BA	1480	C	N3-C2-O2	-7.06	116.96	121.90
18	AS	36	ARG	NE-CZ-NH1	7.06	123.83	120.30
21	AA	1275	A	C5-C6-N1	7.06	121.23	117.70
55	B5	134	ARG	NE-CZ-NH1	7.06	123.83	120.30
21	AA	908	A	C4-C5-C6	-7.05	113.47	117.00
21	AA	948	C	N3-C2-O2	-7.05	116.96	121.90
21	AA	1092	A	C5-C6-N1	7.05	121.23	117.70
53	BA	1312	U	O4'-C1'-N1	7.05	113.84	108.20
53	BA	1966	A	C4-C5-C6	-7.05	113.47	117.00
53	BA	2506	U	O4'-C1'-N1	7.05	113.84	108.20
53	BA	2554	U	C1'-O4'-C4'	-7.05	104.26	109.90
21	AA	1280	A	C5-C6-N1	7.05	121.23	117.70
53	BA	2748	A	C5-C6-N1	7.05	121.23	117.70
21	AA	1483	A	N1-C6-N6	-7.05	114.37	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	146	A	C5-C6-N1	7.05	121.23	117.70
21	AA	353	A	C5-C6-N1	7.05	121.22	117.70
21	AA	1167	A	C5-C6-N1	7.05	121.22	117.70
53	BA	1213	A	N1-C6-N6	-7.05	114.37	118.60
21	AA	1117	A	C4-C5-C6	-7.05	113.48	117.00
53	BA	1111	A	C5-C6-N1	7.05	121.22	117.70
53	BA	666	A	C4-C5-C6	-7.05	113.48	117.00
53	BA	812	C	N3-C2-O2	-7.05	116.97	121.90
53	BA	1918	A	C5-C6-N1	7.05	121.22	117.70
53	BA	2439	A	C5-C6-N1	7.05	121.22	117.70
53	BA	2658	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	408	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	825	A	N1-C6-N6	-7.04	114.37	118.60
53	BA	352	A	N1-C6-N6	-7.04	114.37	118.60
53	BA	1378	A	O4'-C1'-N9	7.04	113.83	108.20
53	BA	1606	C	N1-C2-O2	7.04	123.13	118.90
53	BA	2030	A	C5-C6-N1	7.04	121.22	117.70
53	BA	789	A	C4-C5-C6	-7.04	113.48	117.00
53	BA	1706	C	N1-C2-O2	7.04	123.12	118.90
21	AA	8	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	26	A	N1-C6-N6	-7.04	114.38	118.60
21	AA	876	C	O4'-C1'-N1	7.04	113.83	108.20
53	BA	218	A	C5-C6-N1	7.04	121.22	117.70
53	BA	592	A	C4-C5-C6	-7.04	113.48	117.00
53	BA	1353	A	C5-C6-N1	7.04	121.22	117.70
54	BB	114	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	163	C	N3-C2-O2	-7.04	116.97	121.90
53	BA	217	A	C5-C6-N1	7.04	121.22	117.70
53	BA	1088	A	N1-C6-N6	-7.04	114.38	118.60
53	BA	1572	A	C5-C6-N1	7.04	121.22	117.70
9	AJ	62	ARG	NE-CZ-NH1	7.04	123.82	120.30
21	AA	1129	C	N3-C2-O2	-7.04	116.97	121.90
53	BA	1717	A	C5-C6-N1	7.04	121.22	117.70
53	BA	2119	A	N1-C6-N6	-7.04	114.38	118.60
21	AA	841	C	C1'-O4'-C4'	-7.03	104.27	109.90
21	AA	1274	A	N1-C6-N6	-7.03	114.38	118.60
53	BA	1746	A	C5-C6-N1	7.03	121.22	117.70
53	BA	951	C	O4'-C1'-N1	7.03	113.83	108.20
53	BA	541	A	N1-C6-N6	-7.03	114.38	118.60
21	AA	909	A	C5-C6-N1	7.03	121.21	117.70
53	BA	1928	A	C5-C6-N1	7.03	121.21	117.70
53	BA	2805	C	N3-C2-O2	-7.03	116.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BO	25	ARG	NE-CZ-NH1	7.02	123.81	120.30
53	BA	2765	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1330	U	O4'-C1'-N1	7.02	113.82	108.20
53	BA	454	A	C5-C6-N1	7.02	121.21	117.70
53	BA	2534	A	C5-C6-N1	7.02	121.21	117.70
53	BA	1590	A	C5-C6-N1	7.02	121.21	117.70
21	AA	129	A	C4-C5-C6	-7.02	113.49	117.00
21	AA	181	A	C4-C5-C6	-7.02	113.49	117.00
53	BA	348	A	C5-C6-N1	7.02	121.21	117.70
53	BA	1754	A	C5-C6-N1	7.02	121.21	117.70
40	BS	95	ARG	NE-CZ-NH2	-7.02	116.79	120.30
10	AK	121	ARG	NE-CZ-NH1	7.01	123.81	120.30
21	AA	743	A	C5-C6-N1	7.01	121.21	117.70
53	BA	985	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	1350	A	C5-N7-C8	-7.01	100.39	103.90
53	BA	935	C	N3-C2-O2	-7.01	116.99	121.90
53	BA	1731	G	C8-N9-C4	-7.01	103.59	106.40
53	BA	2893	A	C4-C5-C6	-7.01	113.49	117.00
21	AA	1055	A	C4-C5-C6	-7.01	113.50	117.00
53	BA	14	A	N1-C6-N6	-7.01	114.39	118.60
53	BA	344	A	C4-C5-C6	-7.01	113.50	117.00
21	AA	1217	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	1324	A	N1-C6-N6	-7.01	114.40	118.60
53	BA	56	A	C4-C5-C6	-7.01	113.50	117.00
53	BA	2766	A	C5-C6-N1	7.01	121.20	117.70
53	BA	2740	A	C5-C6-N1	7.00	121.20	117.70
21	AA	882	C	N3-C2-O2	-7.00	117.00	121.90
54	BB	38	C	O4'-C1'-N1	7.00	113.80	108.20
21	AA	190	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	912	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	1216	A	C4-C5-C6	-7.00	113.50	117.00
53	BA	1298	C	N1-C2-O2	7.00	123.10	118.90
53	BA	1565	C	N3-C2-O2	-7.00	117.00	121.90
53	BA	1759	A	C5-C6-N1	7.00	121.20	117.70
53	BA	2088	A	N1-C6-N6	-7.00	114.40	118.60
53	BA	2806	C	N1-C2-O2	7.00	123.10	118.90
13	AN	41	ARG	NE-CZ-NH1	7.00	123.80	120.30
21	AA	469	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	1428	A	C5-C6-N1	7.00	121.20	117.70
21	AA	110	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	796	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	895	G	C5-C6-N1	7.00	115.00	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1082	A	C5-C6-N1	7.00	121.20	117.70
53	BA	2111	U	O4'-C1'-N1	7.00	113.80	108.20
21	AA	460	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	1411	C	N3-C2-O2	-7.00	117.00	121.90
22	A1	13	C	O4'-C1'-N1	7.00	113.80	108.20
53	BA	739	A	N1-C6-N6	-7.00	114.40	118.60
53	BA	928	A	C5-C6-N1	7.00	121.20	117.70
53	BA	1008	A	N1-C6-N6	-7.00	114.40	118.60
53	BA	1889	A	C5-C6-N1	7.00	121.20	117.70
53	BA	2058	A	C4-C5-C6	-7.00	113.50	117.00
53	BA	2851	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	496	A	N1-C6-N6	-7.00	114.40	118.60
13	AN	61	ARG	NE-CZ-NH1	6.99	123.80	120.30
34	BM	16	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	AB	62	ARG	NE-CZ-NH1	6.99	123.80	120.30
53	BA	716	A	C5-C6-N1	6.99	121.19	117.70
53	BA	2377	A	C4-C5-C6	-6.99	113.51	117.00
53	BA	2463	C	N3-C2-O2	-6.99	117.01	121.90
21	AA	1214	C	N3-C4-C5	6.99	124.69	121.90
53	BA	1888	G	O4'-C1'-N9	6.99	113.79	108.20
53	BA	2635	A	N1-C6-N6	-6.99	114.41	118.60
21	AA	1236	A	C5-C6-N1	6.99	121.19	117.70
53	BA	2758	A	C5-C6-N1	6.99	121.19	117.70
53	BA	571	U	O4'-C1'-N1	6.98	113.79	108.20
53	BA	756	A	C5-C6-N1	6.98	121.19	117.70
21	AA	501	C	N3-C2-O2	-6.98	117.01	121.90
53	BA	2101	A	C4-C5-C6	-6.98	113.51	117.00
53	BA	2745	C	N3-C2-O2	-6.98	117.01	121.90
53	BA	2868	A	N1-C6-N6	-6.98	114.41	118.60
37	BP	71	ARG	NE-CZ-NH1	6.98	123.79	120.30
53	BA	22	C	N3-C2-O2	-6.98	117.01	121.90
53	BA	246	C	N3-C2-O2	-6.98	117.01	121.90
21	AA	489	C	N3-C2-O2	-6.98	117.02	121.90
53	BA	503	A	N1-C6-N6	-6.98	114.41	118.60
53	BA	1942	C	N3-C2-O2	-6.98	117.02	121.90
54	BB	49	C	N3-C2-O2	-6.98	117.02	121.90
21	AA	787	A	C5-C6-N1	6.98	121.19	117.70
53	BA	104	A	N1-C6-N6	-6.98	114.41	118.60
53	BA	368	A	C5-C6-N1	6.98	121.19	117.70
53	BA	1278	C	O4'-C1'-N1	6.98	113.78	108.20
53	BA	1847	A	O4'-C1'-N9	6.98	113.78	108.20
53	BA	2845	U	O4'-C1'-N1	6.98	113.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	78	A	N1-C6-N6	-6.98	114.42	118.60
21	AA	694	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	1336	C	N3-C2-O2	-6.98	117.02	121.90
53	BA	316	C	N3-C2-O2	-6.98	117.02	121.90
53	BA	2043	C	N3-C2-O2	-6.98	117.02	121.90
21	AA	250	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	1035	A	C5-C6-N1	6.97	121.19	117.70
53	BA	364	C	N3-C2-O2	-6.97	117.02	121.90
53	BA	1684	G	N1-C6-O6	-6.97	115.72	119.90
21	AA	238	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	1005	A	C4-C5-C6	-6.97	113.51	117.00
53	BA	106	C	N3-C2-O2	-6.97	117.02	121.90
53	BA	1276	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	719	C	N3-C2-O2	-6.97	117.02	121.90
53	BA	631	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	389	A	C4-C5-C6	-6.97	113.52	117.00
21	AA	1277	C	N3-C2-O2	-6.97	117.02	121.90
53	BA	1072	C	N3-C2-O2	-6.97	117.02	121.90
53	BA	1085	A	N1-C6-N6	-6.97	114.42	118.60
53	BA	1477	A	C4-C5-C6	-6.97	113.52	117.00
21	AA	559	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	1308	U	O4'-C1'-N1	6.97	113.77	108.20
53	BA	560	C	N3-C2-O2	-6.97	117.02	121.90
53	BA	2459	A	C5-C6-N1	6.97	121.18	117.70
53	BA	2515	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	274	A	O4'-C1'-N9	6.96	113.77	108.20
21	AA	739	C	N3-C2-O2	-6.96	117.03	121.90
21	AA	1213	A	C4-C5-C6	-6.96	113.52	117.00
53	BA	1746	A	C4-C5-C6	-6.96	113.52	117.00
54	BB	58	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	831	A	C4-C5-C6	-6.96	113.52	117.00
53	BA	19	A	C4-C5-C6	-6.96	113.52	117.00
53	BA	38	A	C4-C5-C6	-6.96	113.52	117.00
53	BA	288	U	O4'-C1'-N1	6.96	113.77	108.20
53	BA	2314	A	C4-C5-C6	-6.96	113.52	117.00
53	BA	2594	C	N3-C2-O2	-6.96	117.03	121.90
21	AA	1409	C	N3-C2-O2	-6.95	117.03	121.90
53	BA	131	A	N1-C6-N6	-6.95	114.43	118.60
53	BA	730	A	C4-C5-C6	-6.95	113.52	117.00
53	BA	814	C	N3-C2-O2	-6.95	117.03	121.90
53	BA	1723	G	N1-C6-O6	-6.95	115.73	119.90
53	BA	2813	A	C4-C5-C6	-6.95	113.52	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AL	113	ARG	NE-CZ-NH1	6.95	123.78	120.30
21	AA	782	A	C5-C6-N1	6.95	121.17	117.70
21	AA	797	C	N3-C2-O2	-6.95	117.03	121.90
26	BE	21	ARG	NE-CZ-NH1	6.95	123.78	120.30
53	BA	239	C	N3-C2-O2	-6.95	117.03	121.90
53	BA	1194	A	C4-C5-C6	-6.95	113.53	117.00
53	BA	2598	A	C5-C6-N1	6.95	121.17	117.70
53	BA	2868	A	C4-C5-C6	-6.95	113.52	117.00
2	AC	131	ARG	NE-CZ-NH1	6.95	123.77	120.30
21	AA	58	C	O4'-C1'-N1	6.95	113.76	108.20
22	A1	48	C	N3-C2-O2	-6.95	117.04	121.90
53	BA	1167	C	N3-C2-O2	-6.95	117.04	121.90
21	AA	676	A	C5-C6-N1	6.95	121.17	117.70
21	AA	1131	G	N3-C2-N2	-6.95	115.04	119.90
53	BA	992	C	N3-C2-O2	-6.95	117.04	121.90
53	BA	1373	A	N1-C6-N6	-6.95	114.43	118.60
53	BA	1348	C	O4'-C1'-N1	6.94	113.75	108.20
53	BA	2809	A	C5-C6-N1	6.94	121.17	117.70
21	AA	135	C	O4'-C1'-N1	6.94	113.75	108.20
21	AA	460	A	O4'-C1'-N9	6.94	113.75	108.20
21	AA	915	A	C4-C5-C6	-6.94	113.53	117.00
53	BA	627	A	N1-C6-N6	-6.94	114.43	118.60
53	BA	2366	A	C5-C6-N1	6.94	121.17	117.70
21	AA	120	A	N1-C6-N6	-6.94	114.44	118.60
53	BA	1128	G	C1'-O4'-C4'	-6.94	104.35	109.90
21	AA	672	U	O4'-C1'-N1	6.94	113.75	108.20
3	AD	110	ARG	NE-CZ-NH1	6.94	123.77	120.30
21	AA	1476	A	C5-C6-N1	6.94	121.17	117.70
53	BA	900	A	N1-C6-N6	-6.94	114.44	118.60
53	BA	1888	G	C5'-C4'-O4'	6.94	117.42	109.10
53	BA	800	A	C5-C6-N1	6.94	121.17	117.70
53	BA	909	A	C5-C6-N1	6.93	121.17	117.70
53	BA	1382	G	O4'-C1'-N9	6.93	113.75	108.20
21	AA	120	A	C5-C6-N1	6.93	121.17	117.70
21	AA	131	A	C4-C5-C6	-6.93	113.53	117.00
53	BA	479	A	C4-C5-C6	-6.93	113.53	117.00
53	BA	2750	A	C4-C5-C6	-6.93	113.53	117.00
54	BB	104	A	C5-C6-N1	6.93	121.17	117.70
21	AA	452	A	C5-C6-N1	6.93	121.17	117.70
21	AA	364	A	C5-C6-N1	6.93	121.17	117.70
21	AA	999	C	N3-C2-O2	-6.93	117.05	121.90
53	BA	996	A	N1-C6-N6	-6.93	114.44	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1625	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	756	C	N1-C2-O2	6.93	123.06	118.90
53	BA	2268	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	435	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	1329	A	N1-C6-N6	-6.92	114.45	118.60
53	BA	6	A	C5-C6-N1	6.92	121.16	117.70
21	AA	89	U	O4'-C1'-N1	6.92	113.74	108.20
21	AA	483	C	O4'-C1'-N1	6.92	113.74	108.20
53	BA	1161	C	O4'-C1'-N1	6.92	113.74	108.20
21	AA	151	A	C5-C6-N1	6.92	121.16	117.70
21	AA	889	A	C5-C6-N1	6.92	121.16	117.70
53	BA	2732	G	N3-C2-N2	-6.92	115.06	119.90
53	BA	2882	A	C5-C6-N1	6.92	121.16	117.70
21	AA	77	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	217	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	452	A	C4-C5-C6	-6.92	113.54	117.00
53	BA	2516	A	C5-C6-N1	6.92	121.16	117.70
53	BA	2738	A	C4-C5-C6	-6.92	113.54	117.00
53	BA	513	A	N1-C6-N6	-6.92	114.45	118.60
53	BA	1502	A	C5-C6-N1	6.92	121.16	117.70
37	BP	112	ARG	NE-CZ-NH1	6.92	123.76	120.30
53	BA	149	A	C4-C5-C6	-6.92	113.54	117.00
53	BA	1759	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	872	A	O4'-C1'-N9	6.91	113.73	108.20
53	BA	526	A	N1-C6-N6	-6.91	114.45	118.60
53	BA	1399	C	N3-C2-O2	-6.91	117.06	121.90
53	BA	2587	A	C5-C6-N1	6.91	121.16	117.70
53	BA	623	C	N3-C2-O2	-6.91	117.06	121.90
53	BA	2023	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	660	C	O4'-C1'-N1	6.91	113.73	108.20
22	A1	30	C	N3-C2-O2	-6.91	117.06	121.90
53	BA	865	C	N3-C2-O2	-6.91	117.06	121.90
5	AF	45	ARG	NE-CZ-NH1	6.91	123.75	120.30
21	AA	93	U	O4'-C1'-N1	6.91	113.73	108.20
21	AA	401	C	N3-C2-O2	-6.91	117.06	121.90
53	BA	2635	A	C4-C5-C6	-6.91	113.55	117.00
53	BA	440	C	N3-C2-O2	-6.91	117.06	121.90
53	BA	751	A	C5-C6-N1	6.91	121.15	117.70
53	BA	2699	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	539	A	N1-C6-N6	-6.90	114.46	118.60
54	BB	15	A	O4'-C1'-N9	6.90	113.72	108.20
21	AA	1287	A	C4-C5-C6	-6.90	113.55	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1492	A	O4'-C1'-N9	6.90	113.72	108.20
53	BA	482	A	C5-C6-N1	6.90	121.15	117.70
53	BA	2362	C	N3-C2-O2	-6.90	117.07	121.90
2	AC	64	ARG	NE-CZ-NH1	6.89	123.75	120.30
53	BA	2498	C	C3'-C2'-C1'	6.89	107.02	101.50
53	BA	2232	C	N3-C2-O2	-6.89	117.08	121.90
53	BA	2037	A	C4-C5-C6	-6.89	113.56	117.00
21	AA	200	G	O4'-C1'-N9	6.89	113.71	108.20
53	BA	1084	A	C5-C6-N1	6.89	121.14	117.70
53	BA	1549	A	C4-C5-C6	-6.89	113.56	117.00
53	BA	1569	A	C4-C5-C6	-6.89	113.56	117.00
53	BA	309	A	C5-C6-N1	6.89	121.14	117.70
53	BA	140	C	N3-C2-O2	-6.89	117.08	121.90
53	BA	274	C	N3-C2-O2	-6.89	117.08	121.90
54	BB	94	A	C4-C5-C6	-6.89	113.56	117.00
53	BA	352	A	C4-C5-C6	-6.88	113.56	117.00
53	BA	668	A	C5-C6-N1	6.88	121.14	117.70
53	BA	676	A	C4-C5-C6	-6.88	113.56	117.00
53	BA	2332	C	N3-C4-N4	-6.88	113.18	118.00
21	AA	95	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	495	A	C4-C5-C6	-6.88	113.56	117.00
53	BA	1872	A	C5-C6-N1	6.88	121.14	117.70
53	BA	2151	U	O4'-C1'-N1	6.88	113.71	108.20
21	AA	228	A	C5-C6-N1	6.88	121.14	117.70
21	AA	722	G	C3'-C2'-C1'	6.88	107.00	101.50
21	AA	32	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	689	C	O4'-C1'-N1	6.88	113.70	108.20
21	AA	1380	U	O4'-C1'-N1	6.88	113.70	108.20
14	AO	57	ARG	NE-CZ-NH1	6.88	123.74	120.30
53	BA	1614	A	C5-C6-N1	6.88	121.14	117.70
53	BA	1960	A	C4-C5-C6	-6.88	113.56	117.00
53	BA	2626	C	N3-C2-O2	-6.88	117.08	121.90
53	BA	457	A	C5-C6-N1	6.88	121.14	117.70
53	BA	531	C	N3-C2-O2	-6.88	117.09	121.90
53	BA	1494	A	N1-C6-N6	-6.88	114.47	118.60
53	BA	2531	A	N1-C6-N6	-6.88	114.47	118.60
53	BA	1571	A	C5-C6-N1	6.88	121.14	117.70
53	BA	2071	A	C4-C5-C6	-6.88	113.56	117.00
24	BC	86	ARG	NE-CZ-NH1	6.87	123.74	120.30
30	BI	133	ARG	NE-CZ-NH1	6.87	123.74	120.30
53	BA	897	C	N1-C2-O2	6.87	123.02	118.90
21	AA	330	C	N1-C2-O2	6.87	123.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	489	C	O4'-C1'-N1	6.87	113.70	108.20
21	AA	533	A	C5-C6-N1	6.87	121.14	117.70
21	AA	630	A	C4-C5-C6	-6.87	113.56	117.00
53	BA	1711	A	C5-C6-N1	6.87	121.14	117.70
21	AA	715	A	N1-C6-N6	-6.87	114.48	118.60
53	BA	532	A	N1-C6-N6	-6.87	114.48	118.60
53	BA	582	A	C4-C5-C6	-6.87	113.56	117.00
53	BA	590	A	C5-C6-N1	6.87	121.14	117.70
7	AH	14	ARG	NE-CZ-NH1	6.87	123.73	120.30
21	AA	873	A	N1-C6-N6	-6.87	114.48	118.60
35	BN	4	ARG	NE-CZ-NH1	6.87	123.73	120.30
53	BA	1229	C	N3-C2-O2	-6.87	117.09	121.90
53	BA	2815	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	181	A	C5-C6-N1	6.87	121.13	117.70
21	AA	1350	A	C8-N9-C4	-6.87	103.05	105.80
53	BA	345	A	C5-C6-N1	6.87	121.13	117.70
53	BA	1075	C	O4'-C1'-N1	6.87	113.69	108.20
54	BB	78	A	C4-C5-C6	-6.87	113.57	117.00
53	BA	890	C	N3-C2-O2	-6.86	117.09	121.90
53	BA	896	A	N1-C6-N6	-6.86	114.48	118.60
53	BA	661	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	80	A	N1-C6-N6	-6.86	114.48	118.60
53	BA	2381	A	N1-C6-N6	-6.86	114.48	118.60
53	BA	2589	A	C4-C5-C6	-6.86	113.57	117.00
53	BA	910	A	C4-C5-C6	-6.86	113.57	117.00
53	BA	1351	C	O4'-C1'-N1	6.86	113.69	108.20
53	BA	2198	A	N1-C6-N6	-6.86	114.48	118.60
21	AA	974	A	O4'-C1'-N9	6.86	113.68	108.20
53	BA	125	A	C5-C6-N1	6.86	121.13	117.70
53	BA	2135	A	C4-C5-C6	-6.86	113.57	117.00
53	BA	1967	C	N3-C2-O2	-6.85	117.10	121.90
53	BA	504	A	C5-C6-N1	6.85	121.13	117.70
53	BA	2077	A	N1-C6-N6	-6.85	114.49	118.60
21	AA	1370	G	N3-C4-C5	-6.85	125.17	128.60
21	AA	1100	C	N3-C2-O2	-6.85	117.11	121.90
21	AA	1340	A	C5-C6-N1	6.85	121.12	117.70
53	BA	490	C	N3-C2-O2	-6.85	117.11	121.90
21	AA	465	A	C4-C5-C6	-6.85	113.58	117.00
21	AA	914	A	C5-C6-N1	6.85	121.12	117.70
21	AA	1412	C	N3-C2-O2	-6.85	117.11	121.90
53	BA	2019	A	C5-C6-N1	6.85	121.12	117.70
21	AA	298	A	C4-C5-C6	-6.84	113.58	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	724	U	O4'-C1'-N1	6.84	113.67	108.20
53	BA	835	C	N3-C2-O2	-6.84	117.11	121.90
53	BA	1354	A	N1-C6-N6	-6.84	114.49	118.60
53	BA	1635	A	C4-C5-C6	-6.84	113.58	117.00
54	BB	45	A	C5-C6-N1	6.84	121.12	117.70
53	BA	2395	C	N1-C2-O2	6.84	123.00	118.90
21	AA	379	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	1150	A	C4-C5-C6	-6.84	113.58	117.00
53	BA	1313	U	N3-C2-O2	-6.84	117.41	122.20
53	BA	1557	C	N3-C2-O2	-6.84	117.11	121.90
53	BA	1912	A	C4-C5-C6	-6.84	113.58	117.00
53	BA	2037	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1462	C	N3-C2-O2	-6.84	117.11	121.90
22	A1	56	C	N3-C2-O2	-6.84	117.11	121.90
53	BA	1202	G	N1-C6-O6	-6.84	115.80	119.90
53	BA	1768	C	N3-C2-O2	-6.84	117.11	121.90
55	B5	53	ARG	NE-CZ-NH1	6.84	123.72	120.30
53	BA	1453	A	C4-C5-C6	-6.83	113.58	117.00
53	BA	877	A	N1-C6-N6	-6.83	114.50	118.60
53	BA	946	C	N3-C2-O2	-6.83	117.12	121.90
53	BA	2035	G	O4'-C1'-N9	6.83	113.67	108.20
21	AA	580	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1397	C	N3-C2-O2	-6.83	117.12	121.90
53	BA	1685	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	790	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	1238	A	C5-C6-N1	6.83	121.11	117.70
53	BA	991	C	N3-C2-O2	-6.83	117.12	121.90
53	BA	1057	A	N1-C6-N6	-6.83	114.50	118.60
53	BA	1829	A	C5-C6-N1	6.83	121.11	117.70
2	AC	163	ARG	NE-CZ-NH1	6.83	123.71	120.30
21	AA	466	A	C5-C6-N1	6.83	121.11	117.70
53	BA	2163	A	C4-C5-C6	-6.83	113.59	117.00
21	AA	923	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	1293	C	N3-C2-O2	-6.82	117.12	121.90
53	BA	680	C	N3-C2-O2	-6.82	117.12	121.90
53	BA	1123	C	N3-C2-O2	-6.82	117.12	121.90
54	BB	46	A	C4-C5-C6	-6.82	113.59	117.00
53	BA	332	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	1403	C	N3-C2-O2	-6.82	117.13	121.90
53	BA	1664	A	C4-C5-C6	-6.82	113.59	117.00
53	BA	1689	A	C5-C6-N1	6.82	121.11	117.70
21	AA	1256	A	C5-C6-N1	6.82	121.11	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AO	87	ARG	NE-CZ-NH1	6.82	123.71	120.30
21	AA	808	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	910	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	1110	A	C4-C5-C6	-6.82	113.59	117.00
53	BA	1549	A	C5-C6-N1	6.82	121.11	117.70
53	BA	1284	A	C5-C6-N1	6.82	121.11	117.70
53	BA	1512	C	N3-C2-O2	-6.82	117.13	121.90
5	AF	2	ARG	NE-CZ-NH1	6.81	123.71	120.30
53	BA	1129	A	C4-C5-C6	-6.81	113.59	117.00
53	BA	1393	A	C4-C5-C6	-6.81	113.59	117.00
24	BC	220	ARG	NE-CZ-NH1	6.81	123.70	120.30
53	BA	670	A	C5-C6-N1	6.81	121.11	117.70
53	BA	1175	A	C4-C5-C6	-6.81	113.59	117.00
53	BA	1306	C	O4'-C1'-N1	6.81	113.65	108.20
21	AA	1152	A	N1-C6-N6	-6.81	114.51	118.60
53	BA	640	C	N3-C2-O2	-6.81	117.13	121.90
53	BA	1139	G	N7-C8-N9	6.81	116.50	113.10
53	BA	1241	A	C5-C6-N1	6.81	121.11	117.70
53	BA	2713	U	O4'-C1'-N1	6.81	113.65	108.20
22	A1	69	A	C5-C6-N1	6.81	121.10	117.70
53	BA	2183	A	C5-C6-N1	6.81	121.10	117.70
53	BA	728	G	C5-C6-N1	6.81	114.90	111.50
21	AA	395	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	1192	C	N3-C2-O2	-6.80	117.14	121.90
53	BA	1291	C	N3-C2-O2	-6.80	117.14	121.90
53	BA	2154	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	1357	A	C5-C6-N1	6.80	121.10	117.70
21	AA	857	C	N3-C2-O2	-6.80	117.14	121.90
50	B2	19	ARG	NE-CZ-NH2	6.80	123.70	120.30
53	BA	255	A	C5-C6-N1	6.80	121.10	117.70
53	BA	513	A	C5-C6-N1	6.80	121.10	117.70
21	AA	923	A	C5-C6-N1	6.80	121.10	117.70
53	BA	1128	G	N1-C6-O6	-6.80	115.82	119.90
18	AS	31	ARG	NE-CZ-NH1	6.80	123.70	120.30
24	BC	132	ARG	NE-CZ-NH1	6.80	123.70	120.30
36	BO	9	ARG	NE-CZ-NH1	6.80	123.70	120.30
53	BA	860	U	O4'-C1'-N1	6.80	113.64	108.20
53	BA	2778	A	C5-C6-N1	6.80	121.10	117.70
54	BB	17	C	N3-C2-O2	-6.80	117.14	121.90
53	BA	2369	A	O4'-C1'-N9	6.79	113.64	108.20
53	BA	310	A	C4-C5-C6	-6.79	113.60	117.00
53	BA	661	A	C5-C6-N1	6.79	121.10	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2459	A	C4-C5-C6	-6.79	113.60	117.00
21	AA	101	A	C5-C6-N1	6.79	121.10	117.70
53	BA	1969	A	C5-C6-N1	6.79	121.09	117.70
53	BA	2899	A	C4-C5-C6	-6.79	113.61	117.00
53	BA	335	C	N3-C2-O2	-6.79	117.15	121.90
53	BA	1009	A	C5-C6-N1	6.79	121.09	117.70
21	AA	869	G	N1-C6-O6	-6.79	115.83	119.90
21	AA	1045	C	N3-C2-O2	-6.79	117.15	121.90
53	BA	125	A	N1-C6-N6	-6.79	114.53	118.60
53	BA	693	A	C4-C5-C6	-6.79	113.61	117.00
53	BA	821	A	C4-C5-C6	-6.79	113.61	117.00
53	BA	1497	U	O4'-C1'-N1	6.79	113.63	108.20
21	AA	1146	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	1301	U	O4'-C1'-N1	6.79	113.63	108.20
21	AA	1410	A	C5-C6-N1	6.79	121.09	117.70
53	BA	1837	C	N3-C2-O2	-6.79	117.15	121.90
53	BA	2115	G	N3-C4-C5	-6.79	125.21	128.60
21	AA	681	A	C5-C6-N1	6.78	121.09	117.70
53	BA	233	A	C4-C5-C6	-6.78	113.61	117.00
53	BA	1292	G	N1-C6-O6	-6.78	115.83	119.90
53	BA	1982	U	O4'-C1'-N1	6.78	113.63	108.20
21	AA	873	A	C5-C6-N1	6.78	121.09	117.70
53	BA	1181	U	O4'-C1'-N1	6.78	113.62	108.20
21	AA	935	A	C5-C6-N1	6.78	121.09	117.70
53	BA	2691	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	856	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	1469	C	N3-C2-O2	-6.78	117.16	121.90
53	BA	614	A	C5-C6-N1	6.78	121.09	117.70
53	BA	1678	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	325	A	C4-C5-C6	-6.78	113.61	117.00
53	BA	1253	A	C5-C6-N1	6.78	121.09	117.70
53	BA	2799	A	C5-C6-N1	6.78	121.09	117.70
21	AA	1146	A	C5-C6-N1	6.77	121.09	117.70
53	BA	2247	A	O4'-C1'-N9	6.77	113.62	108.20
53	BA	347	A	C5-C6-N1	6.77	121.09	117.70
21	AA	1531	A	C5-C6-N1	6.77	121.09	117.70
11	AL	35	ARG	NE-CZ-NH1	6.77	123.68	120.30
22	A1	73	A	C4-C5-C6	-6.77	113.61	117.00
53	BA	217	A	N1-C6-N6	-6.77	114.54	118.60
53	BA	1075	C	N3-C2-O2	-6.77	117.16	121.90
53	BA	786	C	N3-C2-O2	-6.77	117.16	121.90
53	BA	1503	A	C5-C6-N1	6.77	121.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	53	A	C4-C5-C6	-6.77	113.62	117.00
21	AA	1239	A	N1-C6-N6	-6.77	114.54	118.60
21	AA	51	A	C4-C5-C6	-6.76	113.62	117.00
53	BA	616	A	N1-C6-N6	-6.76	114.54	118.60
2	AC	58	ARG	NE-CZ-NH1	6.76	123.68	120.30
21	AA	418	C	N3-C2-O2	-6.76	117.17	121.90
53	BA	432	A	C5-C6-N1	6.76	121.08	117.70
54	BB	58	A	N1-C6-N6	-6.76	114.54	118.60
16	AQ	76	ARG	NE-CZ-NH1	6.76	123.68	120.30
21	AA	1037	C	N3-C4-N4	-6.76	113.27	118.00
53	BA	1028	A	C4-C5-C6	-6.76	113.62	117.00
53	BA	1417	C	O4'-C1'-N1	6.76	113.61	108.20
53	BA	2785	C	N3-C2-O2	-6.76	117.17	121.90
54	BB	66	A	N1-C6-N6	-6.76	114.54	118.60
21	AA	977	A	C5-C6-N1	6.76	121.08	117.70
53	BA	42	A	N1-C6-N6	-6.76	114.54	118.60
53	BA	241	A	O4'-C1'-N9	6.76	113.61	108.20
53	BA	1760	C	N3-C2-O2	-6.76	117.17	121.90
53	BA	505	A	C4-C5-C6	-6.76	113.62	117.00
53	BA	1278	C	N3-C2-O2	-6.76	117.17	121.90
53	BA	149	A	C5-C6-N1	6.75	121.08	117.70
53	BA	2513	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	545	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	1262	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	1452	C	N3-C2-O2	-6.75	117.17	121.90
53	BA	348	A	C4-C5-C6	-6.75	113.62	117.00
53	BA	2306	C	N3-C2-O2	-6.75	117.17	121.90
53	BA	2858	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	393	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1228	C	N3-C2-O2	-6.75	117.17	121.90
53	BA	503	A	C5-C6-N1	6.75	121.08	117.70
53	BA	1536	C	N3-C2-O2	-6.75	117.17	121.90
53	BA	1870	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	178	C	N3-C2-O2	-6.75	117.17	121.90
6	AG	77	ARG	NE-CZ-NH1	6.75	123.67	120.30
53	BA	1367	A	N1-C6-N6	-6.75	114.55	118.60
53	BA	2154	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1434	A	C4-C5-C6	-6.75	113.63	117.00
53	BA	1161	C	N3-C2-O2	-6.75	117.18	121.90
53	BA	2823	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	19	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	371	A	C4-C5-C6	-6.75	113.63	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	422	A	C4-C5-C6	-6.75	113.63	117.00
53	BA	1373	A	C5-C6-N1	6.75	121.07	117.70
53	BA	2765	A	N1-C6-N6	-6.75	114.55	118.60
21	AA	300	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1317	C	N3-C2-O2	-6.74	117.18	121.90
53	BA	661	A	N1-C6-N6	-6.74	114.55	118.60
53	BA	1254	A	C5-C6-N1	6.74	121.07	117.70
53	BA	1919	A	N1-C6-N6	-6.74	114.55	118.60
53	BA	352	A	C5-C6-N1	6.74	121.07	117.70
53	BA	2809	A	C4-C5-C6	-6.74	113.63	117.00
11	AL	11	ARG	NE-CZ-NH1	6.74	123.67	120.30
21	AA	192	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1466	C	N3-C2-O2	-6.74	117.18	121.90
44	BW	76	ARG	NE-CZ-NH1	6.74	123.67	120.30
53	BA	454	A	C4-C5-C6	-6.74	113.63	117.00
53	BA	892	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	912	C	N1-C2-O2	6.74	122.94	118.90
53	BA	726	G	O4'-C1'-N9	6.74	113.59	108.20
53	BA	1417	C	N3-C2-O2	-6.74	117.18	121.90
53	BA	2020	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	923	A	N1-C6-N6	-6.74	114.56	118.60
21	AA	101	A	N1-C6-N6	-6.74	114.56	118.60
21	AA	1036	A	C4-C5-C6	-6.74	113.63	117.00
53	BA	524	G	N1-C6-O6	-6.74	115.86	119.90
53	BA	2717	C	N3-C2-O2	-6.74	117.19	121.90
21	AA	32	A	C4-C5-C6	-6.73	113.63	117.00
51	B3	12	ARG	NE-CZ-NH1	6.73	123.67	120.30
53	BA	199	A	C4-C5-C6	-6.73	113.63	117.00
53	BA	1165	A	C4-C5-C6	-6.73	113.63	117.00
53	BA	2451	A	C4-C5-C6	-6.73	113.63	117.00
35	BN	46	ARG	NE-CZ-NH1	6.73	123.67	120.30
53	BA	1981	A	C5-C6-N1	6.73	121.07	117.70
53	BA	2700	A	C5-C6-N1	6.73	121.06	117.70
26	BE	117	ARG	NE-CZ-NH1	6.73	123.66	120.30
53	BA	2676	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	958	A	C1'-O4'-C4'	-6.73	104.52	109.90
53	BA	973	A	C5-C6-N1	6.73	121.06	117.70
53	BA	2394	C	N3-C2-O2	-6.73	117.19	121.90
53	BA	2765	A	C4-C5-C6	-6.73	113.64	117.00
4	AE	137	ARG	NE-CZ-NH1	6.73	123.66	120.30
53	BA	533	G	N9-C4-C5	6.73	108.09	105.40
21	AA	824	G	N1-C6-O6	-6.72	115.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	983	A	C5-C6-N1	6.72	121.06	117.70
53	BA	1908	C	O4'-C1'-N1	6.72	113.58	108.20
21	AA	65	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	250	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	559	A	C5-C6-N1	6.72	121.06	117.70
53	BA	73	A	C4-C5-C6	-6.72	113.64	117.00
53	BA	239	C	O4'-C1'-N1	6.72	113.58	108.20
21	AA	1234	C	O4'-C1'-N1	6.72	113.58	108.20
53	BA	95	A	C4-C5-C6	-6.72	113.64	117.00
53	BA	387	U	N3-C2-O2	-6.72	117.50	122.20
21	AA	295	C	O4'-C1'-N1	6.72	113.58	108.20
53	BA	483	A	C5-C6-N1	6.72	121.06	117.70
53	BA	1016	G	N1-C6-O6	-6.72	115.87	119.90
53	BA	1089	A	C4-C5-C6	-6.72	113.64	117.00
53	BA	1784	A	N1-C6-N6	-6.72	114.57	118.60
53	BA	1866	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	139	A	C5-C6-N1	6.72	121.06	117.70
21	AA	386	C	N3-C2-O2	-6.72	117.20	121.90
21	AA	334	C	N1-C2-O2	6.72	122.93	118.90
21	AA	742	G	N3-C2-N2	-6.72	115.20	119.90
47	BZ	29	ARG	NE-CZ-NH1	6.72	123.66	120.30
53	BA	1289	C	N3-C2-O2	-6.72	117.20	121.90
21	AA	792	A	C5-C6-N1	6.71	121.06	117.70
53	BA	336	C	N3-C2-O2	-6.71	117.20	121.90
53	BA	398	C	C6-N1-C2	-6.71	117.61	120.30
21	AA	498	A	N1-C6-N6	-6.71	114.57	118.60
21	AA	790	A	C4-C5-C6	-6.71	113.64	117.00
53	BA	2513	A	N1-C6-N6	-6.71	114.57	118.60
21	AA	396	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	1043	G	N1-C6-O6	-6.71	115.87	119.90
21	AA	1362	A	C4-C5-C6	-6.71	113.64	117.00
21	AA	1449	C	N3-C2-O2	-6.71	117.20	121.90
53	BA	289	G	N1-C6-O6	-6.71	115.87	119.90
53	BA	691	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	1176	A	C5-C6-N1	6.71	121.05	117.70
21	AA	1339	A	C4-C5-C6	-6.71	113.65	117.00
53	BA	782	A	N1-C6-N6	-6.71	114.58	118.60
53	BA	2376	A	C4-C5-C6	-6.71	113.64	117.00
21	AA	263	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	607	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	1171	A	C5-C6-N1	6.71	121.05	117.70
41	BT	6	ARG	NE-CZ-NH2	6.71	123.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	984	A	C5-C6-N1	6.71	121.05	117.70
53	BA	1713	A	C5-C6-N1	6.71	121.05	117.70
53	BA	2635	A	C5-C6-N1	6.71	121.05	117.70
53	BA	1780	A	C5-C6-N1	6.70	121.05	117.70
54	BB	110	C	N3-C2-O2	-6.70	117.21	121.90
53	BA	1599	U	O4'-C1'-N1	6.70	113.56	108.20
21	AA	1483	A	C5-C6-N1	6.70	121.05	117.70
22	A1	68	C	N3-C2-O2	-6.70	117.21	121.90
53	BA	2695	U	O4'-C1'-N1	6.70	113.56	108.20
14	AO	76	ARG	NE-CZ-NH1	6.70	123.65	120.30
21	AA	567	G	N3-C4-C5	-6.70	125.25	128.60
21	AA	1397	C	N1-C2-O2	6.70	122.92	118.90
21	AA	751	U	O4'-C1'-N1	6.70	113.56	108.20
53	BA	902	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	1012	A	C5-C6-N1	6.70	121.05	117.70
40	BS	92	ARG	NE-CZ-NH2	6.70	123.65	120.30
53	BA	2347	C	N3-C2-O2	-6.70	117.21	121.90
48	B0	49	ARG	NE-CZ-NH2	6.69	123.65	120.30
53	BA	182	A	C5-C6-N1	6.69	121.05	117.70
49	B1	43	ARG	NE-CZ-NH1	6.69	123.65	120.30
53	BA	223	A	C5-C6-N1	6.69	121.05	117.70
53	BA	669	G	O4'-C1'-N9	6.69	113.55	108.20
53	BA	1076	C	O4'-C1'-N1	6.69	113.55	108.20
53	BA	1142	A	C5-C6-N1	6.69	121.05	117.70
53	BA	2333	A	C4-C5-C6	-6.69	113.66	117.00
21	AA	1149	C	O4'-C1'-N1	6.69	113.55	108.20
22	A1	11	C	N3-C2-O2	-6.69	117.22	121.90
53	BA	1470	A	N1-C6-N6	-6.69	114.59	118.60
53	BA	2710	C	N3-C2-O2	-6.69	117.22	121.90
53	BA	1958	C	N3-C2-O2	-6.69	117.22	121.90
53	BA	2434	A	C5-C6-N1	6.69	121.04	117.70
53	BA	2566	A	C4-C5-C6	-6.69	113.66	117.00
21	AA	143	A	C5-C6-N1	6.68	121.04	117.70
21	AA	569	C	N3-C4-C5	6.68	124.57	121.90
21	AA	1196	A	C4-C5-C6	-6.68	113.66	117.00
53	BA	556	A	C4-C5-C6	-6.68	113.66	117.00
53	BA	2496	C	N3-C2-O2	-6.68	117.22	121.90
53	BA	2670	A	C4-C5-C6	-6.68	113.66	117.00
53	BA	98	G	N1-C6-O6	-6.68	115.89	119.90
53	BA	528	A	N1-C6-N6	-6.68	114.59	118.60
53	BA	2560	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1331	G	N1-C6-O6	-6.68	115.89	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1288	G	N3-C4-C5	-6.68	125.26	128.60
53	BA	2499	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	936	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	1128	C	N3-C2-O2	-6.68	117.22	121.90
53	BA	1505	A	C4-C5-C6	-6.68	113.66	117.00
53	BA	1874	C	O4'-C1'-N1	6.68	113.54	108.20
53	BA	2679	A	C5-C6-N1	6.68	121.04	117.70
53	BA	1742	U	O4'-C1'-N1	6.68	113.54	108.20
53	BA	2013	A	C5-C6-N1	6.68	121.04	117.70
53	BA	1215	G	N3-C2-N2	-6.68	115.23	119.90
53	BA	2097	A	C5-C6-N1	6.68	121.04	117.70
53	BA	231	A	O4'-C1'-N9	6.67	113.54	108.20
53	BA	1076	C	N3-C2-O2	-6.67	117.23	121.90
53	BA	1262	A	C5-C6-N1	6.67	121.04	117.70
53	BA	428	A	C4-C5-C6	-6.67	113.66	117.00
53	BA	14	A	C5-C6-N1	6.67	121.04	117.70
53	BA	421	C	N3-C2-O2	-6.67	117.23	121.90
53	BA	2097	A	C4-C5-C6	-6.67	113.67	117.00
22	A1	66	A	N1-C6-N6	-6.67	114.60	118.60
53	BA	47	C	N3-C2-O2	-6.67	117.23	121.90
53	BA	2169	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	1288	A	C5-C6-N1	6.67	121.03	117.70
53	BA	737	C	N3-C2-O2	-6.67	117.23	121.90
53	BA	2725	A	C5-C6-N1	6.67	121.03	117.70
54	BB	15	A	C5-C6-N1	6.67	121.03	117.70
21	AA	66	A	C4-C5-C6	-6.67	113.67	117.00
53	BA	2660	A	C5-C6-N1	6.67	121.03	117.70
21	AA	1180	A	C5-C6-N1	6.67	121.03	117.70
27	BF	109	ARG	NE-CZ-NH1	6.67	123.63	120.30
21	AA	687	A	C4-C5-C6	-6.66	113.67	117.00
22	A1	75	C	N3-C2-O2	-6.66	117.23	121.90
21	AA	52	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	520	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	777	A	C4-C5-C6	-6.66	113.67	117.00
53	BA	1366	A	C5-C6-N1	6.66	121.03	117.70
53	BA	1780	A	O4'-C1'-N9	6.66	113.53	108.20
53	BA	1919	A	C5-C6-N1	6.66	121.03	117.70
53	BA	1140	C	N3-C2-O2	-6.66	117.24	121.90
53	BA	2515	C	O4'-C1'-N1	6.66	113.53	108.20
21	AA	812	G	N3-C4-C5	-6.66	125.27	128.60
21	AA	469	C	O4'-C1'-N1	6.66	113.53	108.20
21	AA	1418	A	C5-C6-N1	6.66	121.03	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1487	G	N3-C2-N2	-6.66	115.24	119.90
22	A1	41	A	C4-C5-C6	-6.66	113.67	117.00
53	BA	2654	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	87	C	N3-C2-O2	-6.65	117.24	121.90
53	BA	323	C	C1'-O4'-C4'	-6.65	104.58	109.90
53	BA	1967	C	O4'-C1'-N1	6.65	113.52	108.20
53	BA	2612	C	N3-C2-O2	-6.65	117.24	121.90
53	BA	959	A	C5-C6-N1	6.65	121.03	117.70
53	BA	1844	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	673	A	C5-C6-N1	6.65	121.02	117.70
21	AA	1322	C	N3-C2-O2	-6.65	117.25	121.90
53	BA	2225	A	N1-C6-N6	-6.65	114.61	118.60
21	AA	744	C	N3-C2-O2	-6.65	117.25	121.90
44	BW	10	ARG	NE-CZ-NH2	6.65	123.62	120.30
53	BA	84	A	C5-C6-N1	6.65	121.02	117.70
53	BA	1133	A	C4-C5-C6	-6.65	113.68	117.00
53	BA	1229	C	O4'-C1'-N1	6.65	113.52	108.20
53	BA	1803	A	C4-C5-C6	-6.65	113.68	117.00
53	BA	2746	U	O4'-C1'-N1	6.65	113.52	108.20
21	AA	665	A	C4-C5-C6	-6.65	113.68	117.00
21	AA	823	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	1114	C	N3-C2-O2	-6.65	117.25	121.90
53	BA	1252	G	P-O3'-C3'	6.65	127.67	119.70
21	AA	1069	C	N3-C2-O2	-6.64	117.25	121.90
53	BA	2260	C	N3-C2-O2	-6.64	117.25	121.90
19	AT	9	ARG	NE-CZ-NH1	6.64	123.62	120.30
21	AA	306	A	C4-C5-C6	-6.64	113.68	117.00
21	AA	1080	A	C4-C5-C6	-6.64	113.68	117.00
53	BA	104	A	C4-C5-C6	-6.64	113.68	117.00
53	BA	660	C	N3-C2-O2	-6.64	117.25	121.90
53	BA	1469	A	C6-C5-N7	6.64	136.95	132.30
53	BA	1881	C	O4'-C1'-N1	6.64	113.51	108.20
21	AA	1394	A	C4-C5-C6	-6.64	113.68	117.00
53	BA	1732	C	N3-C2-O2	-6.64	117.25	121.90
3	AD	80	ARG	NE-CZ-NH2	-6.64	116.98	120.30
21	AA	23	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	805	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	906	A	N1-C6-N6	-6.64	114.62	118.60
21	AA	1092	A	C4-C5-C6	-6.64	113.68	117.00
21	AA	1162	C	N3-C2-O2	-6.64	117.25	121.90
54	BB	113	C	N3-C2-O2	-6.64	117.25	121.90
53	BA	1053	C	O4'-C1'-N1	6.64	113.51	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AK	105	ARG	NE-CZ-NH1	6.64	123.62	120.30
21	AA	156	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	223	A	C5-C6-N1	6.64	121.02	117.70
21	AA	732	C	N3-C2-O2	-6.64	117.25	121.90
53	BA	2873	A	N1-C6-N6	-6.64	114.62	118.60
21	AA	370	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	665	A	C5-C6-N1	6.63	121.02	117.70
21	AA	695	A	N1-C6-N6	-6.63	114.62	118.60
54	BB	53	A	C4-C5-C6	-6.63	113.68	117.00
21	AA	1004	A	C4-C5-C6	-6.63	113.68	117.00
21	AA	60	A	N1-C6-N6	-6.63	114.62	118.60
21	AA	511	C	N3-C2-O2	-6.63	117.26	121.90
32	BK	108	ARG	NE-CZ-NH1	6.63	123.61	120.30
53	BA	192	C	N1-C2-O2	6.63	122.88	118.90
53	BA	1641	A	C5-C6-N1	6.63	121.01	117.70
53	BA	1969	A	O4'-C1'-N9	6.63	113.50	108.20
53	BA	2241	A	C4-C5-C6	-6.63	113.69	117.00
53	BA	2429	G	C8-N9-C4	-6.63	103.75	106.40
53	BA	2587	A	C4-C5-C6	-6.63	113.69	117.00
53	BA	1691	C	N3-C2-O2	-6.62	117.26	121.90
53	BA	2008	C	N3-C2-O2	-6.62	117.26	121.90
53	BA	2133	G	C5-C6-N1	6.62	114.81	111.50
53	BA	581	C	N3-C2-O2	-6.62	117.26	121.90
53	BA	911	A	N1-C6-N6	-6.62	114.63	118.60
53	BA	1279	G	C5-C6-N1	6.62	114.81	111.50
53	BA	1634	A	C5-C6-N1	6.62	121.01	117.70
53	BA	2270	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	1192	C	O4'-C1'-N1	6.62	113.50	108.20
53	BA	1279	G	N1-C6-O6	-6.62	115.93	119.90
53	BA	1385	A	C4-C5-C6	-6.62	113.69	117.00
53	BA	2206	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	940	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	1508	A	C4-C5-C6	-6.62	113.69	117.00
43	BV	18	ARG	NE-CZ-NH1	6.62	123.61	120.30
53	BA	2759	G	N1-C6-O6	-6.62	115.93	119.90
21	AA	1252	A	C4-C5-C6	-6.62	113.69	117.00
53	BA	974	G	N9-C1'-C2'	6.62	122.60	114.00
53	BA	1615	C	N3-C2-O2	-6.62	117.27	121.90
53	BA	1918	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	285	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	910	C	O4'-C1'-N1	6.61	113.49	108.20
53	BA	575	A	N1-C6-N6	-6.61	114.63	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	998	C	N3-C2-O2	-6.61	117.27	121.90
3	AD	164	ARG	NE-CZ-NH1	6.61	123.61	120.30
21	AA	288	A	N1-C6-N6	-6.61	114.63	118.60
21	AA	1437	A	C5-C6-N1	6.61	121.00	117.70
53	BA	2285	C	N3-C2-O2	-6.61	117.27	121.90
53	BA	1787	A	N1-C6-N6	-6.61	114.64	118.60
53	BA	2749	A	C5-C6-N1	6.61	121.00	117.70
26	BE	49	ARG	NE-CZ-NH1	6.61	123.60	120.30
53	BA	2243	U	O4'-C1'-N1	6.61	113.49	108.20
21	AA	510	A	C4-C5-C6	-6.61	113.70	117.00
28	BG	2	ARG	NE-CZ-NH2	6.61	123.60	120.30
53	BA	2760	C	N3-C2-O2	-6.61	117.28	121.90
53	BA	1231	U	O4'-C1'-N1	6.60	113.48	108.20
53	BA	1664	A	C5-C6-N1	6.60	121.00	117.70
53	BA	2837	A	C5-C6-N1	6.60	121.00	117.70
53	BA	398	C	O4'-C1'-N1	6.60	113.48	108.20
53	BA	758	C	N3-C2-O2	-6.60	117.28	121.90
53	BA	1431	A	C5-C6-N1	6.60	121.00	117.70
53	BA	2070	A	C5-C6-N1	6.60	121.00	117.70
53	BA	1641	A	N1-C6-N6	-6.60	114.64	118.60
53	BA	2753	A	C4-C5-C6	-6.60	113.70	117.00
53	BA	1427	A	C5-C6-N1	6.60	121.00	117.70
21	AA	1115	U	O4'-C1'-N1	6.60	113.48	108.20
21	AA	1317	C	N1-C2-O2	6.60	122.86	118.90
53	BA	915	C	N3-C2-O2	-6.60	117.28	121.90
53	BA	951	C	N3-C2-O2	-6.60	117.28	121.90
53	BA	1470	A	C4-C5-C6	-6.60	113.70	117.00
53	BA	1001	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	746	A	C5-C6-N1	6.59	121.00	117.70
53	BA	1701	A	C4-C5-C6	-6.59	113.70	117.00
53	BA	1908	C	N3-C2-O2	-6.59	117.28	121.90
53	BA	143	C	N3-C2-O2	-6.59	117.28	121.90
21	AA	746	A	C4-C5-C6	-6.59	113.70	117.00
53	BA	415	A	C4-C5-C6	-6.59	113.70	117.00
53	BA	597	G	N1-C6-O6	-6.59	115.95	119.90
53	BA	829	A	C4-C5-C6	-6.59	113.70	117.00
53	BA	599	A	C4-C5-C6	-6.59	113.70	117.00
53	BA	1196	C	O4'-C1'-N1	6.59	113.47	108.20
53	BA	2896	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	816	A	N1-C6-N6	-6.59	114.65	118.60
53	BA	249	C	P-O3'-C3'	6.58	127.60	119.70
53	BA	1396	U	N3-C2-O2	-6.58	117.59	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1508	A	N1-C6-N6	-6.58	114.65	118.60
53	BA	2025	C	N3-C2-O2	-6.58	117.29	121.90
53	BA	733	G	N1-C6-O6	-6.58	115.95	119.90
53	BA	1685	C	O4'-C1'-N1	6.58	113.47	108.20
53	BA	1882	U	O4'-C1'-N1	6.58	113.47	108.20
21	AA	1284	C	O4'-C1'-N1	6.58	113.46	108.20
36	BO	33	ARG	NE-CZ-NH2	6.58	123.59	120.30
53	BA	245	G	C8-N9-C4	-6.58	103.77	106.40
53	BA	1611	C	N3-C2-O2	-6.58	117.29	121.90
14	AO	88	ARG	NE-CZ-NH1	6.58	123.59	120.30
21	AA	1479	C	N3-C2-O2	-6.58	117.30	121.90
53	BA	152	A	C4-C5-C6	-6.58	113.71	117.00
53	BA	516	C	N3-C2-O2	-6.58	117.29	121.90
53	BA	845	A	C5-C6-N1	6.58	120.99	117.70
54	BB	94	A	C5-C6-N1	6.58	120.99	117.70
21	AA	1521	C	N3-C4-C5	6.58	124.53	121.90
53	BA	1301	A	C2-N3-C4	6.58	113.89	110.60
21	AA	533	A	C3'-C2'-C1'	6.58	106.76	101.50
53	BA	1169	A	C5-C6-N1	6.58	120.99	117.70
53	BA	1180	U	O4'-C1'-N1	6.58	113.46	108.20
53	BA	1207	C	N3-C2-O2	-6.58	117.30	121.90
53	BA	1552	A	O4'-C1'-N9	6.58	113.46	108.20
53	BA	1652	A	C5-C6-N1	6.58	120.99	117.70
53	BA	2043	C	N1-C2-O2	6.58	122.84	118.90
53	BA	2171	A	C5-C6-N1	6.58	120.99	117.70
53	BA	776	G	O4'-C1'-N9	6.57	113.46	108.20
53	BA	828	U	N3-C2-O2	-6.57	117.60	122.20
53	BA	1415	U	O4'-C1'-N1	6.57	113.46	108.20
53	BA	2675	A	C4-C5-C6	-6.57	113.71	117.00
53	BA	558	U	O4'-C1'-N1	6.57	113.46	108.20
53	BA	477	A	C5-C6-N1	6.57	120.98	117.70
53	BA	743	A	C4-C5-C6	-6.57	113.72	117.00
53	BA	847	U	N3-C2-O2	-6.57	117.60	122.20
53	BA	111	A	C5-C6-N1	6.57	120.98	117.70
53	BA	1525	A	C5-C6-N1	6.57	120.98	117.70
53	BA	1545	A	C4-C5-C6	-6.57	113.72	117.00
53	BA	2405	G	N1-C6-O6	-6.57	115.96	119.90
19	AT	17	ARG	NE-CZ-NH1	6.57	123.58	120.30
21	AA	117	G	N1-C6-O6	-6.57	115.96	119.90
21	AA	448	A	C4-C5-C6	-6.57	113.72	117.00
53	BA	130	C	O4'-C1'-N1	6.57	113.45	108.20
53	BA	838	C	N1-C2-O2	6.57	122.84	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1275	A	C5-C6-N1	6.57	120.98	117.70
53	BA	1786	A	C5-C6-N1	6.57	120.98	117.70
53	BA	1990	C	N3-C2-O2	-6.57	117.31	121.90
53	BA	2142	A	C5-C6-N1	6.57	120.98	117.70
53	BA	2614	A	C5-C6-N1	6.57	120.98	117.70
21	AA	143	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	906	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	1448	C	N3-C2-O2	-6.56	117.31	121.90
53	BA	164	C	N3-C2-O2	-6.56	117.31	121.90
53	BA	300	A	C5-C6-N1	6.56	120.98	117.70
53	BA	2358	A	C5-C6-N1	6.56	120.98	117.70
53	BA	71	A	C5-C6-N1	6.56	120.98	117.70
21	AA	1492	A	C4-C5-C6	-6.56	113.72	117.00
50	B2	34	ARG	NE-CZ-NH2	-6.56	117.02	120.30
53	BA	145	C	O4'-C1'-N1	6.56	113.45	108.20
53	BA	2212	A	C5-C6-N1	6.56	120.98	117.70
53	BA	2650	U	O4'-C1'-N1	6.56	113.45	108.20
53	BA	2054	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	400	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	900	A	C5-C6-N1	6.56	120.98	117.70
53	BA	429	A	C4-C5-C6	-6.56	113.72	117.00
53	BA	1287	A	C3'-C2'-C1'	6.56	106.75	101.50
53	BA	2590	A	C5-C6-N1	6.56	120.98	117.70
21	AA	136	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	903	G	C8-N9-C4	-6.55	103.78	106.40
53	BA	126	A	C4-C5-C6	-6.55	113.72	117.00
53	BA	1909	C	N3-C2-O2	-6.55	117.31	121.90
53	BA	2352	A	C5-C6-N1	6.55	120.98	117.70
21	AA	587	G	N1-C6-O6	-6.55	115.97	119.90
21	AA	78	A	C5-C6-N1	6.55	120.97	117.70
33	BL	33	ARG	NE-CZ-NH1	6.55	123.57	120.30
53	BA	126	A	C5-C6-N1	6.55	120.97	117.70
53	BA	2263	C	N1-C2-O2	6.55	122.83	118.90
53	BA	2065	C	N3-C2-O2	-6.55	117.32	121.90
53	BA	2342	C	N3-C2-O2	-6.55	117.32	121.90
21	AA	461	A	C4-C5-C6	-6.55	113.73	117.00
53	BA	1920	C	N3-C2-O2	-6.55	117.32	121.90
21	AA	48	C	N1-C2-O2	6.54	122.83	118.90
21	AA	988	G	N1-C6-O6	-6.54	115.97	119.90
53	BA	759	G	N1-C6-O6	-6.54	115.97	119.90
53	BA	2448	A	C5-C6-N1	6.54	120.97	117.70
37	BP	52	ARG	NE-CZ-NH1	6.54	123.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	624	C	N3-C2-O2	-6.54	117.32	121.90
53	BA	1347	A	C4-C5-C6	-6.54	113.73	117.00
53	BA	1893	C	N3-C2-O2	-6.54	117.32	121.90
53	BA	2824	C	N3-C2-O2	-6.54	117.32	121.90
53	BA	919	U	O4'-C1'-N1	6.54	113.43	108.20
54	BB	104	A	C4-C5-C6	-6.54	113.73	117.00
53	BA	284	U	O4'-C1'-N1	6.54	113.43	108.20
21	AA	980	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	1521	C	N3-C2-O2	-6.54	117.32	121.90
53	BA	280	U	N3-C2-O2	-6.54	117.62	122.20
53	BA	541	A	C5-C6-N1	6.54	120.97	117.70
53	BA	2157	G	N3-C4-C5	-6.54	125.33	128.60
53	BA	2284	A	N1-C6-N6	-6.54	114.68	118.60
53	BA	83	A	C4-C5-C6	-6.54	113.73	117.00
53	BA	301	G	O4'-C1'-N9	6.54	113.43	108.20
53	BA	430	A	C5-C6-N1	6.54	120.97	117.70
53	BA	1023	U	O4'-C1'-N1	6.54	113.43	108.20
21	AA	1021	A	C5-C6-N1	6.53	120.97	117.70
53	BA	16	C	N3-C2-O2	-6.53	117.33	121.90
53	BA	627	A	C5-C6-N1	6.53	120.97	117.70
53	BA	2798	U	O4'-C1'-N1	6.53	113.43	108.20
54	BB	3	C	O4'-C1'-N1	6.53	113.43	108.20
53	BA	385	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	865	A	C6-C5-N7	6.53	136.87	132.30
21	AA	1063	C	C6-N1-C2	-6.53	117.69	120.30
22	A1	9	A	N1-C6-N6	-6.53	114.68	118.60
53	BA	2381	A	C4-C5-C6	-6.53	113.73	117.00
53	BA	2591	C	N3-C2-O2	-6.53	117.33	121.90
53	BA	761	A	C5-C6-N1	6.53	120.97	117.70
6	AG	108	ARG	NE-CZ-NH2	-6.53	117.04	120.30
21	AA	72	A	C4-C5-C6	-6.53	113.74	117.00
21	AA	493	A	C5-C6-N1	6.53	120.96	117.70
53	BA	1089	A	N1-C6-N6	-6.53	114.68	118.60
53	BA	1806	C	N3-C2-O2	-6.53	117.33	121.90
53	BA	2359	C	O4'-C1'-N1	6.53	113.42	108.20
21	AA	36	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	366	A	C5-C6-N1	6.53	120.96	117.70
21	AA	441	A	C5-C6-N1	6.53	120.96	117.70
21	AA	931	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1103	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1358	U	C5-C6-N1	-6.53	119.44	122.70
53	BA	1350	C	N3-C2-O2	-6.53	117.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1803	A	C5-C6-N1	6.53	120.96	117.70
21	AA	608	A	C4-C5-C6	-6.52	113.74	117.00
53	BA	1268	A	C5-C6-N1	6.52	120.96	117.70
53	BA	2250	G	N1-C6-O6	-6.52	115.99	119.90
21	AA	556	C	N3-C2-O2	-6.52	117.33	121.90
53	BA	226	A	C5-C6-N1	6.52	120.96	117.70
53	BA	2090	A	C4-C5-C6	-6.52	113.74	117.00
4	AE	44	ARG	NE-CZ-NH1	6.52	123.56	120.30
53	BA	95	A	C5-C6-N1	6.52	120.96	117.70
54	BB	101	A	C5-C6-N1	6.52	120.96	117.70
21	AA	356	A	C5-C6-N1	6.52	120.96	117.70
21	AA	383	A	C5-C6-N1	6.52	120.96	117.70
53	BA	1739	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	99	C	N3-C2-O2	-6.52	117.34	121.90
53	BA	1509	A	C5-C6-N1	6.52	120.96	117.70
21	AA	689	C	N3-C2-O2	-6.51	117.34	121.90
53	BA	753	A	C5-C6-N1	6.51	120.96	117.70
53	BA	1020	A	C5-C6-N1	6.51	120.96	117.70
53	BA	1941	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	1097	C	N3-C2-O2	-6.51	117.34	121.90
53	BA	1885	A	C4-C5-C6	-6.51	113.75	117.00
53	BA	2416	C	N3-C2-O2	-6.51	117.34	121.90
53	BA	2516	A	C4-C5-C6	-6.51	113.75	117.00
53	BA	2748	A	C4-C5-C6	-6.51	113.74	117.00
53	BA	74	A	C5-C6-N1	6.51	120.95	117.70
53	BA	2014	A	C5-C6-N1	6.51	120.95	117.70
53	BA	2477	U	O4'-C1'-N1	6.51	113.41	108.20
21	AA	532	A	C4-C5-C6	-6.51	113.75	117.00
53	BA	119	A	C4-C5-C6	-6.51	113.75	117.00
53	BA	1191	G	N3-C4-C5	-6.51	125.35	128.60
11	AL	8	ARG	NE-CZ-NH2	6.50	123.55	120.30
53	BA	933	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1172	C	N3-C2-O2	-6.50	117.35	121.90
54	BB	35	C	N3-C4-C5	6.50	124.50	121.90
21	AA	305	G	O4'-C1'-N9	6.50	113.40	108.20
21	AA	421	U	N3-C2-O2	-6.50	117.65	122.20
53	BA	492	A	C5-C6-N1	6.50	120.95	117.70
53	BA	2164	C	N1-C2-O2	6.50	122.80	118.90
53	BA	32	C	N3-C2-O2	-6.50	117.35	121.90
53	BA	1727	C	N3-C2-O2	-6.50	117.35	121.90
53	BA	2435	A	N1-C6-N6	-6.50	114.70	118.60
21	AA	374	A	N1-C6-N6	-6.50	114.70	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1269	A	C4-C5-C6	-6.50	113.75	117.00
53	BA	2449	U	O4'-C1'-N1	6.50	113.40	108.20
53	BA	2899	A	C5-C6-N1	6.50	120.95	117.70
21	AA	78	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	374	A	C5-C6-N1	6.50	120.95	117.70
21	AA	432	A	C5-C6-N1	6.50	120.95	117.70
53	BA	2177	C	N3-C2-O2	-6.50	117.35	121.90
22	A1	73	A	C5-C6-N1	6.50	120.95	117.70
21	AA	74	A	C5-C6-N1	6.49	120.95	117.70
53	BA	979	A	C5-C6-N1	6.49	120.95	117.70
53	BA	2741	A	C4-C5-C6	-6.49	113.75	117.00
53	BA	1937	A	O4'-C1'-N9	6.49	113.39	108.20
53	BA	2407	A	C5-C6-N1	6.49	120.95	117.70
21	AA	579	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	1225	A	C4-C5-C6	-6.49	113.75	117.00
31	BJ	95	ARG	NE-CZ-NH1	6.49	123.55	120.30
53	BA	405	U	O4'-C1'-N1	6.49	113.39	108.20
53	BA	2620	C	N3-C2-O2	-6.49	117.36	121.90
53	BA	721	A	C4-C5-C6	-6.49	113.75	117.00
53	BA	1354	A	C5-C6-N1	6.49	120.94	117.70
53	BA	1548	A	C5-C6-N1	6.49	120.94	117.70
22	A1	26	A	C4-C5-C6	-6.49	113.76	117.00
53	BA	328	U	O4'-C1'-N1	6.49	113.39	108.20
53	BA	1404	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	264	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	275	G	C5-C6-N1	6.48	114.74	111.50
21	AA	420	U	O4'-C1'-N1	6.48	113.39	108.20
21	AA	574	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	637	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	1107	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	1269	A	C4-C5-C6	-6.48	113.76	117.00
24	BC	213	ARG	NE-CZ-NH2	-6.48	117.06	120.30
53	BA	515	A	N1-C6-N6	-6.48	114.71	118.60
53	BA	1398	C	N3-C2-O2	-6.48	117.36	121.90
53	BA	2358	A	C4-C5-C6	-6.48	113.76	117.00
53	BA	764	A	N1-C6-N6	-6.48	114.71	118.60
53	BA	981	A	C5-C6-N1	6.48	120.94	117.70
53	BA	1079	C	N3-C2-O2	-6.48	117.36	121.90
53	BA	1564	C	N3-C2-O2	-6.48	117.37	121.90
21	AA	1328	C	N3-C2-O2	-6.47	117.37	121.90
53	BA	1558	C	N1-C2-O2	6.47	122.78	118.90
53	BA	2160	C	N3-C2-O2	-6.47	117.37	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2393	U	O4'-C1'-N1	6.47	113.38	108.20
53	BA	2578	G	N1-C6-O6	-6.47	116.02	119.90
21	AA	1501	C	N1-C2-O2	6.47	122.78	118.90
53	BA	2652	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	403	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	510	A	C5-C6-N1	6.47	120.94	117.70
21	AA	1529	G	C1'-O4'-C4'	-6.47	104.72	109.90
25	BD	128	ARG	NE-CZ-NH2	6.47	123.53	120.30
53	BA	372	G	C8-N9-C4	-6.47	103.81	106.40
53	BA	380	G	N1-C6-O6	-6.47	116.02	119.90
53	BA	1607	C	N1-C2-O2	6.47	122.78	118.90
21	AA	338	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	930	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1413	A	C5-C6-N1	6.47	120.93	117.70
53	BA	395	U	O4'-C1'-N1	6.47	113.37	108.20
53	BA	1144	A	C5-C6-N1	6.47	120.93	117.70
53	BA	1211	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	414	A	C4-C5-C6	-6.47	113.77	117.00
53	BA	147	C	N3-C2-O2	-6.46	117.37	121.90
53	BA	1832	C	N3-C2-O2	-6.46	117.37	121.90
53	BA	2616	C	N3-C2-O2	-6.46	117.38	121.90
53	BA	2822	G	N1-C6-O6	-6.46	116.02	119.90
53	BA	2681	C	N3-C4-C5	6.46	124.48	121.90
21	AA	502	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	728	A	N1-C6-N6	-6.46	114.72	118.60
53	BA	423	A	C5-C6-N1	6.46	120.93	117.70
21	AA	366	A	N1-C6-N6	-6.46	114.72	118.60
13	AN	90	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	223	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	976	G	C5-C6-N1	6.46	114.73	111.50
21	AA	1484	C	O4'-C1'-N1	6.46	113.37	108.20
53	BA	812	C	N1-C2-O2	6.46	122.78	118.90
53	BA	1357	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	1160	G	N3-C2-N2	-6.46	115.38	119.90
24	BC	166	ARG	NE-CZ-NH2	-6.46	117.07	120.30
53	BA	2318	G	N1-C6-O6	-6.46	116.03	119.90
21	AA	63	C	N3-C2-O2	-6.45	117.38	121.90
53	BA	735	A	C4-C5-C6	-6.45	113.77	117.00
53	BA	972	A	C4-C5-C6	-6.45	113.77	117.00
53	BA	1367	A	C5-C6-N1	6.45	120.93	117.70
53	BA	2736	A	C5-C6-N1	6.45	120.93	117.70
22	A1	64	U	O4'-C1'-N1	6.45	113.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BF	149	ARG	NE-CZ-NH1	6.45	123.53	120.30
21	AA	869	G	C5-C6-N1	6.45	114.72	111.50
6	AG	142	ARG	NE-CZ-NH1	6.45	123.53	120.30
21	AA	602	A	C4-C5-C6	-6.45	113.78	117.00
53	BA	945	A	C5-C6-N1	6.45	120.92	117.70
53	BA	1528	A	C4-C5-C6	-6.45	113.78	117.00
53	BA	2404	U	O4'-C1'-N1	6.45	113.36	108.20
53	BA	658	U	O4'-C1'-N1	6.45	113.36	108.20
14	AO	71	ARG	NE-CZ-NH1	6.45	123.52	120.30
53	BA	332	A	N1-C6-N6	-6.45	114.73	118.60
53	BA	635	C	N1-C2-O2	6.44	122.77	118.90
53	BA	786	C	N1-C2-O2	6.44	122.77	118.90
53	BA	1269	A	N1-C6-N6	-6.44	114.73	118.60
53	BA	1610	A	C4-C5-C6	-6.44	113.78	117.00
53	BA	2225	A	O4'-C1'-N9	6.44	113.36	108.20
53	BA	2227	A	C5-C6-N1	6.44	120.92	117.70
16	AQ	10	ARG	NE-CZ-NH1	6.44	123.52	120.30
47	BZ	15	ARG	NE-CZ-NH2	-6.44	117.08	120.30
53	BA	1641	A	C4-C5-C6	-6.44	113.78	117.00
53	BA	204	A	C4-C5-C6	-6.44	113.78	117.00
53	BA	1699	G	N3-C2-N2	-6.44	115.39	119.90
53	BA	1893	C	O4'-C1'-N1	6.44	113.35	108.20
53	BA	941	A	C5'-C4'-O4'	6.44	116.83	109.10
53	BA	1821	A	C4-C5-C6	-6.44	113.78	117.00
53	BA	2814	A	C5-C6-N1	6.44	120.92	117.70
21	AA	1433	A	C4-C5-C6	-6.44	113.78	117.00
53	BA	1943	U	O4'-C1'-N1	6.44	113.35	108.20
53	BA	2776	A	C5-C6-N1	6.44	120.92	117.70
53	BA	52	A	C5-C6-N1	6.44	120.92	117.70
53	BA	1518	C	N3-C2-O2	-6.44	117.39	121.90
53	BA	62	U	N3-C2-O2	-6.43	117.70	122.20
53	BA	1165	A	N1-C6-N6	-6.43	114.74	118.60
2	AC	125	ARG	NE-CZ-NH1	6.43	123.52	120.30
53	BA	1260	A	C4-C5-C6	-6.43	113.78	117.00
53	BA	2469	A	C4-C5-C6	-6.43	113.78	117.00
53	BA	1290	C	N3-C2-O2	-6.43	117.40	121.90
53	BA	1434	A	N1-C6-N6	-6.43	114.74	118.60
53	BA	1794	A	C4-C5-C6	-6.43	113.78	117.00
53	BA	1985	C	N3-C2-O2	-6.43	117.40	121.90
6	AG	91	ARG	NE-CZ-NH1	6.43	123.52	120.30
21	AA	1458	G	N1-C6-O6	-6.43	116.04	119.90
21	AA	1493	A	C4-C5-C6	-6.43	113.78	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	715	A	C5-C6-N1	6.43	120.92	117.70
53	BA	1051	G	C5-C6-N1	6.43	114.71	111.50
28	BG	162	ARG	NE-CZ-NH1	6.43	123.51	120.30
21	AA	69	G	C8-N9-C4	-6.43	103.83	106.40
53	BA	533	G	C8-N9-C4	-6.43	103.83	106.40
21	AA	301	G	O4'-C1'-N9	6.42	113.34	108.20
21	AA	336	A	C5-C6-N1	6.42	120.91	117.70
21	AA	1238	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1301	U	N3-C2-O2	-6.42	117.70	122.20
53	BA	196	A	C5-C6-N1	6.42	120.91	117.70
53	BA	1049	C	N3-C2-O2	-6.42	117.40	121.90
53	BA	1775	U	O4'-C1'-N1	6.42	113.34	108.20
53	BA	2556	C	N3-C2-O2	-6.42	117.40	121.90
13	AN	65	ARG	NE-CZ-NH1	6.42	123.51	120.30
21	AA	960	U	N3-C2-O2	-6.42	117.70	122.20
53	BA	66	C	N3-C2-O2	-6.42	117.40	121.90
53	BA	346	A	O4'-C1'-N9	6.42	113.34	108.20
53	BA	778	G	N3-C4-C5	-6.42	125.39	128.60
21	AA	719	C	N1-C2-O2	6.42	122.75	118.90
53	BA	825	A	C5-C6-N1	6.42	120.91	117.70
53	BA	1005	C	C6-N1-C2	-6.42	117.73	120.30
53	BA	2466	C	N3-C2-O2	-6.42	117.40	121.90
21	AA	631	C	N1-C2-O2	6.42	122.75	118.90
53	BA	228	C	O4'-C1'-N1	6.42	113.34	108.20
53	BA	372	G	O4'-C1'-N9	6.42	113.33	108.20
53	BA	435	C	O4'-C1'-N1	6.42	113.33	108.20
53	BA	564	C	N3-C2-O2	-6.42	117.41	121.90
53	BA	1843	C	N1-C2-O2	6.42	122.75	118.90
53	BA	179	C	N3-C2-O2	-6.42	117.41	121.90
53	BA	433	C	O4'-C1'-N1	6.42	113.33	108.20
53	BA	633	A	C4-C5-C6	-6.42	113.79	117.00
53	BA	897	C	N3-C4-C5	6.42	124.47	121.90
53	BA	2482	A	C5-C6-N1	6.42	120.91	117.70
53	BA	2108	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	492	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	909	A	N1-C6-N6	-6.41	114.75	118.60
21	AA	1443	C	N3-C2-O2	-6.41	117.41	121.90
53	BA	226	A	N1-C6-N6	-6.41	114.75	118.60
53	BA	255	A	C4-C5-C6	-6.41	113.79	117.00
53	BA	13	A	C4-C5-C6	-6.41	113.79	117.00
53	BA	1162	G	N1-C6-O6	-6.41	116.05	119.90
21	AA	73	C	N3-C2-O2	-6.41	117.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1037	C	N1-C2-O2	6.41	122.75	118.90
21	AA	1298	U	N3-C2-O2	-6.41	117.71	122.20
53	BA	318	C	N3-C2-O2	-6.41	117.41	121.90
53	BA	1656	C	N1-C2-O2	6.41	122.75	118.90
53	BA	2825	G	N3-C2-N2	-6.41	115.41	119.90
7	AH	116	ARG	NE-CZ-NH1	6.41	123.50	120.30
53	BA	1490	A	O4'-C1'-N9	6.41	113.33	108.20
53	BA	2347	C	O4'-C1'-N1	6.41	113.33	108.20
53	BA	2887	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	36	C	N1-C2-O2	6.41	122.74	118.90
53	BA	632	A	C5-C6-N1	6.41	120.90	117.70
21	AA	614	C	O4'-C1'-N1	6.40	113.32	108.20
22	A1	18	G	O4'-C1'-N9	6.40	113.32	108.20
53	BA	808	G	O4'-C1'-N9	6.40	113.32	108.20
53	BA	1007	C	N3-C2-O2	-6.40	117.42	121.90
53	BA	1515	A	C4-C5-C6	-6.40	113.80	117.00
53	BA	219	A	C6-C5-N7	6.40	136.78	132.30
53	BA	1006	C	N3-C2-O2	-6.40	117.42	121.90
53	BA	1752	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	518	C	N3-C2-O2	-6.40	117.42	121.90
53	BA	820	A	C4-C5-C6	-6.40	113.80	117.00
53	BA	944	C	N3-C2-O2	-6.40	117.42	121.90
53	BA	43	G	C8-N9-C4	-6.40	103.84	106.40
53	BA	240	C	N1-C2-O2	6.40	122.74	118.90
53	BA	772	C	O4'-C1'-N1	6.40	113.32	108.20
53	BA	964	C	N3-C2-O2	-6.40	117.42	121.90
53	BA	1922	G	N1-C6-O6	-6.40	116.06	119.90
21	AA	693	G	N3-C4-C5	-6.40	125.40	128.60
21	AA	519	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	770	C	O4'-C1'-N1	6.39	113.31	108.20
53	BA	1128	G	O4'-C1'-N9	6.39	113.31	108.20
53	BA	2140	G	N1-C6-O6	-6.39	116.06	119.90
53	BA	1318	U	O4'-C1'-N1	6.39	113.31	108.20
21	AA	307	C	N3-C2-O2	-6.39	117.43	121.90
21	AA	978	A	C5-C6-N1	6.39	120.89	117.70
21	AA	1456	A	C4-C5-C6	-6.39	113.81	117.00
21	AA	1254	A	C4-C5-C6	-6.39	113.81	117.00
22	A1	65	C	N3-C2-O2	-6.39	117.43	121.90
45	BX	27	ARG	NE-CZ-NH1	6.39	123.50	120.30
53	BA	892	A	N1-C6-N6	-6.39	114.77	118.60
53	BA	1703	G	N1-C6-O6	-6.39	116.07	119.90
53	BA	2887	A	C5-C6-N1	6.39	120.89	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1161	C	O4'-C1'-N1	6.39	113.31	108.20
53	BA	1257	C	N3-C2-O2	-6.39	117.43	121.90
53	BA	2602	A	C5-C6-N1	6.39	120.89	117.70
21	AA	993	G	O4'-C1'-N9	6.38	113.31	108.20
53	BA	621	A	C5-C6-N1	6.38	120.89	117.70
53	BA	895	U	O4'-C1'-N1	6.38	113.31	108.20
53	BA	1795	C	O4'-C1'-N1	6.38	113.31	108.20
53	BA	783	A	C5'-C4'-O4'	6.38	116.76	109.10
53	BA	1644	C	N3-C2-O2	-6.38	117.43	121.90
53	BA	2261	C	O4'-C1'-N1	6.38	113.31	108.20
53	BA	97	C	N3-C2-O2	-6.38	117.43	121.90
54	BB	52	A	N1-C6-N6	-6.38	114.77	118.60
21	AA	197	A	N1-C6-N6	-6.38	114.77	118.60
21	AA	225	C	N3-C2-O2	-6.38	117.43	121.90
21	AA	256	U	O4'-C1'-N1	6.38	113.30	108.20
21	AA	934	C	N1-C2-O2	6.38	122.73	118.90
26	BE	79	ARG	NE-CZ-NH1	6.38	123.49	120.30
53	BA	906	U	O4'-C1'-N1	6.38	113.30	108.20
53	BA	2579	C	N3-C2-O2	-6.38	117.44	121.90
53	BA	2757	A	C5-C6-N1	6.38	120.89	117.70
28	BG	68	ARG	NE-CZ-NH1	6.38	123.49	120.30
53	BA	1987	A	C5-C6-N1	6.38	120.89	117.70
53	BA	1548	A	C4-C5-C6	-6.38	113.81	117.00
53	BA	1574	C	N1-C2-O2	6.38	122.72	118.90
53	BA	1686	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	25	C	N3-C2-O2	-6.37	117.44	121.90
53	BA	161	A	C4-C5-C6	-6.37	113.81	117.00
53	BA	584	C	N3-C2-O2	-6.37	117.44	121.90
53	BA	632	A	N1-C6-N6	-6.37	114.78	118.60
53	BA	2059	A	C5-C6-N1	6.37	120.89	117.70
53	BA	2791	G	N1-C6-O6	-6.37	116.08	119.90
55	B5	60	ARG	NE-CZ-NH2	6.37	123.49	120.30
21	AA	271	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	889	A	C4-C5-C6	-6.37	113.81	117.00
53	BA	1127	A	C4-C5-C6	-6.37	113.81	117.00
53	BA	2430	A	C4-C5-C6	-6.37	113.81	117.00
53	BA	2526	G	N1-C6-O6	-6.37	116.08	119.90
21	AA	216	U	O4'-C1'-N1	6.37	113.30	108.20
21	AA	539	A	C5-C6-N1	6.37	120.89	117.70
53	BA	885	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	205	A	C5-C6-N1	6.37	120.89	117.70
21	AA	335	C	N3-C2-O2	-6.37	117.44	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1368	A	C4-C5-C6	-6.37	113.81	117.00
53	BA	582	A	C5-C6-N1	6.37	120.88	117.70
53	BA	2193	G	O4'-C1'-N9	6.37	113.30	108.20
53	BA	1600	C	N3-C2-O2	-6.37	117.44	121.90
53	BA	90	U	O4'-C1'-N1	6.37	113.29	108.20
53	BA	2339	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1250	A	C5-C6-N1	6.36	120.88	117.70
53	BA	2879	A	O4'-C1'-N9	6.36	113.29	108.20
54	BB	60	C	N3-C2-O2	-6.36	117.44	121.90
14	AO	76	ARG	NE-CZ-NH2	-6.36	117.12	120.30
53	BA	772	C	N3-C2-O2	-6.36	117.45	121.90
53	BA	1592	C	N3-C2-O2	-6.36	117.45	121.90
53	BA	1733	G	C5-C6-N1	6.36	114.68	111.50
53	BA	2054	A	C5-C6-N1	6.36	120.88	117.70
53	BA	2199	A	C5-C6-N1	6.36	120.88	117.70
21	AA	84	U	O4'-C1'-N1	6.36	113.29	108.20
21	AA	1407	C	N3-C2-O2	-6.36	117.45	121.90
53	BA	282	A	C5-C6-N1	6.36	120.88	117.70
53	BA	732	C	O4'-C1'-N1	6.36	113.29	108.20
53	BA	1104	C	N3-C2-O2	-6.36	117.45	121.90
53	BA	2087	G	C5-C6-N1	6.36	114.68	111.50
53	BA	2101	A	C5-C6-N1	6.36	120.88	117.70
21	AA	274	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	1513	A	C5-C6-N1	6.36	120.88	117.70
53	BA	1974	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	119	A	C4-C5-C6	-6.36	113.82	117.00
53	BA	1698	A	C5-C6-N1	6.36	120.88	117.70
53	BA	267	C	N3-C2-O2	-6.36	117.45	121.90
53	BA	650	C	N1-C2-O2	6.36	122.71	118.90
21	AA	1521	C	N1-C2-O2	6.35	122.71	118.90
34	BM	38	ARG	NE-CZ-NH1	6.35	123.48	120.30
53	BA	1744	A	C5-C6-N1	6.35	120.88	117.70
21	AA	417	G	N1-C6-O6	-6.35	116.09	119.90
21	AA	1171	A	C4-C5-C6	-6.35	113.82	117.00
53	BA	626	A	C4-C5-C6	-6.35	113.82	117.00
53	BA	2029	G	C8-N9-C4	-6.35	103.86	106.40
53	BA	2152	G	C5-C6-N1	6.35	114.68	111.50
21	AA	1237	C	N3-C2-O2	-6.35	117.45	121.90
53	BA	25	U	O4'-C1'-N1	6.35	113.28	108.20
53	BA	181	A	C5-C6-N1	6.35	120.88	117.70
53	BA	2006	C	C6-N1-C2	-6.35	117.76	120.30
21	AA	328	C	N3-C2-O2	-6.35	117.46	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	575	G	P-O3'-C3'	6.35	127.32	119.70
21	AA	733	G	N1-C6-O6	-6.35	116.09	119.90
39	BR	79	ARG	NE-CZ-NH2	6.35	123.47	120.30
53	BA	231	A	C4-C5-C6	-6.35	113.83	117.00
53	BA	644	A	C4-C5-C6	-6.35	113.83	117.00
53	BA	1640	A	C4-C5-C6	-6.35	113.83	117.00
54	BB	8	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	640	A	C5-C6-N1	6.35	120.87	117.70
53	BA	1386	C	N3-C2-O2	-6.35	117.46	121.90
53	BA	1389	G	O4'-C1'-N9	6.35	113.28	108.20
53	BA	1591	A	C6-C5-N7	6.35	136.74	132.30
53	BA	1749	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	188	C	N1-C2-O2	6.34	122.71	118.90
21	AA	716	A	C5-C6-N1	6.34	120.87	117.70
21	AA	733	G	O4'-C1'-N9	6.34	113.28	108.20
22	A1	31	C	N3-C2-O2	-6.34	117.46	121.90
53	BA	49	A	C5-C6-N1	6.34	120.87	117.70
53	BA	201	C	N3-C4-C5	6.34	124.44	121.90
53	BA	1032	A	C4-C5-C6	-6.34	113.83	117.00
53	BA	2027	G	N1-C6-O6	-6.34	116.09	119.90
53	BA	622	G	N3-C4-C5	-6.34	125.43	128.60
53	BA	819	A	C4-C5-C6	-6.34	113.83	117.00
53	BA	971	G	N1-C6-O6	-6.34	116.10	119.90
53	BA	1351	C	N3-C2-O2	-6.34	117.46	121.90
53	BA	1711	A	N1-C6-N6	-6.34	114.80	118.60
53	BA	1801	A	C4-C5-C6	-6.34	113.83	117.00
53	BA	2277	G	C8-N9-C4	-6.34	103.86	106.40
53	BA	2455	G	C8-N9-C4	-6.34	103.86	106.40
21	AA	178	C	O4'-C1'-N1	6.34	113.27	108.20
45	BX	56	ARG	NE-CZ-NH2	-6.34	117.13	120.30
53	BA	1269	A	C5-C6-N1	6.34	120.87	117.70
53	BA	2721	A	C4-C5-C6	-6.34	113.83	117.00
25	BD	46	ARG	NE-CZ-NH1	6.34	123.47	120.30
53	BA	510	C	N3-C2-O2	-6.34	117.46	121.90
53	BA	679	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	635	A	C4-C5-C6	-6.34	113.83	117.00
53	BA	190	A	N1-C6-N6	-6.34	114.80	118.60
53	BA	1496	A	C4-C5-C6	-6.34	113.83	117.00
53	BA	2725	A	C4-C5-C6	-6.34	113.83	117.00
53	BA	2753	A	C5-C6-N1	6.34	120.87	117.70
53	BA	2825	G	C8-N9-C4	-6.34	103.86	106.40
54	BB	71	C	N3-C2-O2	-6.34	117.46	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	241	G	C5-C6-N1	6.33	114.67	111.50
53	BA	749	A	C4-C5-C6	-6.33	113.83	117.00
53	BA	995	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	560	A	C4-C5-C6	-6.33	113.83	117.00
21	AA	1263	C	N3-C2-O2	-6.33	117.47	121.90
53	BA	1508	A	C4-C5-C6	-6.33	113.83	117.00
53	BA	2041	U	O4'-C1'-N1	6.33	113.27	108.20
21	AA	568	G	N1-C6-O6	-6.33	116.10	119.90
53	BA	504	A	O4'-C1'-N9	6.33	113.27	108.20
53	BA	2582	G	C8-N9-C4	-6.33	103.87	106.40
54	BB	19	C	N3-C2-O2	-6.33	117.47	121.90
53	BA	2585	U	N1-C1'-C2'	-6.33	105.04	112.00
21	AA	207	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	251	G	C5-C6-N1	6.33	114.66	111.50
21	AA	1254	A	N1-C6-N6	-6.33	114.80	118.60
53	BA	256	A	C5-C6-N1	6.33	120.86	117.70
53	BA	984	A	C4-C5-C6	-6.33	113.83	117.00
53	BA	1762	A	C4-C5-C6	-6.33	113.84	117.00
53	BA	2205	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	381	C	N1-C2-O2	6.33	122.70	118.90
21	AA	1044	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	1480	A	C4-C5-C6	-6.33	113.84	117.00
53	BA	501	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	519	C	C3'-C2'-C1'	6.33	106.56	101.50
21	AA	1176	A	C4-C5-C6	-6.33	113.84	117.00
53	BA	787	C	N3-C4-C5	6.33	124.43	121.90
53	BA	899	A	C5-C6-N1	6.33	120.86	117.70
53	BA	1158	C	N1-C2-O2	6.33	122.69	118.90
53	BA	1936	A	C4-C5-C6	-6.33	113.84	117.00
53	BA	343	C	N3-C2-O2	-6.32	117.47	121.90
53	BA	753	A	C4-C5-C6	-6.32	113.84	117.00
53	BA	1140	C	C3'-C2'-C1'	6.32	106.56	101.50
53	BA	2095	A	C4-C5-C6	-6.32	113.84	117.00
53	BA	514	A	C4-C5-C6	-6.32	113.84	117.00
53	BA	727	A	C5-C6-N1	6.32	120.86	117.70
53	BA	2288	A	C5-C6-N1	6.32	120.86	117.70
53	BA	2534	A	C4-C5-C6	-6.32	113.84	117.00
23	A2	79	A	C4-C5-C6	-6.32	113.84	117.00
53	BA	1414	C	O4'-C1'-N1	6.32	113.25	108.20
53	BA	1552	A	N1-C6-N6	-6.32	114.81	118.60
3	AD	183	ARG	NE-CZ-NH1	6.32	123.46	120.30
21	AA	523	A	C5-C6-N1	6.32	120.86	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1665	A	N1-C6-N6	-6.32	114.81	118.60
21	AA	49	U	O4'-C1'-N1	6.32	113.25	108.20
21	AA	844	G	C5-C6-N1	6.32	114.66	111.50
54	BB	118	C	O4'-C1'-N1	6.32	113.25	108.20
53	BA	739	A	C5-C6-N1	6.31	120.86	117.70
53	BA	1088	A	C5-C6-N1	6.31	120.86	117.70
40	BS	25	ARG	NE-CZ-NH1	6.31	123.46	120.30
53	BA	2901	C	N3-C2-O2	-6.31	117.48	121.90
54	BB	31	C	C6-N1-C2	-6.31	117.78	120.30
21	AA	498	A	C5-C6-N1	6.31	120.86	117.70
21	AA	750	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	1352	C	N1-C2-O2	6.31	122.69	118.90
50	B2	12	ARG	NE-CZ-NH2	6.31	123.46	120.30
53	BA	2383	G	C5-C6-N1	6.31	114.66	111.50
38	BQ	47	ARG	NE-CZ-NH1	6.31	123.45	120.30
53	BA	115	C	N3-C2-O2	-6.31	117.48	121.90
53	BA	484	C	N3-C2-O2	-6.31	117.48	121.90
53	BA	2332	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	321	A	C4-C5-C6	-6.31	113.85	117.00
53	BA	559	G	O4'-C1'-N9	6.31	113.25	108.20
21	AA	338	A	N1-C6-N6	-6.30	114.82	118.60
44	BW	40	ARG	NE-CZ-NH1	6.30	123.45	120.30
53	BA	1934	C	N3-C2-O2	-6.30	117.49	121.90
53	BA	2029	G	N7-C8-N9	6.30	116.25	113.10
21	AA	1398	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	285	C	O4'-C1'-N1	6.30	113.24	108.20
21	AA	411	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	807	A	C4-C5-C6	-6.30	113.85	117.00
53	BA	922	C	N3-C2-O2	-6.30	117.49	121.90
53	BA	957	C	N3-C4-C5	6.30	124.42	121.90
34	BM	44	ARG	NE-CZ-NH1	6.30	123.45	120.30
53	BA	296	U	O4'-C1'-N1	6.30	113.24	108.20
53	BA	848	C	N3-C2-O2	-6.30	117.49	121.90
53	BA	1544	A	C4-C5-C6	-6.30	113.85	117.00
53	BA	1783	A	C4-C5-C6	-6.30	113.85	117.00
53	BA	1848	A	C5-C6-N1	6.30	120.85	117.70
53	BA	2298	A	C5-C6-N1	6.30	120.85	117.70
21	AA	836	G	N1-C6-O6	-6.30	116.12	119.90
53	BA	398	C	N3-C2-O2	-6.30	117.49	121.90
53	BA	1064	C	N3-C2-O2	-6.30	117.49	121.90
53	BA	1070	A	C5-C6-N1	6.30	120.85	117.70
21	AA	861	G	C5-C6-N1	6.29	114.65	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1983	G	N3-C4-C5	-6.29	125.45	128.60
26	BE	40	ARG	NE-CZ-NH1	6.29	123.45	120.30
53	BA	715	A	C4-C5-C6	-6.29	113.85	117.00
53	BA	1243	C	N1-C2-O2	6.29	122.68	118.90
53	BA	1461	C	N3-C2-O2	-6.29	117.50	121.90
53	BA	1618	A	C5-C6-N1	6.29	120.85	117.70
53	BA	2521	C	N3-C2-O2	-6.29	117.49	121.90
53	BA	1539	U	C1'-O4'-C4'	-6.29	104.87	109.90
53	BA	1735	A	C4-C5-C6	-6.29	113.85	117.00
53	BA	2033	A	C6-C5-N7	6.29	136.70	132.30
53	BA	2758	A	C4-C5-C6	-6.29	113.85	117.00
53	BA	2764	A	C5-C6-N1	6.29	120.85	117.70
53	BA	1677	A	C4-C5-C6	-6.29	113.86	117.00
53	BA	1879	C	N1-C2-O2	6.29	122.67	118.90
53	BA	633	A	C5-C6-N1	6.29	120.84	117.70
53	BA	2270	A	N1-C6-N6	-6.29	114.83	118.60
53	BA	2551	C	N3-C2-O2	-6.29	117.50	121.90
21	AA	1303	C	N3-C2-O2	-6.29	117.50	121.90
53	BA	975	A	C4-C5-C6	-6.29	113.86	117.00
32	BK	49	ARG	NE-CZ-NH1	6.29	123.44	120.30
53	BA	817	C	N1-C2-O2	6.29	122.67	118.90
53	BA	1142	A	C4-C5-C6	-6.29	113.86	117.00
53	BA	1868	C	N3-C2-O2	-6.29	117.50	121.90
53	BA	2626	C	O4'-C1'-N1	6.29	113.23	108.20
23	A2	88	U	C5-C6-N1	-6.28	119.56	122.70
53	BA	334	C	N3-C2-O2	-6.28	117.50	121.90
53	BA	870	U	O4'-C1'-N1	6.28	113.23	108.20
53	BA	1146	C	N3-C2-O2	-6.28	117.50	121.90
53	BA	1172	C	O4'-C1'-N1	6.28	113.23	108.20
21	AA	563	A	C4-C5-C6	-6.28	113.86	117.00
53	BA	1216	G	N1-C6-O6	-6.28	116.13	119.90
21	AA	434	U	O4'-C1'-N1	6.28	113.22	108.20
53	BA	508	A	C4-C5-C6	-6.28	113.86	117.00
53	BA	1429	G	N1-C6-O6	-6.28	116.13	119.90
53	BA	2146	C	N1-C2-O2	6.28	122.67	118.90
21	AA	40	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	10	A	C5-C6-N1	6.28	120.84	117.70
21	AA	430	A	N1-C6-N6	-6.28	114.83	118.60
21	AA	1325	C	N3-C2-O2	-6.28	117.51	121.90
21	AA	1255	G	O4'-C1'-N9	6.28	113.22	108.20
21	AA	1300	G	O4'-C1'-N9	6.28	113.22	108.20
21	AA	1331	G	N9-C4-C5	6.28	107.91	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	322	A	C5-C6-N1	6.28	120.84	117.70
53	BA	459	U	O4'-C1'-N1	6.28	113.22	108.20
53	BA	1536	C	N1-C2-O2	6.28	122.67	118.90
53	BA	2215	C	N3-C2-O2	-6.28	117.51	121.90
53	BA	2856	A	N1-C6-N6	-6.28	114.83	118.60
54	BB	61	G	N3-C2-N2	-6.28	115.51	119.90
21	AA	195	A	C6-C5-N7	6.27	136.69	132.30
21	AA	82	G	N1-C6-O6	-6.27	116.14	119.90
53	BA	19	A	C5-C6-N1	6.27	120.84	117.70
53	BA	788	A	C5-C6-N1	6.27	120.84	117.70
53	BA	1244	A	N1-C6-N6	-6.27	114.84	118.60
53	BA	2432	A	C5-C6-N1	6.27	120.84	117.70
53	BA	601	C	N3-C2-O2	-6.27	117.51	121.90
53	BA	2095	A	C5-C6-N1	6.27	120.83	117.70
53	BA	2146	C	N3-C2-O2	-6.27	117.51	121.90
53	BA	2495	G	C5-C6-N1	6.27	114.64	111.50
53	BA	901	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	430	A	C4-C5-C6	-6.27	113.87	117.00
21	AA	1404	C	N3-C2-O2	-6.27	117.51	121.90
22	A1	20	G	O4'-C1'-N9	6.27	113.21	108.20
53	BA	150	U	O4'-C1'-N1	6.27	113.21	108.20
53	BA	203	A	C5-C6-N1	6.27	120.83	117.70
53	BA	1561	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	667	G	N9-C4-C5	6.27	107.91	105.40
53	BA	908	C	N1-C2-O2	6.27	122.66	118.90
21	AA	1362	A	C5-C6-N1	6.26	120.83	117.70
53	BA	575	A	C4-C5-C6	-6.26	113.87	117.00
53	BA	1320	C	C6-N1-C2	-6.26	117.79	120.30
21	AA	18	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	996	A	C5-C6-N1	6.26	120.83	117.70
21	AA	1296	C	N3-C2-O2	-6.26	117.52	121.90
53	BA	322	A	C4-C5-C6	-6.26	113.87	117.00
53	BA	1431	A	C4-C5-C6	-6.26	113.87	117.00
53	BA	2556	C	O4'-C1'-N1	6.26	113.21	108.20
21	AA	308	C	N3-C2-O2	-6.26	117.52	121.90
53	BA	1730	C	N1-C2-O2	6.26	122.66	118.90
53	BA	2000	C	N1-C2-O2	6.26	122.66	118.90
53	BA	2738	A	C5-C6-N1	6.26	120.83	117.70
53	BA	2322	A	C5-C6-N1	6.26	120.83	117.70
53	BA	497	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	311	C	N1-C2-O2	6.26	122.65	118.90
21	AA	590	U	O4'-C1'-N1	6.26	113.20	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1038	C	N1-C2-O2	6.26	122.65	118.90
22	A1	69	A	C4-C5-C6	-6.26	113.87	117.00
53	BA	397	U	O4'-C1'-N1	6.26	113.20	108.20
53	BA	1647	U	N1-C2-N3	6.26	118.65	114.90
21	AA	435	A	C5-C6-N1	6.25	120.83	117.70
53	BA	1614	A	O4'-C1'-N9	6.25	113.20	108.20
53	BA	2214	C	N1-C2-O2	6.25	122.65	118.90
53	BA	2258	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	28	A	C4-C5-C6	-6.25	113.87	117.00
53	BA	236	C	N1-C2-O2	6.25	122.65	118.90
53	BA	1272	A	C5-C6-N1	6.25	120.83	117.70
53	BA	1757	A	C5-C6-N1	6.25	120.83	117.70
53	BA	1993	U	C5-C6-N1	-6.25	119.57	122.70
21	AA	1105	A	C5-C6-N1	6.25	120.83	117.70
35	BN	71	ARG	NE-CZ-NH2	6.25	123.43	120.30
53	BA	739	A	C4-C5-C6	-6.25	113.88	117.00
53	BA	2879	A	C4-C5-C6	-6.25	113.87	117.00
7	AH	87	ARG	NE-CZ-NH1	6.25	123.42	120.30
53	BA	177	G	N3-C4-C5	-6.25	125.47	128.60
53	BA	570	G	C1'-O4'-C4'	-6.25	104.90	109.90
53	BA	732	C	N3-C2-O2	-6.25	117.53	121.90
53	BA	1965	C	N3-C2-O2	-6.25	117.53	121.90
53	BA	2346	A	C5-C6-N1	6.25	120.82	117.70
21	AA	277	C	O4'-C1'-N1	6.25	113.20	108.20
53	BA	524	G	O4'-C1'-N9	6.25	113.20	108.20
53	BA	2646	C	N1-C2-O2	6.25	122.65	118.90
54	BB	42	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	1331	G	O4'-C1'-N9	6.24	113.19	108.20
53	BA	426	C	N3-C2-O2	-6.24	117.53	121.90
53	BA	610	C	N3-C2-O2	-6.24	117.53	121.90
53	BA	1743	G	C5-C6-N1	6.24	114.62	111.50
21	AA	850	U	C5-C6-N1	-6.24	119.58	122.70
53	BA	1353	A	C4-C5-C6	-6.24	113.88	117.00
53	BA	2086	U	O4'-C1'-N1	6.24	113.19	108.20
53	BA	2350	C	O4'-C1'-N1	6.24	113.19	108.20
21	AA	272	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	1480	A	C5-C6-N1	6.24	120.82	117.70
53	BA	1551	A	C4-C5-C6	-6.24	113.88	117.00
53	BA	2866	U	O4'-C1'-N1	6.24	113.19	108.20
53	BA	1059	G	O4'-C1'-N9	6.24	113.19	108.20
53	BA	1270	C	O4'-C1'-N1	6.24	113.19	108.20
53	BA	2119	A	C5-C6-N1	6.24	120.82	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1369	C	O4'-C1'-N1	6.24	113.19	108.20
43	BV	19	ARG	NH1-CZ-NH2	-6.24	112.54	119.40
21	AA	784	A	N1-C6-N6	-6.23	114.86	118.60
21	AA	1094	G	O4'-C1'-N9	6.23	113.19	108.20
53	BA	1526	C	N3-C2-O2	-6.23	117.54	121.90
11	AL	109	ARG	NE-CZ-NH1	6.23	123.42	120.30
21	AA	1310	G	N1-C6-O6	-6.23	116.16	119.90
21	AA	1428	A	C4-C5-C6	-6.23	113.88	117.00
53	BA	429	A	C5-C6-N1	6.23	120.82	117.70
53	BA	1336	A	C5-C6-N1	6.23	120.82	117.70
53	BA	1936	A	C5-C6-N1	6.23	120.82	117.70
54	BB	68	C	N3-C2-O2	-6.23	117.54	121.90
53	BA	1732	C	N1-C2-O2	6.23	122.64	118.90
53	BA	2657	A	C5-C6-N1	6.23	120.81	117.70
21	AA	708	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1379	G	N1-C6-O6	-6.23	116.16	119.90
22	A1	59	U	N3-C2-O2	-6.23	117.84	122.20
53	BA	1142	A	P-O3'-C3'	6.23	127.17	119.70
21	AA	962	C	N3-C2-O2	-6.23	117.54	121.90
53	BA	1472	C	N3-C2-O2	-6.23	117.54	121.90
12	AM	56	ARG	NE-CZ-NH1	6.22	123.41	120.30
21	AA	16	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	336	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1150	A	C5-C6-N1	6.22	120.81	117.70
53	BA	314	C	N3-C2-O2	-6.22	117.54	121.90
53	BA	608	A	C4-C5-C6	-6.22	113.89	117.00
53	BA	2341	G	C5-C6-N1	6.22	114.61	111.50
53	BA	2589	A	O4'-C1'-N9	6.22	113.18	108.20
53	BA	2781	A	C4-C5-C6	-6.22	113.89	117.00
53	BA	1103	A	C4-C5-C6	-6.22	113.89	117.00
53	BA	2777	G	C5-C6-N1	6.22	114.61	111.50
53	BA	402	A	N1-C6-N6	-6.22	114.87	118.60
53	BA	483	A	N1-C6-N6	-6.22	114.87	118.60
53	BA	840	C	N3-C2-O2	-6.22	117.55	121.90
53	BA	1028	A	N1-C6-N6	-6.22	114.87	118.60
21	AA	1517	G	C5-C6-N1	6.22	114.61	111.50
53	BA	1363	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	422	C	N3-C2-O2	-6.22	117.55	121.90
53	BA	125	A	O4'-C1'-N9	6.22	113.17	108.20
53	BA	1679	A	C5-C6-N1	6.22	120.81	117.70
53	BA	1854	A	C5-C6-N1	6.22	120.81	117.70
53	BA	1998	A	C5-C6-N1	6.22	120.81	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2446	G	C5-C6-N1	6.22	114.61	111.50
3	AD	43	ARG	NE-CZ-NH1	6.21	123.41	120.30
53	BA	800	A	C4-C5-C6	-6.21	113.89	117.00
54	BB	44	G	C5-C6-N1	6.21	114.61	111.50
21	AA	739	C	N1-C2-O2	6.21	122.63	118.90
53	BA	1945	G	N1-C6-O6	-6.21	116.17	119.90
21	AA	251	G	N1-C6-O6	-6.21	116.17	119.90
53	BA	2681	C	N3-C2-O2	-6.21	117.55	121.90
53	BA	1830	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	1141	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	1483	A	C4-C5-C6	-6.21	113.90	117.00
53	BA	2072	C	O4'-C1'-N1	6.21	113.17	108.20
21	AA	932	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	1350	A	O4'-C1'-N9	6.21	113.17	108.20
53	BA	66	C	O4'-C1'-N1	6.21	113.17	108.20
53	BA	820	A	C5-C6-N1	6.21	120.80	117.70
53	BA	1938	A	C4-C5-C6	-6.21	113.90	117.00
53	BA	918	A	C5-C6-N1	6.21	120.80	117.70
53	BA	1116	G	N9-C4-C5	6.21	107.88	105.40
53	BA	1960	A	C5-C6-N1	6.21	120.80	117.70
21	AA	373	A	N1-C6-N6	-6.20	114.88	118.60
53	BA	1136	G	N3-C4-C5	-6.20	125.50	128.60
21	AA	109	A	C4-C5-C6	-6.20	113.90	117.00
22	A1	71	C	N3-C2-O2	-6.20	117.56	121.90
53	BA	49	A	P-O3'-C3'	6.20	127.14	119.70
53	BA	709	U	O4'-C1'-N1	6.20	113.16	108.20
27	BF	166	ARG	NE-CZ-NH1	6.20	123.40	120.30
53	BA	1233	C	O4'-C1'-N1	6.20	113.16	108.20
53	BA	1802	A	N1-C6-N6	-6.20	114.88	118.60
53	BA	2518	A	C4-C5-C6	-6.20	113.90	117.00
9	AJ	5	ARG	NE-CZ-NH2	-6.20	117.20	120.30
21	AA	1261	A	C5-C6-N1	6.20	120.80	117.70
53	BA	1293	C	N1-C2-O2	6.20	122.62	118.90
53	BA	1791	A	C4-C5-C6	-6.20	113.90	117.00
53	BA	2872	A	C5-C6-N1	6.20	120.80	117.70
22	A1	20	G	C5-C6-N1	6.20	114.60	111.50
33	BL	123	ARG	NE-CZ-NH1	6.20	123.40	120.30
53	BA	559	G	N1-C6-O6	-6.20	116.18	119.90
53	BA	670	A	P-O3'-C3'	6.20	127.13	119.70
21	AA	759	A	C5-C6-N1	6.19	120.80	117.70
53	BA	2517	C	N1-C2-O2	6.19	122.62	118.90
53	BA	276	U	O4'-C1'-N1	6.19	113.15	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1144	A	C4-C5-C6	-6.19	113.90	117.00
53	BA	1902	C	O4'-C1'-N1	6.19	113.16	108.20
53	BA	2198	A	C4-C5-C6	-6.19	113.90	117.00
21	AA	58	C	N3-C2-O2	-6.19	117.57	121.90
24	BC	268	ARG	NE-CZ-NH1	6.19	123.39	120.30
53	BA	349	U	O4'-C1'-N1	6.19	113.15	108.20
53	BA	1607	C	O4'-C1'-N1	6.19	113.15	108.20
53	BA	1796	U	O4'-C1'-N1	6.19	113.15	108.20
53	BA	2030	A	C4-C5-C6	-6.19	113.91	117.00
53	BA	2261	C	P-O3'-C3'	6.19	127.13	119.70
53	BA	1615	C	C5'-C4'-O4'	6.19	116.53	109.10
53	BA	2171	A	O4'-C1'-N9	6.19	113.15	108.20
21	AA	52	C	O4'-C1'-N1	6.19	113.15	108.20
21	AA	419	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	487	A	C5-C6-N1	6.19	120.79	117.70
21	AA	1155	A	C5-C6-N1	6.19	120.79	117.70
28	BG	94	ARG	NE-CZ-NH1	6.19	123.39	120.30
21	AA	1431	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	1509	C	N3-C2-O2	-6.18	117.57	121.90
53	BA	629	G	N3-C4-C5	-6.18	125.51	128.60
53	BA	793	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	55	A	C5-C6-N1	6.18	120.79	117.70
21	AA	284	C	N3-C2-O2	-6.18	117.58	121.90
53	BA	905	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	389	A	C5-C6-N1	6.18	120.79	117.70
21	AA	553	A	C5-C6-N1	6.18	120.79	117.70
53	BA	404	A	N1-C6-N6	-6.18	114.89	118.60
53	BA	915	C	N1-C2-O2	6.18	122.61	118.90
53	BA	2447	G	O4'-C1'-N9	6.18	113.14	108.20
4	AE	156	ARG	NE-CZ-NH2	6.18	123.39	120.30
53	BA	434	U	O4'-C1'-N1	6.18	113.14	108.20
53	BA	668	A	C4-C5-C6	-6.18	113.91	117.00
53	BA	1247	A	C5-C6-N1	6.18	120.79	117.70
54	BB	99	A	C5-C6-N1	6.18	120.79	117.70
21	AA	924	C	N3-C2-O2	-6.17	117.58	121.90
53	BA	177	G	O4'-C1'-N9	6.17	113.14	108.20
53	BA	762	U	P-O3'-C3'	6.17	127.11	119.70
53	BA	1297	C	O4'-C1'-N1	6.17	113.14	108.20
21	AA	679	C	N3-C2-O2	-6.17	117.58	121.90
36	BO	16	ARG	NE-CZ-NH1	6.17	123.39	120.30
53	BA	2268	A	C5-C6-N1	6.17	120.79	117.70
53	BA	2450	A	C5-C6-N1	6.17	120.79	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	468	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	918	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	1311	A	C6-C5-N7	6.17	136.62	132.30
53	BA	611	C	N3-C2-O2	-6.17	117.58	121.90
53	BA	782	A	C5-C6-N1	6.17	120.79	117.70
53	BA	1528	A	C5-C6-N1	6.17	120.79	117.70
53	BA	2156	G	C5-C6-N1	6.17	114.58	111.50
21	AA	1202	U	O4'-C1'-N1	6.17	113.14	108.20
54	BB	91	C	C1'-O4'-C4'	-6.17	104.96	109.90
54	BB	91	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	85	U	O4'-C1'-N1	6.17	113.13	108.20
21	AA	206	C	N1-C2-O2	6.17	122.60	118.90
21	AA	265	G	N1-C6-O6	-6.17	116.20	119.90
21	AA	1282	C	N3-C2-O2	-6.17	117.58	121.90
53	BA	1646	C	N3-C2-O2	-6.17	117.58	121.90
53	BA	2184	A	C4-C5-C6	-6.17	113.92	117.00
54	BB	39	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	311	C	N3-C2-O2	-6.17	117.58	121.90
53	BA	956	G	N3-C4-C5	-6.17	125.52	128.60
53	BA	2019	A	C4-C5-C6	-6.17	113.92	117.00
53	BA	2496	C	N1-C2-O2	6.17	122.60	118.90
21	AA	51	A	C5-C6-N1	6.17	120.78	117.70
53	BA	181	A	C4'-C3'-C2'	-6.17	96.44	102.60
53	BA	257	C	N3-C2-O2	-6.17	117.58	121.90
53	BA	414	C	N3-C2-O2	-6.16	117.58	121.90
53	BA	738	G	N1-C6-O6	-6.16	116.20	119.90
53	BA	1507	C	N3-C2-O2	-6.16	117.58	121.90
53	BA	903	C	N3-C2-O2	-6.16	117.59	121.90
53	BA	1395	A	C4-C5-C6	-6.16	113.92	117.00
53	BA	535	G	C5-C6-N1	6.16	114.58	111.50
53	BA	686	U	O4'-C1'-N1	6.16	113.13	108.20
21	AA	210	C	O4'-C1'-N1	6.16	113.13	108.20
21	AA	603	U	C5-C6-N1	-6.16	119.62	122.70
21	AA	1346	A	C5-C6-N1	6.16	120.78	117.70
21	AA	1384	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	1385	G	N1-C6-O6	-6.16	116.21	119.90
53	BA	238	C	N3-C2-O2	-6.16	117.59	121.90
53	BA	1371	G	N3-C2-N2	-6.16	115.59	119.90
21	AA	47	C	N3-C4-C5	6.16	124.36	121.90
21	AA	576	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	729	A	C4-C5-C6	-6.16	113.92	117.00
33	BL	126	ARG	NE-CZ-NH1	6.16	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	816	C	O4'-C1'-N1	6.16	113.12	108.20
53	BA	1940	U	N3-C2-O2	-6.16	117.89	122.20
53	BA	2503	A	P-O3'-C3'	6.16	127.09	119.70
54	BB	93	C	N3-C2-O2	-6.16	117.59	121.90
53	BA	458	G	C5-C6-N1	6.15	114.58	111.50
53	BA	2666	C	N1-C2-O2	6.15	122.59	118.90
6	AG	137	ARG	NE-CZ-NH2	-6.15	117.22	120.30
53	BA	112	U	C5-C6-N1	-6.15	119.62	122.70
53	BA	1926	U	N1-C2-N3	6.15	118.59	114.90
21	AA	76	G	N1-C6-O6	-6.15	116.21	119.90
21	AA	342	C	N3-C2-O2	-6.15	117.59	121.90
22	A1	36	C	O4'-C1'-N1	6.15	113.12	108.20
27	BF	70	ARG	NE-CZ-NH2	6.15	123.38	120.30
53	BA	518	G	N1-C6-O6	-6.15	116.21	119.90
53	BA	2425	A	C5'-C4'-C3'	-6.15	106.16	116.00
54	BB	89	U	C5-C6-N1	-6.15	119.62	122.70
2	AC	126	ARG	NE-CZ-NH1	6.15	123.37	120.30
21	AA	1388	C	O4'-C1'-N1	6.15	113.12	108.20
21	AA	477	C	N3-C2-O2	-6.15	117.60	121.90
53	BA	2611	C	N3-C2-O2	-6.15	117.60	121.90
53	BA	2856	A	C5-C6-N1	6.15	120.77	117.70
21	AA	612	C	N3-C2-O2	-6.14	117.60	121.90
53	BA	2184	A	C5-C6-N1	6.14	120.77	117.70
53	BA	2411	A	C5-C6-N1	6.14	120.77	117.70
21	AA	896	C	N1-C2-O2	6.14	122.58	118.90
21	AA	1292	G	N1-C6-O6	-6.14	116.21	119.90
21	AA	1298	U	C1'-O4'-C4'	-6.14	104.99	109.90
53	BA	1262	A	C4-C5-C6	-6.14	113.93	117.00
53	BA	1507	C	N3-C4-C5	6.14	124.36	121.90
53	BA	1583	A	C4-C5-C6	-6.14	113.93	117.00
53	BA	1833	C	N3-C2-O2	-6.14	117.60	121.90
53	BA	2364	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	1448	C	N1-C2-O2	6.14	122.58	118.90
53	BA	885	C	O4'-C1'-N1	6.14	113.11	108.20
21	AA	269	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	735	C	N3-C2-O2	-6.14	117.60	121.90
22	A1	6	A	C5-C6-N1	6.14	120.77	117.70
53	BA	1086	A	C5-C6-N1	6.14	120.77	117.70
53	BA	2841	C	N1-C2-O2	6.14	122.58	118.90
53	BA	443	A	N1-C6-N6	-6.14	114.92	118.60
53	BA	1332	G	O4'-C1'-N9	6.14	113.11	108.20
53	BA	1338	G	C5-C6-N1	6.14	114.57	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	163	C	O4'-C1'-N1	6.14	113.11	108.20
21	AA	536	C	N3-C2-O2	-6.14	117.61	121.90
21	AA	630	A	C6-C5-N7	6.14	136.60	132.30
21	AA	855	U	C5-C6-N1	-6.14	119.63	122.70
53	BA	174	U	O4'-C1'-N1	6.14	113.11	108.20
53	BA	512	G	O4'-C1'-N9	6.14	113.11	108.20
21	AA	53	A	O4'-C1'-N9	6.13	113.11	108.20
21	AA	67	C	N3-C4-C5	6.13	124.35	121.90
21	AA	1019	A	C5-C6-N1	6.13	120.77	117.70
53	BA	1695	G	N3-C4-C5	-6.13	125.53	128.60
53	BA	2362	C	C5'-C4'-O4'	6.13	116.46	109.10
53	BA	2439	A	C4-C5-C6	-6.13	113.93	117.00
21	AA	573	A	C5-C6-N1	6.13	120.77	117.70
1	AB	73	ARG	NE-CZ-NH1	6.13	123.37	120.30
21	AA	752	G	C8-N9-C4	-6.13	103.95	106.40
53	BA	847	U	O4'-C1'-N1	6.13	113.11	108.20
53	BA	1397	U	O4'-C1'-N1	6.13	113.11	108.20
53	BA	2314	A	N1-C6-N6	-6.13	114.92	118.60
53	BA	436	C	N3-C2-O2	-6.13	117.61	121.90
53	BA	456	C	N3-C4-C5	6.13	124.35	121.90
1	AB	112	ARG	NE-CZ-NH1	6.13	123.36	120.30
14	AO	53	ARG	NE-CZ-NH2	-6.13	117.24	120.30
21	AA	687	A	C5-C6-N1	6.13	120.76	117.70
21	AA	892	A	C5-C6-N1	6.13	120.77	117.70
53	BA	181	A	C4-C5-C6	-6.13	113.94	117.00
53	BA	565	C	O4'-C1'-N1	6.13	113.10	108.20
53	BA	1034	G	C5-C6-N1	6.13	114.56	111.50
53	BA	1237	A	C4-C5-C6	-6.13	113.94	117.00
21	AA	456	A	N1-C6-N6	-6.13	114.92	118.60
21	AA	864	A	C5-C6-N1	6.13	120.76	117.70
53	BA	2094	A	C5-C6-N1	6.13	120.76	117.70
53	BA	2662	A	N1-C6-N6	-6.13	114.92	118.60
53	BA	2839	G	C8-N9-C4	-6.13	103.95	106.40
21	AA	526	C	N3-C2-O2	-6.12	117.61	121.90
22	A1	3	G	O4'-C1'-N9	6.12	113.10	108.20
53	BA	2021	C	N3-C2-O2	-6.12	117.61	121.90
53	BA	2129	C	N3-C2-O2	-6.12	117.61	121.90
53	BA	2425	A	O4'-C1'-N9	6.12	113.10	108.20
21	AA	200	G	C5-C6-N1	6.12	114.56	111.50
21	AA	1468	A	C5-C6-N1	6.12	120.76	117.70
53	BA	1270	C	N3-C2-O2	-6.12	117.61	121.90
53	BA	2612	C	N1-C2-O2	6.12	122.57	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1259	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	1413	A	C4-C5-C6	-6.12	113.94	117.00
53	BA	1608	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	131	A	C5-C6-N1	6.12	120.76	117.70
21	AA	866	C	N3-C2-O2	-6.12	117.62	121.90
21	AA	1177	G	N3-C2-N2	-6.12	115.62	119.90
53	BA	141	G	N1-C6-O6	-6.12	116.23	119.90
53	BA	573	U	P-O3'-C3'	6.12	127.04	119.70
53	BA	1735	A	C5-C6-N1	6.12	120.76	117.70
21	AA	525	C	N3-C2-O2	-6.12	117.62	121.90
53	BA	1916	A	C4-C5-C6	-6.12	113.94	117.00
12	AM	78	ARG	NE-CZ-NH2	6.12	123.36	120.30
21	AA	1095	U	C5-C6-N1	-6.12	119.64	122.70
53	BA	118	A	O4'-C1'-N9	6.12	113.09	108.20
53	BA	900	A	C5-C6-N1	6.12	120.76	117.70
53	BA	980	A	C5-C6-N1	6.12	120.76	117.70
53	BA	1181	U	C5-C6-N1	-6.12	119.64	122.70
53	BA	2684	U	O4'-C1'-N1	6.12	113.09	108.20
21	AA	50	A	C4-C5-C6	-6.11	113.94	117.00
21	AA	621	A	C6-C5-N7	6.11	136.58	132.30
21	AA	1149	C	N3-C2-O2	-6.11	117.62	121.90
53	BA	479	A	C6-C5-N7	6.11	136.58	132.30
53	BA	1504	A	C5-C6-N1	6.11	120.76	117.70
53	BA	2440	C	N1-C2-O2	6.11	122.57	118.90
21	AA	20	U	O4'-C1'-N1	6.11	113.09	108.20
21	AA	1179	A	C5-C6-N1	6.11	120.75	117.70
21	AA	1217	C	N1-C2-O2	6.11	122.57	118.90
53	BA	1302	A	C5-C6-N1	6.11	120.75	117.70
29	BH	51	ARG	NE-CZ-NH1	6.11	123.35	120.30
53	BA	1292	G	C5-C6-N1	6.11	114.55	111.50
21	AA	144	G	N3-C4-C5	-6.11	125.55	128.60
21	AA	267	C	N3-C2-O2	-6.11	117.63	121.90
21	AA	895	G	N1-C6-O6	-6.11	116.24	119.90
21	AA	896	C	N3-C2-O2	-6.11	117.63	121.90
21	AA	1508	A	C5-C6-N1	6.11	120.75	117.70
13	AN	13	ARG	NE-CZ-NH1	6.10	123.35	120.30
21	AA	678	U	O4'-C1'-N1	6.10	113.08	108.20
21	AA	1109	C	N1-C2-O2	6.10	122.56	118.90
53	BA	109	C	N3-C2-O2	-6.10	117.63	121.90
53	BA	562	U	N3-C2-O2	-6.10	117.93	122.20
53	BA	1676	A	C5-C6-N1	6.10	120.75	117.70
54	BB	10	G	O4'-C1'-N9	6.10	113.08	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	36	C	N3-C2-O2	-6.10	117.63	121.90
52	B4	19	ARG	NE-CZ-NH1	6.10	123.35	120.30
53	BA	1126	A	C4-C5-C6	-6.10	113.95	117.00
53	BA	1970	A	C5-C6-N1	6.10	120.75	117.70
53	BA	2382	G	O4'-C1'-N9	6.10	113.08	108.20
53	BA	2392	A	C5-C6-N1	6.10	120.75	117.70
53	BA	2565	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	475	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1399	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1484	C	N3-C2-O2	-6.10	117.63	121.90
38	BQ	54	ARG	NE-CZ-NH1	6.10	123.35	120.30
53	BA	787	C	N1-C2-O2	6.10	122.56	118.90
53	BA	1359	A	C5-C6-N1	6.10	120.75	117.70
53	BA	2380	C	O4'-C1'-N1	6.10	113.08	108.20
53	BA	2799	A	C4-C5-C6	-6.10	113.95	117.00
53	BA	1834	U	O4'-C1'-N1	6.10	113.08	108.20
53	BA	2354	C	N3-C2-O2	-6.10	117.63	121.90
27	BF	124	ARG	NE-CZ-NH1	-6.09	117.25	120.30
53	BA	821	A	C5-C6-N1	6.09	120.75	117.70
53	BA	972	A	C5-C6-N1	6.09	120.75	117.70
53	BA	1030	C	N3-C2-O2	-6.09	117.63	121.90
53	BA	1158	C	N3-C4-C5	6.09	124.34	121.90
21	AA	832	G	N1-C6-O6	-6.09	116.24	119.90
21	AA	978	A	C4-C5-C6	-6.09	113.95	117.00
53	BA	603	A	N1-C6-N6	-6.09	114.94	118.60
53	BA	2378	A	C5-C6-N1	6.09	120.75	117.70
21	AA	1329	A	C5-C6-N1	6.09	120.75	117.70
21	AA	1529	G	O4'-C1'-N9	6.09	113.07	108.20
53	BA	1419	A	N1-C6-N6	-6.09	114.94	118.60
53	BA	2633	G	N1-C6-O6	-6.09	116.25	119.90
21	AA	451	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	562	U	O4'-C1'-N1	6.09	113.07	108.20
22	A1	11	C	N3-C4-C5	6.09	124.34	121.90
27	BF	132	ARG	NE-CZ-NH1	6.09	123.34	120.30
31	BJ	35	ARG	NE-CZ-NH1	6.09	123.34	120.30
53	BA	1466	U	O4'-C1'-N1	6.09	113.07	108.20
54	BB	68	C	O4'-C1'-N1	6.09	113.07	108.20
53	BA	1	G	N3-C4-C5	-6.09	125.56	128.60
53	BA	985	C	N1-C2-O2	6.09	122.55	118.90
53	BA	2712	C	N3-C2-O2	-6.09	117.64	121.90
53	BA	2735	G	C5-C6-N1	6.09	114.54	111.50
21	AA	901	A	C4-C5-C6	-6.08	113.96	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1237	C	N1-C2-O2	6.08	122.55	118.90
53	BA	1670	C	N3-C2-O2	-6.08	117.64	121.90
53	BA	2496	C	N3-C4-C5	6.08	124.33	121.90
21	AA	382	A	C5-C6-N1	6.08	120.74	117.70
21	AA	652	U	O4'-C1'-N1	6.08	113.07	108.20
48	B0	39	ARG	NE-CZ-NH1	6.08	123.34	120.30
53	BA	227	A	C4-C5-C6	-6.08	113.96	117.00
53	BA	2834	G	C5-C6-N1	6.08	114.54	111.50
21	AA	266	G	N3-C2-N2	-6.08	115.64	119.90
21	AA	946	A	C5-C6-N1	6.08	120.74	117.70
21	AA	1437	A	N1-C6-N6	-6.08	114.95	118.60
53	BA	629	G	N1-C6-O6	-6.08	116.25	119.90
21	AA	53	A	C5-C6-N1	6.08	120.74	117.70
53	BA	391	A	N1-C6-N6	-6.08	114.95	118.60
53	BA	2795	C	N3-C2-O2	-6.08	117.65	121.90
3	AD	12	ARG	NE-CZ-NH1	6.08	123.34	120.30
21	AA	409	U	O4'-C1'-N1	6.08	113.06	108.20
21	AA	602	A	C6-C5-N7	6.08	136.55	132.30
21	AA	1305	G	C5-C6-N1	6.08	114.54	111.50
21	AA	1389	C	N3-C2-O2	-6.08	117.65	121.90
53	BA	105	C	N3-C2-O2	-6.08	117.65	121.90
53	BA	144	A	C4-C5-C6	-6.08	113.96	117.00
53	BA	223	A	C4-C5-C6	-6.08	113.96	117.00
53	BA	743	A	C6-C5-N7	6.08	136.55	132.30
53	BA	929	U	O4'-C1'-N1	6.08	113.06	108.20
53	BA	1682	G	O4'-C1'-N9	6.08	113.06	108.20
53	BA	2153	C	N3-C2-O2	-6.08	117.65	121.90
53	BA	2527	C	O4'-C1'-N1	6.08	113.06	108.20
21	AA	1042	A	O4'-C1'-N9	6.07	113.06	108.20
32	BK	17	ARG	NE-CZ-NH1	6.07	123.34	120.30
46	BY	48	ARG	NE-CZ-NH1	6.07	123.34	120.30
53	BA	151	C	N3-C2-O2	-6.07	117.65	121.90
53	BA	165	A	C6-C5-N7	6.07	136.55	132.30
53	BA	609	A	C5-C6-N1	6.07	120.74	117.70
53	BA	2406	A	C1'-O4'-C4'	-6.07	105.04	109.90
10	AK	105	ARG	NE-CZ-NH2	-6.07	117.26	120.30
21	AA	403	C	O4'-C1'-N1	6.07	113.06	108.20
21	AA	916	U	O4'-C1'-N1	6.07	113.06	108.20
37	BP	50	ARG	NE-CZ-NH1	6.07	123.33	120.30
53	BA	787	C	N3-C2-O2	-6.07	117.65	121.90
53	BA	1411	U	C5-C6-N1	-6.07	119.67	122.70
53	BA	1741	C	N3-C2-O2	-6.07	117.65	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	272	A	C5-C6-N1	6.07	120.73	117.70
53	BA	2598	A	C4-C5-C6	-6.07	113.97	117.00
54	BB	32	U	O4'-C1'-N1	6.07	113.06	108.20
21	AA	150	U	O4'-C1'-N1	6.07	113.05	108.20
53	BA	488	G	N1-C6-O6	-6.07	116.26	119.90
53	BA	634	C	O4'-C1'-N1	6.07	113.06	108.20
53	BA	1111	A	N1-C6-N6	-6.07	114.96	118.60
53	BA	1287	A	C1'-O4'-C4'	-6.07	105.05	109.90
21	AA	759	A	C4-C5-C6	-6.07	113.97	117.00
22	A1	62	C	N3-C2-O2	-6.07	117.65	121.90
53	BA	225	C	N3-C2-O2	-6.07	117.66	121.90
53	BA	269	C	N3-C2-O2	-6.07	117.65	121.90
53	BA	2893	A	N1-C6-N6	-6.07	114.96	118.60
54	BB	61	G	N9-C4-C5	6.07	107.83	105.40
38	BQ	29	ARG	NE-CZ-NH1	6.06	123.33	120.30
21	AA	1102	A	C5-C6-N1	6.06	120.73	117.70
53	BA	412	A	C6-C5-N7	6.06	136.54	132.30
53	BA	1337	G	N1-C6-O6	-6.06	116.26	119.90
53	BA	2055	C	N1-C2-O2	6.06	122.54	118.90
53	BA	118	A	C4-C5-C6	-6.06	113.97	117.00
53	BA	128	C	N3-C2-O2	-6.06	117.66	121.90
54	BB	41	G	C5-C6-N1	6.06	114.53	111.50
37	BP	100	ARG	NE-CZ-NH2	-6.06	117.27	120.30
53	BA	603	A	C5-C6-N1	6.06	120.73	117.70
53	BA	2617	U	O4'-C1'-N1	6.06	113.05	108.20
21	AA	1067	A	C6-C5-N7	6.06	136.54	132.30
21	AA	1218	C	N3-C2-O2	-6.06	117.66	121.90
53	BA	1365	A	C4-C5-C6	-6.06	113.97	117.00
53	BA	1480	C	N1-C2-O2	6.06	122.53	118.90
53	BA	2446	G	N1-C6-O6	-6.06	116.27	119.90
21	AA	1120	C	N3-C2-O2	-6.06	117.66	121.90
53	BA	835	C	N1-C2-O2	6.06	122.53	118.90
53	BA	1370	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	770	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	940	C	O4'-C1'-N1	6.05	113.04	108.20
21	AA	1210	C	N3-C2-O2	-6.05	117.66	121.90
53	BA	963	U	C1'-O4'-C4'	-6.05	105.06	109.90
53	BA	2336	A	C5-C6-N1	6.05	120.73	117.70
53	BA	2503	A	O4'-C1'-N9	6.05	113.04	108.20
54	BB	52	A	C5-C6-N1	6.05	120.73	117.70
54	BB	71	C	O4'-C1'-N1	6.05	113.04	108.20
21	AA	1211	U	C5-C6-N1	-6.05	119.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1318	A	C5-C6-N1	6.05	120.73	117.70
53	BA	2574	G	N7-C8-N9	6.05	116.13	113.10
53	BA	2133	G	N1-C6-O6	-6.05	116.27	119.90
53	BA	347	A	C4-C5-C6	-6.05	113.98	117.00
53	BA	2546	U	O4'-C1'-N1	6.05	113.04	108.20
19	AT	59	ARG	NE-CZ-NH1	6.05	123.32	120.30
21	AA	383	A	C4-C5-C6	-6.05	113.98	117.00
21	AA	545	C	N1-C2-O2	6.05	122.53	118.90
21	AA	611	C	N1-C2-O2	6.05	122.53	118.90
21	AA	1237	C	C3'-C2'-C1'	6.05	106.34	101.50
53	BA	408	G	C5-C6-N1	6.05	114.52	111.50
53	BA	947	A	C4-C5-C6	-6.05	113.98	117.00
53	BA	2572	A	C4-C5-C6	-6.05	113.98	117.00
21	AA	667	G	C8-N9-C4	-6.04	103.98	106.40
21	AA	1501	C	N3-C4-C5	6.04	124.32	121.90
22	A1	10	G	N3-C4-C5	-6.04	125.58	128.60
53	BA	1007	C	N3-C4-C5	6.04	124.32	121.90
53	BA	2679	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	967	C	N1-C2-O2	6.04	122.53	118.90
53	BA	253	C	N3-C2-O2	-6.04	117.67	121.90
53	BA	752	A	N1-C6-N6	-6.04	114.97	118.60
54	BB	109	A	C4-C5-C6	-6.04	113.98	117.00
54	BB	111	U	O4'-C1'-N1	6.04	113.03	108.20
21	AA	139	A	C4-C5-C6	-6.04	113.98	117.00
53	BA	351	C	N3-C2-O2	-6.04	117.67	121.90
53	BA	943	A	C5-C6-N1	6.04	120.72	117.70
53	BA	968	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	192	A	C4-C5-C6	-6.04	113.98	117.00
53	BA	246	C	O4'-C1'-N1	6.04	113.03	108.20
53	BA	1230	A	C4-C5-C6	-6.04	113.98	117.00
53	BA	1547	C	N3-C2-O2	-6.04	117.67	121.90
53	BA	2706	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	121	U	O4'-C1'-N1	6.04	113.03	108.20
53	BA	53	A	C4-C5-C6	-6.04	113.98	117.00
53	BA	2564	A	C4-C5-C6	-6.04	113.98	117.00
53	BA	767	U	O4'-C1'-N1	6.04	113.03	108.20
53	BA	1115	G	C8-N9-C4	-6.04	103.99	106.40
53	BA	2265	U	O4'-C1'-N1	6.04	113.03	108.20
22	A1	72	C	N3-C2-O2	-6.03	117.68	121.90
53	BA	357	C	N3-C2-O2	-6.03	117.68	121.90
53	BA	692	C	N3-C2-O2	-6.03	117.68	121.90
53	BA	2435	A	C5-C6-N1	6.03	120.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	243	A	N1-C6-N6	-6.03	114.98	118.60
23	A2	88	U	O4'-C1'-N1	6.03	113.03	108.20
21	AA	886	G	N1-C6-O6	-6.03	116.28	119.90
53	BA	1675	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	555	U	C5-C6-N1	-6.03	119.69	122.70
21	AA	737	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	729	A	O4'-C1'-N9	6.03	113.02	108.20
21	AA	1365	G	N1-C6-O6	-6.03	116.28	119.90
22	A1	36	C	C6-N1-C2	-6.03	117.89	120.30
53	BA	338	G	C4'-C3'-C2'	-6.03	96.57	102.60
53	BA	2157	G	C5-C6-N1	6.03	114.51	111.50
53	BA	2619	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	1397	C	O4'-C1'-N1	6.02	113.02	108.20
53	BA	1142	A	O4'-C1'-N9	6.02	113.02	108.20
53	BA	2081	U	N1-C2-N3	6.02	118.51	114.90
53	BA	2413	G	C5-C6-N1	6.02	114.51	111.50
53	BA	927	A	C5-C6-N1	6.02	120.71	117.70
53	BA	2374	C	N1-C2-O2	6.02	122.51	118.90
54	BB	87	U	C5-C6-N1	-6.02	119.69	122.70
21	AA	749	A	C6-C5-N7	6.02	136.51	132.30
21	AA	862	C	N3-C2-O2	-6.02	117.69	121.90
53	BA	167	A	C5-C6-N1	6.02	120.71	117.70
53	BA	2870	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	193	C	C3'-C2'-C1'	6.02	106.31	101.50
21	AA	431	A	C5-C6-N1	6.02	120.71	117.70
21	AA	1487	G	O4'-C1'-N9	6.02	113.02	108.20
53	BA	127	A	C5-C6-N1	6.02	120.71	117.70
53	BA	447	A	C5-C6-N1	6.02	120.71	117.70
21	AA	183	C	N1-C2-O2	6.02	122.51	118.90
21	AA	702	A	C5-C6-N1	6.02	120.71	117.70
22	A1	6	A	C4-C5-C6	-6.02	113.99	117.00
53	BA	309	A	N1-C6-N6	-6.02	114.99	118.60
53	BA	394	C	O4'-C1'-N1	6.02	113.01	108.20
53	BA	2364	C	O4'-C1'-N1	6.02	113.01	108.20
53	BA	2600	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	261	U	N3-C2-O2	-6.02	117.99	122.20
53	BA	752	A	C5-C6-N1	6.02	120.71	117.70
53	BA	1590	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	1525	G	N1-C6-O6	-6.01	116.29	119.90
53	BA	69	C	N3-C2-O2	-6.01	117.69	121.90
53	BA	565	C	N3-C2-O2	-6.01	117.69	121.90
53	BA	1324	G	O4'-C1'-N9	6.01	113.01	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1354	A	C4-C5-C6	-6.01	113.99	117.00
53	BA	1575	C	N3-C2-O2	-6.01	117.69	121.90
53	BA	1718	G	C5-C6-N1	6.01	114.51	111.50
53	BA	2467	C	O4'-C1'-N1	6.01	113.01	108.20
21	AA	1236	A	N1-C6-N6	-6.01	114.99	118.60
53	BA	1700	A	C5-C6-N1	6.01	120.71	117.70
21	AA	1113	C	N3-C2-O2	-6.01	117.69	121.90
53	BA	1362	C	N3-C2-O2	-6.01	117.69	121.90
53	BA	2416	C	C6-N1-C2	-6.01	117.89	120.30
21	AA	145	G	C5-C6-N1	6.01	114.50	111.50
21	AA	437	U	O4'-C1'-N1	6.01	113.01	108.20
53	BA	1173	U	O4'-C1'-N1	6.01	113.01	108.20
21	AA	1226	C	N3-C2-O2	-6.01	117.69	121.90
53	BA	1846	G	O4'-C1'-N9	6.01	113.01	108.20
53	BA	1876	A	C4-C5-C6	-6.01	114.00	117.00
21	AA	1031	C	O4'-C1'-N1	6.01	113.01	108.20
26	BE	88	ARG	NE-CZ-NH2	6.01	123.30	120.30
53	BA	533	G	N1-C6-O6	-6.01	116.30	119.90
53	BA	613	A	C3'-C2'-C1'	6.01	106.31	101.50
53	BA	1098	A	O4'-C1'-N9	6.01	113.01	108.20
53	BA	1477	A	N1-C6-N6	-6.01	115.00	118.60
53	BA	1757	A	C4-C5-C6	-6.01	114.00	117.00
53	BA	2066	C	O4'-C1'-N1	6.01	113.00	108.20
53	BA	2170	A	C5-C6-N1	6.01	120.70	117.70
53	BA	1799	G	N9-C4-C5	6.00	107.80	105.40
53	BA	2	G	C5-C6-N1	6.00	114.50	111.50
53	BA	103	A	C6-C5-N7	6.00	136.50	132.30
21	AA	385	C	N3-C2-O2	-6.00	117.70	121.90
53	BA	253	C	N1-C2-O2	6.00	122.50	118.90
53	BA	570	G	C5'-C4'-O4'	6.00	116.30	109.10
53	BA	1054	A	N1-C6-N6	-6.00	115.00	118.60
53	BA	1056	G	P-O3'-C3'	6.00	126.90	119.70
53	BA	1153	C	N1-C2-O2	6.00	122.50	118.90
42	BU	85	ARG	NE-CZ-NH2	6.00	123.30	120.30
53	BA	443	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	903	G	N7-C8-N9	6.00	116.10	113.10
21	AA	1152	A	C5-C6-N1	6.00	120.70	117.70
53	BA	1459	G	O4'-C1'-N9	6.00	113.00	108.20
21	AA	443	C	N3-C2-O2	-6.00	117.70	121.90
53	BA	663	G	N3-C2-N2	-6.00	115.70	119.90
21	AA	849	G	N1-C6-O6	-6.00	116.30	119.90
21	AA	1328	C	N3-C4-C5	6.00	124.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	57	C	N1-C2-O2	6.00	122.50	118.90
21	AA	150	U	C5-C6-N1	-5.99	119.70	122.70
24	BC	213	ARG	NE-CZ-NH1	5.99	123.30	120.30
21	AA	251	G	N3-C4-C5	-5.99	125.60	128.60
53	BA	14	A	C4-C5-C6	-5.99	114.00	117.00
4	AE	111	ARG	NE-CZ-NH1	5.99	123.30	120.30
21	AA	1370	G	C5-C6-N1	5.99	114.50	111.50
53	BA	76	C	N1-C2-O2	5.99	122.50	118.90
53	BA	580	U	O4'-C1'-N1	5.99	112.99	108.20
53	BA	1141	U	O4'-C1'-N1	5.99	112.99	108.20
53	BA	2342	C	N1-C2-O2	5.99	122.49	118.90
53	BA	2814	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	1042	A	C4-C5-C6	-5.99	114.01	117.00
53	BA	616	A	C5-C6-N1	5.99	120.69	117.70
53	BA	723	C	N3-C2-O2	-5.99	117.71	121.90
53	BA	2880	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	523	A	C4-C5-C6	-5.99	114.01	117.00
53	BA	1052	C	N1-C2-O2	5.99	122.49	118.90
53	BA	2266	A	C4-C5-C6	-5.99	114.01	117.00
1	AB	34	ARG	NE-CZ-NH1	5.99	123.29	120.30
21	AA	636	U	C5-C6-N1	-5.99	119.71	122.70
21	AA	211	G	N1-C6-O6	-5.98	116.31	119.90
21	AA	1081	A	C5-C6-N1	5.98	120.69	117.70
21	AA	824	G	C5-C6-N1	5.98	114.49	111.50
53	BA	1772	A	C4-C5-C6	-5.98	114.01	117.00
53	BA	1829	A	C4-C5-C6	-5.98	114.01	117.00
53	BA	1940	U	C1'-O4'-C4'	-5.98	105.11	109.90
53	BA	2283	C	O4'-C1'-N1	5.98	112.99	108.20
21	AA	82	G	O4'-C1'-N9	5.98	112.98	108.20
21	AA	228	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	296	U	C5-C6-N1	-5.98	119.71	122.70
21	AA	322	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	578	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	753	A	C5-C6-N1	5.98	120.69	117.70
21	AA	754	C	N1-C2-O2	5.98	122.49	118.90
21	AA	961	U	O4'-C1'-N1	5.98	112.98	108.20
53	BA	64	A	C5-C6-N1	5.98	120.69	117.70
53	BA	401	A	C4-C5-C6	-5.98	114.01	117.00
53	BA	704	G	O4'-C1'-N9	5.98	112.98	108.20
53	BA	1340	U	N3-C2-O2	-5.98	118.01	122.20
53	BA	1494	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	905	U	C5-C6-N1	-5.98	119.71	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BM	6	ARG	NE-CZ-NH1	5.98	123.29	120.30
53	BA	756	A	N1-C6-N6	-5.98	115.01	118.60
53	BA	1197	G	C5-C6-N1	5.98	114.49	111.50
21	AA	32	A	C5-C6-N1	5.98	120.69	117.70
21	AA	614	C	N3-C2-O2	-5.98	117.72	121.90
21	AA	1043	G	C5-C6-N1	5.98	114.49	111.50
21	AA	79	G	N3-C2-N2	-5.97	115.72	119.90
21	AA	296	U	N3-C2-O2	-5.97	118.02	122.20
21	AA	352	C	N1-C2-O2	5.97	122.48	118.90
53	BA	1383	A	C5-C6-N1	5.97	120.69	117.70
53	BA	2816	G	N1-C6-O6	-5.97	116.31	119.90
54	BB	115	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	35	G	C5-C6-N1	5.97	114.49	111.50
21	AA	172	A	C5-C6-N1	5.97	120.69	117.70
21	AA	1191	A	C5-C6-N1	5.97	120.69	117.70
53	BA	105	C	C3'-C2'-C1'	5.97	106.28	101.50
21	AA	1145	A	N1-C6-N6	-5.97	115.02	118.60
53	BA	167	A	N1-C6-N6	-5.97	115.02	118.60
53	BA	1084	A	C4-C5-C6	-5.97	114.01	117.00
53	BA	1227	G	O4'-C1'-N9	5.97	112.98	108.20
53	BA	1994	C	N3-C2-O2	-5.97	117.72	121.90
53	BA	901	C	O4'-C1'-N1	5.97	112.97	108.20
53	BA	1493	C	N3-C2-O2	-5.97	117.72	121.90
53	BA	1606	C	C6-N1-C2	-5.97	117.91	120.30
53	BA	2451	A	C5-C6-N1	5.97	120.69	117.70
53	BA	2771	C	N1-C2-O2	5.97	122.48	118.90
53	BA	2900	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	28	A	C6-C5-N7	5.97	136.48	132.30
22	A1	10	G	N1-C6-O6	-5.97	116.32	119.90
24	BC	174	ARG	NE-CZ-NH1	5.97	123.28	120.30
53	BA	234	U	N1-C2-N3	5.97	118.48	114.90
53	BA	918	A	N1-C6-N6	-5.97	115.02	118.60
53	BA	1221	C	N3-C2-O2	-5.97	117.72	121.90
53	BA	2531	A	C5-C6-N1	5.97	120.68	117.70
21	AA	378	G	C5'-C4'-O4'	5.96	116.26	109.10
21	AA	573	A	O4'-C4'-C3'	5.96	110.87	106.10
21	AA	715	A	C5-C6-N1	5.96	120.68	117.70
53	BA	184	C	N3-C2-O2	-5.96	117.72	121.90
53	BA	870	U	C5-C6-N1	-5.96	119.72	122.70
53	BA	2178	C	N3-C2-O2	-5.96	117.72	121.90
53	BA	2503	A	C5-C6-N1	5.96	120.68	117.70
54	BB	31	C	N3-C2-O2	-5.96	117.72	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	867	C	N3-C2-O2	-5.96	117.73	121.90
53	BA	2087	G	N3-C4-C5	-5.96	125.62	128.60
21	AA	324	G	C8-N9-C4	-5.96	104.02	106.40
53	BA	1912	A	C1'-O4'-C4'	-5.96	105.13	109.90
21	AA	1503	A	C4-C5-C6	-5.96	114.02	117.00
53	BA	191	A	N1-C6-N6	-5.96	115.02	118.60
21	AA	569	C	N3-C2-O2	-5.96	117.73	121.90
53	BA	2303	G	N1-C6-O6	-5.96	116.33	119.90
21	AA	190	A	C6-C5-N7	5.96	136.47	132.30
21	AA	831	A	C6-C5-N7	5.96	136.47	132.30
21	AA	1032	G	C3'-C2'-C1'	5.96	106.27	101.50
53	BA	1080	A	C5-C6-N1	5.96	120.68	117.70
53	BA	1272	A	C4-C5-C6	-5.96	114.02	117.00
53	BA	2191	A	C4-C5-C6	-5.96	114.02	117.00
53	BA	2502	G	N1-C6-O6	-5.96	116.33	119.90
53	BA	2518	A	C2-N3-C4	5.96	113.58	110.60
21	AA	1273	C	N3-C2-O2	-5.96	117.73	121.90
53	BA	806	C	N3-C2-O2	-5.96	117.73	121.90
53	BA	1874	C	N3-C2-O2	-5.96	117.73	121.90
53	BA	2179	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	408	A	C5-C6-N1	5.95	120.68	117.70
21	AA	1223	C	N3-C2-O2	-5.95	117.73	121.90
53	BA	2086	U	N1-C2-N3	5.95	118.47	114.90
53	BA	2208	C	N3-C2-O2	-5.95	117.73	121.90
53	BA	2581	G	N1-C6-O6	-5.95	116.33	119.90
53	BA	2764	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	160	A	C5-C6-N1	5.95	120.68	117.70
53	BA	145	C	N3-C2-O2	-5.95	117.73	121.90
53	BA	1233	C	N3-C4-C5	5.95	124.28	121.90
53	BA	1285	A	C5-C6-N1	5.95	120.67	117.70
53	BA	2676	C	N1-C2-O2	5.95	122.47	118.90
54	BB	108	A	C5-C6-N1	5.95	120.67	117.70
21	AA	507	C	N3-C2-O2	-5.95	117.73	121.90
22	A1	10	G	C5-C6-N1	5.95	114.47	111.50
53	BA	586	A	C4-C5-C6	-5.95	114.03	117.00
53	BA	1453	A	C2-N3-C4	5.95	113.57	110.60
53	BA	2539	C	N3-C2-O2	-5.95	117.74	121.90
54	BB	26	C	N3-C2-O2	-5.95	117.74	121.90
21	AA	830	G	N1-C6-O6	-5.95	116.33	119.90
53	BA	725	G	N3-C4-C5	-5.95	125.63	128.60
53	BA	1914	C	N1-C2-O2	5.95	122.47	118.90
53	BA	2212	A	N9-C4-C5	5.95	108.18	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2516	A	C6-C5-N7	5.95	136.46	132.30
21	AA	117	G	C8-N9-C4	-5.95	104.02	106.40
21	AA	1100	C	N1-C2-O2	5.95	122.47	118.90
21	AA	1179	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	1287	A	C5-C6-N1	5.95	120.67	117.70
21	AA	1326	U	O4'-C1'-N1	5.95	112.96	108.20
21	AA	1519	A	C5-C6-N1	5.95	120.67	117.70
53	BA	8	C	N3-C2-O2	-5.95	117.74	121.90
53	BA	1218	G	C5-C6-N1	5.95	114.47	111.50
53	BA	2087	G	N1-C6-O6	-5.95	116.33	119.90
21	AA	597	G	N9-C4-C5	5.94	107.78	105.40
53	BA	1323	C	N1-C2-O2	5.94	122.47	118.90
53	BA	1457	U	O4'-C1'-N1	5.94	112.95	108.20
21	AA	661	G	N1-C6-O6	-5.94	116.33	119.90
53	BA	1089	A	C5-C6-N1	5.94	120.67	117.70
53	BA	1462	C	N3-C2-O2	-5.94	117.74	121.90
53	BA	2244	U	C5-C6-N1	-5.94	119.73	122.70
21	AA	1280	A	C4-C5-C6	-5.94	114.03	117.00
53	BA	613	A	C4-C5-C6	-5.94	114.03	117.00
53	BA	624	C	N1-C2-O2	5.94	122.46	118.90
53	BA	1275	A	C4-C5-C6	-5.94	114.03	117.00
53	BA	1299	G	O4'-C1'-N9	5.94	112.95	108.20
53	BA	2053	G	C5'-C4'-O4'	5.94	116.23	109.10
53	BA	2308	G	O4'-C1'-N9	5.94	112.95	108.20
53	BA	2399	G	O4'-C1'-N9	5.94	112.95	108.20
53	BA	2433	A	C5-C6-N1	5.94	120.67	117.70
21	AA	1511	G	C5-C6-N1	5.94	114.47	111.50
53	BA	471	A	C5-C6-N1	5.94	120.67	117.70
53	BA	640	C	N1-C2-O2	5.94	122.46	118.90
53	BA	1411	U	O4'-C1'-N1	5.94	112.95	108.20
53	BA	2418	A	C6-C5-N7	5.94	136.46	132.30
53	BA	2494	G	C5-C6-N1	5.94	114.47	111.50
54	BB	73	A	C4-C5-C6	-5.94	114.03	117.00
53	BA	974	G	N7-C8-N9	5.94	116.07	113.10
53	BA	1699	G	O4'-C1'-N9	5.94	112.95	108.20
53	BA	1872	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	200	G	N1-C6-O6	-5.93	116.34	119.90
21	AA	1267	C	O4'-C1'-N1	5.93	112.95	108.20
53	BA	1156	A	P-O3'-C3'	5.93	126.82	119.70
53	BA	1503	A	C4-C5-C6	-5.93	114.03	117.00
53	BA	1919	A	C4-C5-C6	-5.93	114.03	117.00
11	AL	98	ARG	NE-CZ-NH1	5.93	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	74	A	N1-C6-N6	-5.93	115.04	118.60
21	AA	1468	A	O4'-C1'-N9	5.93	112.94	108.20
53	BA	2153	C	N3-C4-C5	5.93	124.27	121.90
21	AA	372	C	O4'-C1'-N1	5.93	112.94	108.20
21	AA	914	A	C4-C5-C6	-5.93	114.04	117.00
53	BA	241	A	N1-C6-N6	-5.93	115.04	118.60
53	BA	421	C	N1-C2-O2	5.93	122.46	118.90
53	BA	2577	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	760	G	N1-C6-O6	-5.93	116.34	119.90
48	B0	51	ARG	NE-CZ-NH1	5.93	123.26	120.30
21	AA	1402	C	N1-C2-O2	5.93	122.46	118.90
53	BA	271	G	O4'-C1'-N9	5.93	112.94	108.20
53	BA	710	U	C5-C6-N1	-5.93	119.74	122.70
53	BA	2305	U	O4'-C1'-N1	5.93	112.94	108.20
53	BA	2366	A	N1-C6-N6	-5.93	115.04	118.60
53	BA	2537	U	N3-C2-O2	-5.93	118.05	122.20
53	BA	2680	U	O4'-C1'-N1	5.93	112.94	108.20
21	AA	808	C	N1-C2-O2	5.92	122.45	118.90
53	BA	1819	A	N1-C6-N6	-5.92	115.05	118.60
53	BA	1877	A	C4-C5-C6	-5.92	114.04	117.00
24	BC	211	ARG	NE-CZ-NH1	5.92	123.26	120.30
53	BA	2180	U	O4'-C1'-N1	5.92	112.94	108.20
21	AA	673	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	812	G	C4'-C3'-C2'	-5.92	96.68	102.60
53	BA	214	G	N1-C6-O6	-5.92	116.35	119.90
53	BA	1197	G	N1-C6-O6	-5.92	116.35	119.90
53	BA	2621	G	N1-C6-O6	-5.92	116.35	119.90
54	BB	60	C	C6-N1-C2	-5.92	117.93	120.30
21	AA	211	G	N3-C4-C5	-5.92	125.64	128.60
21	AA	520	A	C5-C6-N1	5.92	120.66	117.70
21	AA	740	U	O4'-C1'-N1	5.92	112.94	108.20
21	AA	1272	G	N9-C4-C5	5.92	107.77	105.40
21	AA	1319	A	C5-C6-N1	5.92	120.66	117.70
53	BA	60	G	O4'-C1'-N9	5.92	112.93	108.20
53	BA	216	A	C4-C5-C6	-5.92	114.04	117.00
53	BA	452	G	N1-C6-O6	-5.92	116.35	119.90
53	BA	1076	C	N1-C2-O2	5.92	122.45	118.90
53	BA	1809	A	C5-C6-N1	5.92	120.66	117.70
21	AA	911	U	C5-C6-N1	-5.92	119.74	122.70
21	AA	1107	C	O4'-C1'-N1	5.92	112.93	108.20
53	BA	664	G	N1-C6-O6	-5.92	116.35	119.90
21	AA	29	U	O4'-C1'-N1	5.92	112.93	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	488	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	509	A	C5-C6-N1	5.92	120.66	117.70
53	BA	1260	A	C5-C6-N1	5.92	120.66	117.70
53	BA	2206	C	N1-C2-O2	5.92	122.45	118.90
21	AA	1089	G	N9-C4-C5	5.91	107.77	105.40
21	AA	1466	C	O4'-C1'-N1	5.91	112.93	108.20
53	BA	742	A	C5-C6-N1	5.91	120.66	117.70
53	BA	1754	A	C4-C5-C6	-5.91	114.04	117.00
53	BA	1890	A	C4-C5-C6	-5.91	114.04	117.00
53	BA	236	C	N3-C4-C5	5.91	124.27	121.90
53	BA	934	U	O4'-C1'-N1	5.91	112.93	108.20
53	BA	1139	G	N3-C2-N2	-5.91	115.76	119.90
53	BA	2430	A	C1'-O4'-C4'	-5.91	105.17	109.90
21	AA	620	C	O4'-C1'-N1	5.91	112.93	108.20
21	AA	651	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	811	C	O4'-C1'-N1	5.91	112.93	108.20
21	AA	1167	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	1169	A	C4-C5-C6	-5.91	114.05	117.00
53	BA	553	G	N1-C6-O6	-5.91	116.36	119.90
53	BA	1836	C	C5'-C4'-O4'	5.91	116.19	109.10
53	BA	2237	G	N1-C6-O6	-5.91	116.36	119.90
53	BA	854	C	N1-C2-O2	5.91	122.44	118.90
21	AA	964	A	C5-C6-N1	5.91	120.65	117.70
53	BA	451	U	C4'-C3'-C2'	-5.91	96.69	102.60
53	BA	1577	C	N3-C2-O2	-5.91	117.77	121.90
53	BA	2385	C	N3-C2-O2	-5.91	117.77	121.90
53	BA	2815	C	O4'-C1'-N1	5.91	112.92	108.20
53	BA	2821	A	C4-C5-C6	-5.91	114.05	117.00
54	BB	15	A	C3'-C2'-C1'	5.91	106.22	101.50
21	AA	234	C	N3-C2-O2	-5.90	117.77	121.90
39	BR	90	ARG	NE-CZ-NH2	5.90	123.25	120.30
53	BA	1062	G	N3-C4-C5	-5.90	125.65	128.60
53	BA	2594	C	N1-C2-O2	5.90	122.44	118.90
35	BN	90	ARG	NH1-CZ-NH2	-5.90	112.91	119.40
53	BA	534	U	O4'-C1'-N1	5.90	112.92	108.20
53	BA	683	U	O4'-C1'-N1	5.90	112.92	108.20
53	BA	941	A	C4-C5-C6	-5.90	114.05	117.00
53	BA	1021	A	C5-C6-N1	5.90	120.65	117.70
53	BA	2228	G	C5-C6-N1	5.90	114.45	111.50
21	AA	356	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	364	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	718	A	C4-C5-C6	-5.90	114.05	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1533	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	684	U	O4'-C1'-N1	5.90	112.92	108.20
21	AA	1360	A	C4-C5-C6	-5.90	114.05	117.00
53	BA	470	A	C5-C6-N1	5.90	120.65	117.70
53	BA	2112	G	C5-C6-N1	5.90	114.45	111.50
53	BA	966	G	N1-C6-O6	-5.90	116.36	119.90
53	BA	2236	U	O4'-C1'-N1	5.90	112.92	108.20
21	AA	90	C	N3-C2-O2	-5.89	117.77	121.90
21	AA	136	C	O4'-C1'-N1	5.89	112.92	108.20
21	AA	837	U	N3-C2-O2	-5.89	118.07	122.20
53	BA	504	A	C4-C5-C6	-5.89	114.05	117.00
53	BA	575	A	C5-C6-N1	5.89	120.65	117.70
53	BA	1052	C	N3-C2-O2	-5.89	117.77	121.90
53	BA	2045	C	N3-C2-O2	-5.89	117.77	121.90
53	BA	2651	C	N1-C2-O2	5.89	122.44	118.90
21	AA	1366	C	N3-C2-O2	-5.89	117.78	121.90
53	BA	606	U	O4'-C1'-N1	5.89	112.91	108.20
53	BA	2573	C	N1-C2-O2	5.89	122.44	118.90
53	BA	2578	G	N3-C4-C5	-5.89	125.65	128.60
53	BA	2522	U	C5-C6-N1	-5.89	119.75	122.70
21	AA	563	A	C2-N3-C4	5.89	113.54	110.60
21	AA	977	A	O4'-C1'-N9	5.89	112.91	108.20
53	BA	1179	G	C8-N9-C4	-5.89	104.04	106.40
53	BA	1704	C	N3-C2-O2	-5.89	117.78	121.90
53	BA	2001	C	N3-C4-C5	5.89	124.26	121.90
53	BA	2052	A	C2-N3-C4	5.89	113.55	110.60
53	BA	2275	C	N1-C2-O2	5.89	122.43	118.90
53	BA	2562	U	O4'-C1'-N1	5.89	112.91	108.20
21	AA	1507	A	C5-C6-N1	5.89	120.64	117.70
53	BA	2147	A	C6-C5-N7	5.89	136.42	132.30
21	AA	1122	U	O4'-C1'-N1	5.89	112.91	108.20
53	BA	993	G	C5-C6-N1	5.89	114.44	111.50
53	BA	1345	C	N3-C2-O2	-5.89	117.78	121.90
53	BA	1887	C	N3-C2-O2	-5.89	117.78	121.90
17	AR	69	TYR	CB-CG-CD1	-5.88	117.47	121.00
21	AA	1025	U	O4'-C1'-N1	5.88	112.91	108.20
53	BA	1487	U	C5'-C4'-O4'	5.88	116.16	109.10
53	BA	1616	A	C5-C6-N1	5.88	120.64	117.70
53	BA	80	G	C5-C6-N1	5.88	114.44	111.50
53	BA	2236	U	N1-C2-N3	5.88	118.43	114.90
53	BA	2320	U	O4'-C1'-N1	5.88	112.91	108.20
21	AA	1035	A	C4-C5-C6	-5.88	114.06	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	119	A	C5'-C4'-C3'	-5.88	106.59	116.00
53	BA	569	U	N3-C2-O2	-5.88	118.08	122.20
53	BA	990	A	C4-C5-C6	-5.88	114.06	117.00
53	BA	1145	C	N3-C2-O2	-5.88	117.78	121.90
53	BA	2727	A	C4-C5-C6	-5.88	114.06	117.00
53	BA	2755	C	O4'-C1'-N1	5.88	112.91	108.20
53	BA	337	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	456	A	C5-C6-N1	5.88	120.64	117.70
53	BA	461	C	O4'-C1'-N1	5.88	112.90	108.20
53	BA	1233	C	N1-C2-O2	5.88	122.43	118.90
53	BA	1789	A	C5-C6-N1	5.88	120.64	117.70
21	AA	655	A	C5-C6-N1	5.88	120.64	117.70
21	AA	810	C	N3-C2-O2	-5.88	117.79	121.90
44	BW	54	ARG	NE-CZ-NH1	5.88	123.24	120.30
53	BA	2543	G	N3-C4-C5	-5.88	125.66	128.60
54	BB	11	C	N1-C2-O2	5.88	122.43	118.90
21	AA	996	A	C4-C5-C6	-5.88	114.06	117.00
53	BA	275	C	N3-C2-O2	-5.87	117.79	121.90
53	BA	1328	A	C4-C5-C6	-5.87	114.06	117.00
53	BA	2501	C	N3-C4-N4	-5.87	113.89	118.00
53	BA	2617	U	N1-C2-N3	5.87	118.42	114.90
21	AA	660	C	N3-C2-O2	-5.87	117.79	121.90
53	BA	433	C	C3'-C2'-C1'	5.87	106.20	101.50
53	BA	1185	G	C3'-C2'-C1'	5.87	106.20	101.50
53	BA	1522	A	C4-C5-C6	-5.87	114.06	117.00
53	BA	1446	C	N3-C2-O2	-5.87	117.79	121.90
53	BA	1900	A	C5-C6-N1	5.87	120.64	117.70
53	BA	2882	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	236	A	N1-C6-N6	-5.87	115.08	118.60
21	AA	926	G	C3'-C2'-C1'	5.87	106.19	101.50
23	A2	83	U	C5-C6-N1	-5.87	119.77	122.70
53	BA	935	C	N3-C4-N4	-5.87	113.89	118.00
53	BA	1243	C	O4'-C1'-N1	5.87	112.89	108.20
21	AA	233	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	1507	A	N1-C6-N6	-5.87	115.08	118.60
53	BA	2222	C	N3-C2-O2	-5.87	117.79	121.90
53	BA	2380	C	N3-C2-O2	-5.87	117.79	121.90
46	BY	47	ARG	NE-CZ-NH1	5.87	123.23	120.30
53	BA	886	A	C4-C5-C6	-5.87	114.07	117.00
53	BA	2427	C	N3-C2-O2	-5.87	117.80	121.90
53	BA	2774	C	O4'-C1'-N1	5.87	112.89	108.20
1	AB	207	ARG	NE-CZ-NH1	5.86	123.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	38	A	C6-C5-N7	5.86	136.40	132.30
53	BA	1691	C	N3-C4-C5	5.86	124.25	121.90
53	BA	2332	C	N1-C2-O2	5.86	122.42	118.90
21	AA	637	C	N1-C2-O2	5.86	122.42	118.90
22	A1	8	U	N3-C2-O2	-5.86	118.10	122.20
53	BA	690	G	N1-C6-O6	-5.86	116.38	119.90
21	AA	747	A	C5-C6-N1	5.86	120.63	117.70
53	BA	354	A	C4-C5-C6	-5.86	114.07	117.00
53	BA	419	U	O4'-C1'-N1	5.86	112.89	108.20
53	BA	2108	A	C5-C6-N1	5.86	120.63	117.70
21	AA	37	U	C4'-C3'-C2'	-5.86	96.74	102.60
53	BA	2055	C	N3-C4-C5	5.86	124.24	121.90
21	AA	533	A	O4'-C4'-C3'	5.86	110.79	106.10
21	AA	1050	G	N3-C2-N2	-5.86	115.80	119.90
21	AA	1248	A	C5-C6-N1	5.86	120.63	117.70
42	BU	21	ARG	NE-CZ-NH1	5.86	123.23	120.30
53	BA	522	A	C5-C6-N1	5.86	120.63	117.70
53	BA	940	G	C5'-C4'-O4'	5.86	116.13	109.10
53	BA	2430	A	N1-C6-N6	-5.86	115.09	118.60
21	AA	1161	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	1400	C	N3-C2-O2	-5.86	117.80	121.90
53	BA	441	U	C5-C6-N1	-5.86	119.77	122.70
53	BA	1229	C	N1-C2-O2	5.86	122.41	118.90
53	BA	2797	U	N3-C2-O2	-5.86	118.10	122.20
21	AA	1022	A	C4-C5-C6	-5.85	114.07	117.00
53	BA	172	A	C4-C5-C6	-5.85	114.07	117.00
53	BA	816	C	C5'-C4'-O4'	5.85	116.12	109.10
53	BA	1569	A	C6-C5-N7	5.85	136.40	132.30
53	BA	2207	C	O4'-C1'-N1	5.85	112.88	108.20
53	BA	2433	A	C4-C5-C6	-5.85	114.07	117.00
53	BA	2727	A	C6-C5-N7	5.85	136.40	132.30
21	AA	1102	A	C4-C5-C6	-5.85	114.07	117.00
21	AA	1136	C	N1-C2-O2	5.85	122.41	118.90
53	BA	1537	G	O4'-C1'-N9	5.85	112.88	108.20
53	BA	1822	C	N3-C2-O2	-5.85	117.80	121.90
53	BA	2060	A	C5-C6-N1	5.85	120.63	117.70
53	BA	2174	C	N3-C2-O2	-5.85	117.80	121.90
30	BI	7	TYR	CB-CG-CD1	-5.85	117.49	121.00
53	BA	109	C	N1-C2-O2	5.85	122.41	118.90
53	BA	1728	C	O4'-C1'-N1	5.85	112.88	108.20
53	BA	384	A	N1-C6-N6	-5.85	115.09	118.60
53	BA	1152	C	O4'-C1'-N1	5.85	112.88	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	478	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	768	A	N1-C6-N6	-5.84	115.09	118.60
22	A1	29	U	O4'-C1'-N1	5.84	112.88	108.20
53	BA	112	U	O4'-C1'-N1	5.84	112.88	108.20
21	AA	26	A	C4-C5-C6	-5.84	114.08	117.00
53	BA	1399	C	O4'-C1'-N1	5.84	112.87	108.20
53	BA	1467	U	O4'-C1'-N1	5.84	112.87	108.20
53	BA	1947	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	597	G	N1-C6-O6	-5.84	116.40	119.90
21	AA	1155	A	C4-C5-C6	-5.84	114.08	117.00
53	BA	1023	U	N1-C2-N3	5.84	118.40	114.90
53	BA	2609	U	C5-C6-N1	-5.84	119.78	122.70
21	AA	515	G	O4'-C1'-N9	5.84	112.87	108.20
21	AA	90	C	N1-C2-O2	5.84	122.40	118.90
21	AA	1206	G	N3-C4-C5	-5.84	125.68	128.60
53	BA	998	C	O4'-C1'-N1	5.84	112.87	108.20
53	BA	1074	G	N7-C8-N9	5.84	116.02	113.10
53	BA	1571	A	C4-C5-C6	-5.84	114.08	117.00
53	BA	1618	A	C4-C5-C6	-5.84	114.08	117.00
53	BA	1630	A	C5-C6-N1	5.84	120.62	117.70
53	BA	1887	C	O4'-C1'-N1	5.84	112.87	108.20
53	BA	2690	U	N3-C2-O2	-5.84	118.11	122.20
54	BB	66	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	648	A	C6-C5-N7	5.83	136.38	132.30
53	BA	778	G	C8-N9-C4	-5.83	104.07	106.40
53	BA	2638	G	C5-C6-N1	5.83	114.42	111.50
54	BB	50	A	C6-C5-N7	5.83	136.38	132.30
21	AA	429	U	N1-C1'-C2'	5.83	121.58	114.00
53	BA	443	A	C5-C6-N1	5.83	120.62	117.70
53	BA	485	C	N3-C2-O2	-5.83	117.82	121.90
53	BA	1913	A	C4-C5-C6	-5.83	114.08	117.00
53	BA	2510	C	N1-C2-O2	5.83	122.40	118.90
21	AA	300	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	658	C	N1-C2-O2	5.83	122.40	118.90
53	BA	269	C	N3-C4-C5	5.83	124.23	121.90
21	AA	1534	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	328	C	N1-C2-O2	5.83	122.40	118.90
21	AA	569	C	N1-C2-O2	5.83	122.40	118.90
21	AA	1093	A	C6-C5-N7	5.83	136.38	132.30
21	AA	1284	C	N3-C2-O2	-5.83	117.82	121.90
23	A2	92	U	N3-C2-O2	-5.83	118.12	122.20
53	BA	2076	U	O4'-C1'-N1	5.83	112.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2283	C	N3-C2-O2	-5.83	117.82	121.90
54	BB	97	C	N1-C2-O2	5.83	122.40	118.90
21	AA	872	A	C4-C5-C6	-5.83	114.09	117.00
53	BA	1611	C	C5'-C4'-O4'	5.83	116.09	109.10
53	BA	1962	C	N1-C2-O2	5.83	122.40	118.90
53	BA	156	A	C5-C6-N1	5.83	120.61	117.70
53	BA	686	U	N3-C2-O2	-5.83	118.12	122.20
53	BA	1026	G	C5-C6-N1	5.83	114.41	111.50
53	BA	1691	C	O4'-C1'-N1	5.83	112.86	108.20
53	BA	2132	U	O4'-C1'-N1	5.83	112.86	108.20
21	AA	503	C	N3-C2-O2	-5.82	117.82	121.90
53	BA	671	C	N1-C2-O2	5.82	122.39	118.90
53	BA	675	A	C4-C5-C6	-5.82	114.09	117.00
53	BA	1315	C	N3-C4-N4	-5.82	113.92	118.00
54	BB	38	C	N3-C2-O2	-5.82	117.82	121.90
21	AA	54	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	764	C	N3-C2-O2	-5.82	117.82	121.90
21	AA	853	C	O4'-C1'-N1	5.82	112.86	108.20
21	AA	866	C	N3-C4-C5	5.82	124.23	121.90
53	BA	888	C	N1-C2-O2	5.82	122.39	118.90
53	BA	1178	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	576	C	O4'-C1'-N1	5.82	112.86	108.20
53	BA	1088	A	C4-C5-C6	-5.82	114.09	117.00
53	BA	2566	A	P-O3'-C3'	5.82	126.68	119.70
22	A1	11	C	N1-C2-O2	5.82	122.39	118.90
53	BA	1544	A	N1-C6-N6	-5.82	115.11	118.60
53	BA	2617	U	N3-C2-O2	-5.82	118.13	122.20
53	BA	195	A	C6-C5-N7	5.82	136.37	132.30
53	BA	281	C	N3-C2-O2	-5.82	117.83	121.90
53	BA	2369	A	C5-C6-N1	5.82	120.61	117.70
53	BA	2554	U	C5'-C4'-O4'	5.82	116.08	109.10
54	BB	56	G	N1-C6-O6	-5.82	116.41	119.90
21	AA	568	G	C5-C6-N1	5.81	114.41	111.50
53	BA	991	C	O4'-C1'-N1	5.81	112.85	108.20
53	BA	2052	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	239	U	O4'-C1'-N1	5.81	112.85	108.20
21	AA	1275	A	C4-C5-C6	-5.81	114.09	117.00
53	BA	779	U	C5-C6-N1	-5.81	119.79	122.70
53	BA	919	U	N1-C2-N3	5.81	118.39	114.90
53	BA	1366	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	528	C	N3-C2-O2	-5.81	117.83	121.90
53	BA	704	G	N1-C6-O6	-5.81	116.41	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	740	C	N3-C2-O2	-5.81	117.83	121.90
53	BA	1173	U	C5-C6-N1	-5.81	119.79	122.70
21	AA	482	A	N1-C6-N6	-5.81	115.11	118.60
21	AA	793	U	C1'-O4'-C4'	-5.81	105.25	109.90
21	AA	857	C	N1-C2-O2	5.81	122.39	118.90
53	BA	39	G	N1-C6-O6	-5.81	116.42	119.90
53	BA	79	C	O4'-C1'-N1	5.81	112.85	108.20
53	BA	587	C	N3-C2-O2	-5.81	117.83	121.90
53	BA	1510	G	N3-C2-N2	-5.81	115.83	119.90
53	BA	2368	C	N3-C2-O2	-5.81	117.83	121.90
53	BA	2736	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	498	A	C4-C5-C6	-5.81	114.10	117.00
21	AA	892	A	C4-C5-C6	-5.81	114.10	117.00
21	AA	943	U	O4'-C1'-N1	5.81	112.85	108.20
53	BA	615	U	C5-C6-N1	-5.81	119.80	122.70
53	BA	2725	A	N1-C6-N6	-5.81	115.12	118.60
22	A1	59	U	C3'-C2'-C1'	5.81	106.14	101.50
53	BA	808	G	C5-C6-N1	5.81	114.40	111.50
21	AA	116	A	C5-C6-N1	5.80	120.60	117.70
21	AA	189	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1353	G	C5-C6-N1	5.80	114.40	111.50
53	BA	155	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	1060	U	C5-C6-N1	-5.80	119.80	122.70
53	BA	1385	A	C5-C6-N1	5.80	120.60	117.70
53	BA	1494	A	C5-C6-N1	5.80	120.60	117.70
54	BB	65	U	O4'-C1'-N1	5.80	112.84	108.20
53	BA	642	U	O4'-C1'-N1	5.80	112.84	108.20
53	BA	943	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	2144	G	N1-C6-O6	-5.80	116.42	119.90
53	BA	2303	G	O4'-C1'-N9	5.80	112.84	108.20
21	AA	135	C	N3-C2-O2	-5.80	117.84	121.90
50	B2	35	ARG	NE-CZ-NH1	5.80	123.20	120.30
53	BA	563	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	747	U	O4'-C1'-N1	5.80	112.84	108.20
21	AA	328	C	N3-C4-C5	5.80	124.22	121.90
21	AA	399	G	C8-N9-C4	-5.80	104.08	106.40
21	AA	1250	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	1597	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	1840	G	N3-C2-N2	-5.80	115.84	119.90
53	BA	1969	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	2506	U	N3-C2-O2	-5.80	118.14	122.20
21	AA	1007	U	N3-C2-O2	-5.80	118.14	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1378	A	C6-C5-N7	5.80	136.36	132.30
21	AA	34	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	975	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1297	G	C5-C6-N1	5.80	114.40	111.50
21	AA	1468	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	107	G	C5-C6-N1	5.80	114.40	111.50
53	BA	527	C	N3-C2-O2	-5.80	117.84	121.90
53	BA	815	C	C5'-C4'-C3'	-5.80	106.72	116.00
53	BA	1139	G	C8-N9-C4	-5.80	104.08	106.40
53	BA	1584	U	C5-C6-N1	-5.80	119.80	122.70
53	BA	2700	A	C4-C5-C6	-5.80	114.10	117.00
22	A1	23	A	C5-C6-N1	5.79	120.60	117.70
53	BA	49	A	C4-C5-C6	-5.79	114.10	117.00
53	BA	2034	U	O4'-C1'-N1	5.79	112.84	108.20
53	BA	2638	G	N3-C4-C5	-5.79	125.70	128.60
21	AA	1145	A	C4-C5-C6	-5.79	114.10	117.00
21	AA	1273	C	O4'-C1'-N1	5.79	112.83	108.20
53	BA	310	A	C5-C6-N1	5.79	120.60	117.70
53	BA	452	G	N9-C4-C5	5.79	107.72	105.40
53	BA	2085	U	O4'-C1'-N1	5.79	112.83	108.20
53	BA	2116	G	C8-N9-C4	-5.79	104.08	106.40
53	BA	2885	G	O4'-C1'-N9	5.79	112.83	108.20
21	AA	990	C	N3-C2-O2	-5.79	117.85	121.90
53	BA	1208	C	O4'-C1'-N1	5.79	112.83	108.20
53	BA	1373	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	59	A	C4-C5-C6	-5.79	114.11	117.00
38	BQ	91	ARG	NE-CZ-NH2	-5.79	117.41	120.30
53	BA	444	C	N3-C2-O2	-5.79	117.85	121.90
53	BA	643	A	C5-C6-N1	5.79	120.59	117.70
53	BA	807	U	O4'-C1'-N1	5.79	112.83	108.20
53	BA	1550	C	N3-C2-O2	-5.79	117.85	121.90
54	BB	70	C	N3-C2-O2	-5.79	117.85	121.90
21	AA	103	U	O4'-C1'-N1	5.79	112.83	108.20
53	BA	896	A	C4-C5-C6	-5.79	114.11	117.00
53	BA	2022	U	O4'-C1'-N1	5.79	112.83	108.20
21	AA	366	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	968	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	1525	G	C5-C6-N1	5.79	114.39	111.50
53	BA	96	C	O4'-C1'-N1	5.79	112.83	108.20
53	BA	796	C	N3-C2-O2	-5.79	117.85	121.90
53	BA	952	G	C5-C6-N1	5.79	114.39	111.50
53	BA	2352	A	C4-C5-C6	-5.79	114.11	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	766	A	C5-C6-N1	5.78	120.59	117.70
21	AA	1366	C	N1-C2-O2	5.78	122.37	118.90
53	BA	146	A	C4-C5-C6	-5.78	114.11	117.00
53	BA	840	C	N1-C2-O2	5.78	122.37	118.90
53	BA	924	G	N1-C6-O6	-5.78	116.43	119.90
53	BA	1268	A	C4-C5-C6	-5.78	114.11	117.00
53	BA	1937	A	C6-C5-N7	5.78	136.35	132.30
53	BA	2023	C	N1-C2-O2	5.78	122.37	118.90
53	BA	2766	A	C4-C5-C6	-5.78	114.11	117.00
53	BA	2841	C	N3-C4-C5	5.78	124.21	121.90
21	AA	339	C	N3-C2-O2	-5.78	117.85	121.90
53	BA	2272	U	C4-C5-C6	5.78	123.17	119.70
21	AA	398	U	O4'-C1'-N1	5.78	112.83	108.20
21	AA	1530	G	N1-C6-O6	-5.78	116.43	119.90
42	BU	5	ARG	NE-CZ-NH1	5.78	123.19	120.30
53	BA	820	A	N1-C6-N6	-5.78	115.13	118.60
53	BA	835	C	N3-C4-C5	5.78	124.21	121.90
53	BA	1064	C	N1-C2-O2	5.78	122.37	118.90
53	BA	2498	C	C6-N1-C2	-5.78	117.99	120.30
53	BA	2562	U	C5-C6-N1	-5.78	119.81	122.70
53	BA	2731	G	O4'-C1'-N9	5.78	112.82	108.20
53	BA	2787	C	N3-C2-O2	-5.78	117.85	121.90
21	AA	483	C	N3-C2-O2	-5.78	117.86	121.90
53	BA	1599	U	N1-C2-N3	5.78	118.37	114.90
53	BA	2871	U	N3-C2-O2	-5.78	118.15	122.20
53	BA	727	A	O4'-C1'-N9	5.78	112.82	108.20
53	BA	1572	A	N1-C6-N6	-5.78	115.13	118.60
21	AA	429	U	C3'-C2'-C1'	-5.78	96.88	101.50
21	AA	1005	A	N1-C6-N6	-5.78	115.14	118.60
21	AA	1203	C	N3-C2-O2	-5.78	117.86	121.90
53	BA	220	G	C5-C6-N1	5.78	114.39	111.50
53	BA	1775	U	C5-C6-N1	-5.78	119.81	122.70
53	BA	2614	A	C4-C5-C6	-5.78	114.11	117.00
53	BA	879	G	C8-N9-C4	-5.77	104.09	106.40
53	BA	635	C	N3-C4-C5	5.77	124.21	121.90
53	BA	660	C	N1-C2-O2	5.77	122.36	118.90
53	BA	2007	U	O4'-C1'-N1	5.77	112.82	108.20
53	BA	2498	C	N3-C2-O2	-5.77	117.86	121.90
53	BA	2610	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	573	A	C3'-C2'-C1'	5.77	106.12	101.50
21	AA	802	A	C4-C5-C6	-5.77	114.11	117.00
53	BA	1903	G	O4'-C1'-N9	5.77	112.82	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	487	A	C4-C5-C6	-5.77	114.11	117.00
21	AA	1200	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	1474	U	O4'-C1'-N1	5.77	112.82	108.20
24	BC	202	ARG	NE-CZ-NH1	5.77	123.19	120.30
53	BA	621	A	C4-C5-C6	-5.77	114.11	117.00
53	BA	734	A	C4-C5-C6	-5.77	114.11	117.00
53	BA	1117	C	N3-C4-N4	-5.77	113.96	118.00
53	BA	1207	C	N1-C2-O2	5.77	122.36	118.90
53	BA	2272	U	C5-C6-N1	-5.77	119.81	122.70
53	BA	2435	A	C4-C5-C6	-5.77	114.11	117.00
53	BA	2660	A	O4'-C1'-N9	5.77	112.82	108.20
7	AH	113	ARG	NE-CZ-NH1	5.77	123.18	120.30
17	AR	47	ARG	NE-CZ-NH1	5.77	123.18	120.30
21	AA	1350	A	C5-C6-N1	5.77	120.58	117.70
53	BA	164	C	O4'-C1'-N1	5.77	112.81	108.20
53	BA	327	G	N1-C6-O6	-5.77	116.44	119.90
53	BA	330	A	O4'-C1'-N9	5.77	112.81	108.20
53	BA	795	C	N1-C2-O2	5.77	122.36	118.90
53	BA	1681	G	O4'-C1'-N9	5.77	112.81	108.20
53	BA	1685	C	N3-C4-C5	5.77	124.21	121.90
53	BA	2173	A	C4-C5-C6	-5.77	114.12	117.00
53	BA	2324	U	O4'-C1'-N1	5.77	112.81	108.20
53	BA	2412	A	C5-C6-N1	5.77	120.58	117.70
53	BA	2444	G	N1-C6-O6	-5.77	116.44	119.90
53	BA	2792	A	C4-C5-C6	-5.77	114.12	117.00
53	BA	226	A	C4-C5-C6	-5.77	114.12	117.00
21	AA	1525	G	N3-C4-C5	-5.76	125.72	128.60
53	BA	725	G	N1-C6-O6	-5.76	116.44	119.90
53	BA	1083	U	N3-C2-O2	-5.76	118.17	122.20
53	BA	1706	C	N3-C4-C5	5.76	124.21	121.90
53	BA	1793	C	N3-C2-O2	-5.76	117.86	121.90
54	BB	41	G	N3-C4-C5	-5.76	125.72	128.60
21	AA	1151	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	617	G	C5-C6-N1	5.76	114.38	111.50
21	AA	1015	G	N3-C2-N2	-5.76	115.87	119.90
53	BA	432	A	C4-C5-C6	-5.76	114.12	117.00
53	BA	1191	G	C5-C6-N1	5.76	114.38	111.50
53	BA	1731	G	N3-C4-C5	-5.76	125.72	128.60
53	BA	1821	A	C5-C6-N1	5.76	120.58	117.70
21	AA	790	A	O4'-C4'-C3'	5.76	110.71	106.10
21	AA	1198	G	N1-C6-O6	-5.76	116.44	119.90
53	BA	484	C	N1-C2-O2	5.76	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1424	G	N1-C6-O6	-5.76	116.44	119.90
54	BB	34	A	C6-C5-N7	5.76	136.33	132.30
21	AA	536	C	N1-C2-O2	5.76	122.36	118.90
21	AA	1377	A	C4-C5-C6	-5.76	114.12	117.00
53	BA	415	A	C6-C5-N7	5.76	136.33	132.30
53	BA	1568	G	N1-C6-O6	-5.76	116.44	119.90
53	BA	2000	C	O4'-C1'-N1	5.76	112.81	108.20
12	AM	69	ARG	NE-CZ-NH1	5.76	123.18	120.30
21	AA	770	C	C4'-C3'-C2'	-5.76	96.84	102.60
21	AA	860	A	C5-C6-N1	5.76	120.58	117.70
21	AA	1064	G	C5-C6-N1	5.76	114.38	111.50
53	BA	2561	U	O4'-C1'-N1	5.76	112.81	108.20
53	BA	96	C	N3-C2-O2	-5.75	117.87	121.90
53	BA	179	C	N1-C2-O2	5.75	122.35	118.90
53	BA	208	C	N1-C2-O2	5.75	122.35	118.90
53	BA	1534	U	N1-C2-N3	5.75	118.35	114.90
21	AA	186	C	N3-C2-O2	-5.75	117.87	121.90
27	BF	29	ARG	NE-CZ-NH1	5.75	123.18	120.30
53	BA	158	U	C5-C6-N1	-5.75	119.82	122.70
53	BA	1541	C	N3-C2-O2	-5.75	117.87	121.90
53	BA	1800	C	N3-C2-O2	-5.75	117.87	121.90
53	BA	2215	C	C5'-C4'-O4'	5.75	116.00	109.10
53	BA	2511	U	C5-C4-O4	-5.75	122.45	125.90
53	BA	2731	G	C3'-C2'-C1'	5.75	106.10	101.50
53	BA	2825	G	N3-C4-C5	-5.75	125.72	128.60
21	AA	531	U	O4'-C1'-N1	5.75	112.80	108.20
53	BA	345	A	C3'-C2'-C1'	5.75	106.10	101.50
53	BA	407	G	N1-C6-O6	-5.75	116.45	119.90
53	BA	1378	A	P-O3'-C3'	5.75	126.60	119.70
53	BA	1999	C	O4'-C1'-N1	5.75	112.80	108.20
21	AA	106	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	830	G	N3-C4-C5	-5.75	125.72	128.60
21	AA	854	U	N1-C2-N3	5.75	118.35	114.90
21	AA	1101	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	1301	U	C5-C6-N1	-5.75	119.83	122.70
53	BA	1420	A	C3'-C2'-C1'	5.75	106.10	101.50
53	BA	1553	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	462	G	O4'-C1'-N9	5.75	112.80	108.20
53	BA	449	A	C6-C5-N7	5.75	136.32	132.30
53	BA	792	A	C5-C6-N1	5.75	120.57	117.70
53	BA	1410	G	N1-C6-O6	-5.75	116.45	119.90
53	BA	1461	C	O4'-C1'-N1	5.75	112.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2214	C	O4'-C1'-N1	5.75	112.80	108.20
21	AA	1287	A	C6-C5-N7	5.75	136.32	132.30
32	BK	64	ARG	NE-CZ-NH1	5.75	123.17	120.30
53	BA	311	A	C4-C5-C6	-5.75	114.13	117.00
53	BA	914	G	N3-C2-N2	-5.75	115.88	119.90
53	BA	1214	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	203	G	C4'-C3'-C2'	-5.74	96.86	102.60
53	BA	249	C	N1-C2-O2	5.74	122.35	118.90
53	BA	524	G	C5-C6-N1	5.74	114.37	111.50
53	BA	1141	U	N1-C2-N3	5.74	118.35	114.90
53	BA	1793	C	O4'-C1'-N1	5.74	112.80	108.20
53	BA	2431	U	O4'-C1'-N1	5.74	112.80	108.20
54	BB	101	A	C4-C5-C6	-5.74	114.13	117.00
53	BA	8	C	N3-C4-C5	5.74	124.20	121.90
53	BA	774	G	C5-C6-N1	5.74	114.37	111.50
53	BA	913	U	C5-C6-N1	-5.74	119.83	122.70
53	BA	2891	U	O4'-C1'-N1	5.74	112.79	108.20
15	AP	25	ARG	NE-CZ-NH1	-5.74	117.43	120.30
21	AA	100	G	N1-C6-O6	-5.74	116.45	119.90
21	AA	343	U	N1-C2-N3	5.74	118.34	114.90
53	BA	1795	C	N1-C2-O2	5.74	122.34	118.90
21	AA	519	C	O4'-C1'-N1	5.74	112.79	108.20
21	AA	1096	C	N1-C2-O2	5.74	122.34	118.90
21	AA	1318	A	C4-C5-C6	-5.74	114.13	117.00
53	BA	76	C	N3-C2-O2	-5.74	117.88	121.90
53	BA	509	C	N1-C2-O2	5.74	122.34	118.90
53	BA	1526	C	N1-C2-O2	5.74	122.34	118.90
53	BA	2674	G	N1-C6-O6	-5.74	116.46	119.90
53	BA	2705	A	C4-C5-C6	-5.74	114.13	117.00
53	BA	118	A	C5'-C4'-O4'	5.74	115.98	109.10
17	AR	60	ARG	NE-CZ-NH1	5.74	123.17	120.30
21	AA	1070	U	O4'-C1'-N1	5.74	112.79	108.20
53	BA	64	A	C4-C5-C6	-5.74	114.13	117.00
53	BA	1179	G	N3-C2-N2	-5.74	115.89	119.90
53	BA	1189	A	N1-C6-N6	-5.74	115.16	118.60
53	BA	761	A	C4-C5-C6	-5.73	114.13	117.00
53	BA	1173	U	N1-C2-N3	5.73	118.34	114.90
53	BA	1574	C	C5'-C4'-O4'	5.73	115.98	109.10
21	AA	1472	U	O4'-C1'-N1	5.73	112.79	108.20
53	BA	532	A	C5-C6-N1	5.73	120.57	117.70
53	BA	2278	A	C5-C6-N1	5.73	120.57	117.70
54	BB	3	C	N3-C2-O2	-5.73	117.89	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	899	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	1037	C	O4'-C1'-N1	5.73	112.78	108.20
53	BA	245	G	N7-C8-N9	5.73	115.97	113.10
53	BA	688	U	O4'-C1'-N1	5.73	112.78	108.20
53	BA	1473	G	N1-C6-O6	-5.73	116.46	119.90
21	AA	1200	C	O4'-C1'-N1	5.73	112.78	108.20
53	BA	1748	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	179	A	C6-C5-N7	5.73	136.31	132.30
21	AA	393	A	C4-C5-C6	-5.73	114.14	117.00
21	AA	470	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	612	C	N1-C2-O2	5.73	122.34	118.90
53	BA	1016	G	O4'-C1'-N9	5.73	112.78	108.20
53	BA	1111	A	C4-C5-C6	-5.73	114.14	117.00
53	BA	1499	C	O4'-C1'-N1	5.73	112.78	108.20
21	AA	991	U	O4'-C1'-N1	5.73	112.78	108.20
21	AA	1206	G	C5-C6-N1	5.73	114.36	111.50
53	BA	205	G	N3-C4-C5	-5.73	125.74	128.60
53	BA	1323	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	617	G	N1-C6-O6	-5.72	116.47	119.90
21	AA	1476	A	C4-C5-C6	-5.72	114.14	117.00
53	BA	304	U	O4'-C1'-N1	5.72	112.78	108.20
53	BA	320	A	C4-C5-C6	-5.72	114.14	117.00
53	BA	399	U	O4'-C1'-N1	5.72	112.78	108.20
53	BA	1639	C	N1-C2-O2	5.72	122.33	118.90
53	BA	1990	C	N1-C2-O2	5.72	122.33	118.90
53	BA	2440	C	C2-N3-C4	-5.72	117.04	119.90
8	AI	10	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
21	AA	564	C	N3-C2-O2	-5.72	117.89	121.90
40	BS	84	ARG	NE-CZ-NH1	5.72	123.16	120.30
53	BA	298	G	N3-C4-C5	-5.72	125.74	128.60
53	BA	478	A	C5-C6-N1	5.72	120.56	117.70
53	BA	675	A	N1-C6-N6	-5.72	115.17	118.60
53	BA	775	G	N3-C4-C5	-5.72	125.74	128.60
21	AA	296	U	O4'-C1'-N1	5.72	112.78	108.20
21	AA	1390	U	O4'-C1'-N1	5.72	112.78	108.20
38	BQ	27	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
53	BA	1325	U	O4'-C1'-N1	5.72	112.78	108.20
21	AA	769	G	N7-C8-N9	5.72	115.96	113.10
53	BA	375	G	C5-C6-N1	5.72	114.36	111.50
53	BA	1092	C	N3-C2-O2	-5.72	117.90	121.90
53	BA	1319	C	N3-C2-O2	-5.72	117.90	121.90
54	BB	43	C	N3-C2-O2	-5.72	117.90	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	215	C	N3-C2-O2	-5.72	117.90	121.90
53	BA	1127	A	N1-C6-N6	-5.72	115.17	118.60
53	BA	1208	C	N3-C2-O2	-5.72	117.90	121.90
53	BA	1578	U	N1-C2-N3	5.72	118.33	114.90
53	BA	2606	C	N3-C4-C5	5.72	124.19	121.90
53	BA	2865	U	N3-C2-O2	-5.72	118.20	122.20
21	AA	971	G	C3'-C2'-C1'	-5.71	96.93	101.50
53	BA	916	G	C8-N9-C4	-5.71	104.11	106.40
53	BA	1087	G	N3-C2-N2	-5.71	115.90	119.90
53	BA	1122	G	N3-C2-N2	-5.71	115.90	119.90
53	BA	1773	A	N1-C6-N6	-5.71	115.17	118.60
21	AA	726	C	N1-C2-O2	5.71	122.33	118.90
21	AA	742	G	C8-N9-C4	-5.71	104.11	106.40
21	AA	1243	C	N3-C2-O2	-5.71	117.90	121.90
53	BA	229	C	N3-C2-O2	-5.71	117.90	121.90
53	BA	502	A	C5-C6-N1	5.71	120.56	117.70
21	AA	1140	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	492	C	N1-C2-O2	5.71	122.33	118.90
51	B3	39	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	AC	87	ARG	NE-CZ-NH1	5.71	123.15	120.30
53	BA	511	U	O4'-C4'-C3'	5.71	110.67	106.10
53	BA	1414	C	N3-C2-O2	-5.71	117.90	121.90
53	BA	1805	A	C5-C6-N1	5.71	120.55	117.70
53	BA	264	C	N3-C2-O2	-5.71	117.91	121.90
53	BA	470	A	C4-C5-C6	-5.71	114.15	117.00
53	BA	539	G	C5'-C4'-O4'	5.71	115.95	109.10
53	BA	2059	A	C4-C5-C6	-5.71	114.15	117.00
53	BA	2609	U	O4'-C1'-N1	5.71	112.77	108.20
21	AA	1430	A	C6-C5-N7	5.71	136.29	132.30
53	BA	2848	G	N1-C6-O6	-5.71	116.48	119.90
53	BA	190	A	C5-C6-N1	5.70	120.55	117.70
53	BA	465	G	N1-C6-O6	-5.70	116.48	119.90
53	BA	1283	G	N3-C4-C5	-5.70	125.75	128.60
53	BA	2829	A	C4-C5-C6	-5.70	114.15	117.00
3	AD	164	ARG	NE-CZ-NH2	5.70	123.15	120.30
21	AA	379	C	N1-C2-O2	5.70	122.32	118.90
21	AA	962	C	N1-C2-O2	5.70	122.32	118.90
21	AA	1291	U	O4'-C1'-N1	5.70	112.76	108.20
53	BA	1059	G	N9-C4-C5	5.70	107.68	105.40
53	BA	1556	C	N3-C2-O2	-5.70	117.91	121.90
53	BA	956	G	N1-C6-O6	-5.70	116.48	119.90
53	BA	1074	G	C8-N9-C4	-5.70	104.12	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2443	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	883	C	N1-C2-O2	5.70	122.32	118.90
53	BA	767	U	C5-C6-N1	-5.70	119.85	122.70
53	BA	1406	U	C5-C6-N1	-5.70	119.85	122.70
53	BA	2150	C	N3-C2-O2	-5.70	117.91	121.90
53	BA	1788	C	N3-C2-O2	-5.70	117.91	121.90
53	BA	2442	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	86	G	N9-C4-C5	5.70	107.68	105.40
21	AA	1288	A	C4-C5-C6	-5.70	114.15	117.00
53	BA	766	U	O4'-C1'-N1	5.70	112.76	108.20
53	BA	1545	A	C5-C6-N1	5.70	120.55	117.70
53	BA	1704	C	O4'-C1'-N1	5.70	112.76	108.20
53	BA	2243	U	C5-C6-N1	-5.70	119.85	122.70
53	BA	2304	G	N1-C6-O6	-5.69	116.48	119.90
21	AA	44	A	C4-C5-C6	-5.69	114.15	117.00
21	AA	95	C	N3-C4-C5	5.69	124.18	121.90
53	BA	540	C	N1-C2-O2	5.69	122.32	118.90
53	BA	630	G	C5-C6-N1	5.69	114.35	111.50
53	BA	1240	U	O4'-C1'-N1	5.69	112.75	108.20
53	BA	1488	C	N1-C2-O2	5.69	122.31	118.90
21	AA	220	G	N3-C2-N2	-5.69	115.92	119.90
21	AA	1007	U	C5-C6-N1	-5.69	119.86	122.70
53	BA	1598	A	C5-C6-N1	5.69	120.55	117.70
53	BA	1932	A	C6-C5-N7	5.69	136.28	132.30
53	BA	2490	G	N3-C2-N2	-5.69	115.92	119.90
21	AA	554	A	C4-C5-C6	-5.69	114.16	117.00
21	AA	1054	C	N1-C2-O2	5.69	122.31	118.90
22	A1	23	A	N1-C6-N6	-5.69	115.19	118.60
53	BA	360	U	O4'-C1'-N1	5.69	112.75	108.20
53	BA	676	A	C5-C6-N1	5.69	120.55	117.70
53	BA	750	A	C4-C5-C6	-5.69	114.16	117.00
53	BA	2589	A	C6-C5-N7	5.69	136.28	132.30
53	BA	2649	C	C6-N1-C2	-5.69	118.02	120.30
53	BA	2698	U	O4'-C1'-N1	5.69	112.75	108.20
53	BA	876	C	N1-C2-O2	5.69	122.31	118.90
53	BA	1590	A	C6-C5-N7	5.69	136.28	132.30
21	AA	806	C	N3-C2-O2	-5.69	117.92	121.90
21	AA	868	C	N3-C2-O2	-5.69	117.92	121.90
21	AA	908	A	N1-C6-N6	-5.68	115.19	118.60
53	BA	362	A	C5-C6-N1	5.68	120.54	117.70
53	BA	937	C	N3-C2-O2	-5.68	117.92	121.90
53	BA	1394	U	C5-C6-N1	-5.68	119.86	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1637	A	C5-C6-N1	5.68	120.54	117.70
53	BA	2112	G	N3-C4-C5	-5.68	125.76	128.60
53	BA	2806	C	N3-C4-C5	5.68	124.17	121.90
21	AA	267	C	N1-C2-O2	5.68	122.31	118.90
21	AA	426	U	O4'-C1'-N1	5.68	112.75	108.20
21	AA	511	C	O4'-C1'-N1	5.68	112.75	108.20
21	AA	866	C	N1-C2-O2	5.68	122.31	118.90
21	AA	1178	G	C8-N9-C4	-5.68	104.13	106.40
53	BA	1308	A	O4'-C1'-N9	5.68	112.75	108.20
53	BA	1410	G	C8-N9-C4	-5.68	104.13	106.40
53	BA	1686	C	N1-C2-O2	5.68	122.31	118.90
53	BA	2096	C	N3-C2-O2	-5.68	117.92	121.90
53	BA	2602	A	O4'-C1'-N9	5.68	112.75	108.20
22	A1	25	C	O4'-C1'-N1	5.68	112.74	108.20
53	BA	129	C	N3-C2-O2	-5.68	117.92	121.90
53	BA	1057	A	C5-C6-N1	5.68	120.54	117.70
53	BA	1384	A	C6-C5-N7	5.68	136.28	132.30
21	AA	1188	A	C4-C5-C6	-5.68	114.16	117.00
53	BA	782	A	O4'-C1'-N9	5.68	112.74	108.20
53	BA	1234	U	O4'-C1'-N1	5.68	112.74	108.20
53	BA	1838	C	N3-C2-O2	-5.68	117.93	121.90
53	BA	2488	G	O4'-C1'-N9	5.68	112.74	108.20
53	BA	361	G	N1-C6-O6	-5.68	116.49	119.90
53	BA	1031	G	N9-C4-C5	5.68	107.67	105.40
21	AA	853	C	N3-C2-O2	-5.67	117.93	121.90
53	BA	852	U	O4'-C1'-N1	5.67	112.74	108.20
53	BA	1109	C	N1-C2-O2	5.67	122.31	118.90
53	BA	2407	A	C4-C5-C6	-5.67	114.16	117.00
53	BA	1810	A	C4-C5-C6	-5.67	114.16	117.00
21	AA	970	C	N1-C2-O2	5.67	122.30	118.90
21	AA	1019	A	C4-C5-C6	-5.67	114.16	117.00
53	BA	1012	U	C5-C6-N1	-5.67	119.86	122.70
53	BA	1104	C	O4'-C1'-N1	5.67	112.74	108.20
53	BA	1412	U	C5-C6-N1	-5.67	119.86	122.70
53	BA	1812	U	O4'-C1'-N1	5.67	112.74	108.20
21	AA	288	A	C5-C6-N1	5.67	120.53	117.70
21	AA	1451	U	N3-C2-O2	-5.67	118.23	122.20
53	BA	1214	A	C5-C6-N1	5.67	120.53	117.70
53	BA	2357	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	595	A	O4'-C1'-N9	5.67	112.73	108.20
21	AA	1016	A	C5-C6-N1	5.67	120.53	117.70
53	BA	984	A	C6-C5-N7	5.67	136.27	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1155	A	C5-C6-N1	5.67	120.53	117.70
53	BA	2513	A	C5-C6-N1	5.67	120.53	117.70
53	BA	2825	G	N7-C8-N9	5.67	115.93	113.10
21	AA	83	C	N1-C2-O2	5.67	122.30	118.90
21	AA	688	G	C8-N9-C4	-5.67	104.13	106.40
21	AA	1346	A	C4-C5-C6	-5.67	114.17	117.00
29	BH	50	ARG	NE-CZ-NH1	5.67	123.13	120.30
53	BA	2755	C	N1-C2-O2	5.67	122.30	118.90
8	AI	32	ARG	NE-CZ-NH1	5.66	123.13	120.30
53	BA	1970	A	C4-C5-C6	-5.66	114.17	117.00
53	BA	2058	A	O4'-C1'-N9	5.66	112.73	108.20
53	BA	2578	G	C5-C6-N1	5.66	114.33	111.50
21	AA	319	G	O4'-C1'-N9	5.66	112.73	108.20
53	BA	2248	C	O4'-C1'-N1	5.66	112.73	108.20
53	BA	2561	U	N3-C2-O2	-5.66	118.24	122.20
21	AA	144	G	C5-C6-N1	5.66	114.33	111.50
21	AA	940	C	N1-C2-O2	5.66	122.30	118.90
53	BA	1284	A	N1-C6-N6	-5.66	115.20	118.60
53	BA	2350	C	N3-C2-O2	-5.66	117.94	121.90
53	BA	2763	G	N3-C2-N2	-5.66	115.94	119.90
21	AA	199	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	235	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	265	G	N3-C4-C5	-5.66	125.77	128.60
22	A1	25	C	N1-C2-O2	5.66	122.30	118.90
51	B3	7	ARG	NE-CZ-NH1	5.66	123.13	120.30
53	BA	28	A	C4-C5-C6	-5.66	114.17	117.00
53	BA	903	C	N1-C2-O2	5.66	122.30	118.90
53	BA	1168	G	C5-C6-N1	5.66	114.33	111.50
53	BA	1518	C	O4'-C1'-N1	5.66	112.73	108.20
21	AA	968	A	C2-N3-C4	5.66	113.43	110.60
21	AA	1066	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1519	A	C4-C5-C6	-5.66	114.17	117.00
53	BA	66	C	N1-C2-O2	5.66	122.29	118.90
53	BA	267	C	O4'-C1'-N1	5.66	112.72	108.20
53	BA	1141	U	C3'-C2'-C1'	5.66	106.02	101.50
53	BA	1996	C	N3-C2-O2	-5.66	117.94	121.90
53	BA	2723	C	O4'-C1'-N1	5.66	112.72	108.20
53	BA	8	C	N1-C2-O2	5.65	122.29	118.90
53	BA	528	A	C5-C6-N1	5.65	120.53	117.70
53	BA	2515	C	C4'-C3'-C2'	-5.65	96.95	102.60
3	AD	164	ARG	NH1-CZ-NH2	-5.65	113.18	119.40
21	AA	911	U	O4'-C1'-N1	5.65	112.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	935	A	C4-C5-C6	-5.65	114.17	117.00
53	BA	757	G	C8-N9-C4	-5.65	104.14	106.40
53	BA	1083	U	N1-C2-N3	5.65	118.29	114.90
21	AA	765	G	N3-C2-N2	-5.65	115.94	119.90
21	AA	883	C	N3-C4-C5	5.65	124.16	121.90
21	AA	1082	A	C4-C5-C6	-5.65	114.17	117.00
53	BA	453	A	C4-C5-C6	-5.65	114.17	117.00
53	BA	1186	G	N1-C6-O6	-5.65	116.51	119.90
54	BB	29	A	C6-C5-N7	5.65	136.25	132.30
21	AA	1518	A	O4'-C1'-N9	5.65	112.72	108.20
53	BA	919	U	C5-C6-N1	-5.65	119.88	122.70
53	BA	1181	U	N1-C2-N3	5.65	118.29	114.90
21	AA	1404	C	N3-C4-C5	5.65	124.16	121.90
53	BA	2072	C	N1-C2-O2	5.65	122.29	118.90
53	BA	2386	A	C4-C5-C6	-5.65	114.18	117.00
53	BA	2581	G	C8-N9-C4	-5.65	104.14	106.40
21	AA	633	G	N3-C2-N2	-5.65	115.95	119.90
53	BA	299	A	C5-C6-N1	5.64	120.52	117.70
53	BA	2874	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	549	C	N1-C2-O2	5.64	122.28	118.90
21	AA	1201	A	C5-C6-N1	5.64	120.52	117.70
21	AA	1327	C	N1-C2-O2	5.64	122.28	118.90
21	AA	1493	A	C1'-O4'-C4'	-5.64	105.39	109.90
53	BA	44	A	C6-C5-N7	5.64	136.25	132.30
53	BA	510	C	N1-C2-O2	5.64	122.29	118.90
53	BA	990	A	C5-C6-N1	5.64	120.52	117.70
53	BA	2642	G	O4'-C1'-N9	5.64	112.71	108.20
53	BA	2882	A	C6-C5-N7	5.64	136.25	132.30
53	BA	436	C	N1-C2-O2	5.64	122.28	118.90
53	BA	1824	G	N1-C6-O6	-5.64	116.52	119.90
53	BA	2415	G	C4'-C3'-C2'	-5.64	96.96	102.60
53	BA	2425	A	C6-C5-N7	5.64	136.25	132.30
21	AA	889	A	N1-C6-N6	-5.64	115.22	118.60
53	BA	466	A	C4-C5-C6	-5.64	114.18	117.00
53	BA	574	A	C4-C5-C6	-5.64	114.18	117.00
53	BA	614	A	N1-C6-N6	-5.64	115.22	118.60
53	BA	1164	C	N3-C2-O2	-5.64	117.95	121.90
53	BA	1501	G	C5-C6-N1	5.64	114.32	111.50
53	BA	2860	A	C4-C5-C6	-5.64	114.18	117.00
53	BA	21	A	C5-C6-N1	5.64	120.52	117.70
53	BA	192	C	O4'-C1'-N1	5.64	112.71	108.20
53	BA	927	A	C4-C5-C6	-5.64	114.18	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1359	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	642	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	1013	G	N1-C6-O6	-5.64	116.52	119.90
53	BA	538	A	C5-C6-N1	5.64	120.52	117.70
53	BA	1215	G	C8-N9-C4	-5.64	104.15	106.40
53	BA	1677	A	O4'-C1'-N9	5.64	112.71	108.20
53	BA	2573	C	O4'-C1'-N1	5.64	112.71	108.20
21	AA	530	G	N3-C4-C5	-5.63	125.78	128.60
53	BA	160	A	C6-C5-N7	5.63	136.24	132.30
53	BA	1157	G	C5-C6-N1	5.63	114.32	111.50
53	BA	1459	G	N3-C4-C5	-5.63	125.78	128.60
53	BA	1898	U	C5-C6-N1	-5.63	119.88	122.70
53	BA	2473	U	O4'-C1'-N1	5.63	112.71	108.20
21	AA	439	U	O4'-C1'-N1	5.63	112.71	108.20
53	BA	1521	G	N1-C6-O6	-5.63	116.52	119.90
21	AA	100	G	C5-C6-N1	5.63	114.32	111.50
21	AA	1130	A	C4-C5-C6	-5.63	114.18	117.00
53	BA	173	A	C5-C6-N1	5.63	120.52	117.70
53	BA	1495	A	C5-C6-N1	5.63	120.52	117.70
53	BA	2153	C	N1-C2-O2	5.63	122.28	118.90
54	BB	54	G	C4'-C3'-C2'	-5.63	96.97	102.60
21	AA	9	G	N3-C2-N2	-5.63	115.96	119.90
21	AA	616	G	N1-C6-O6	-5.63	116.52	119.90
21	AA	1117	A	C1'-O4'-C4'	-5.63	105.40	109.90
53	BA	1390	U	C5'-C4'-C3'	-5.63	106.99	116.00
53	BA	1858	A	C5-C6-N1	5.63	120.52	117.70
21	AA	392	C	N3-C2-O2	-5.63	117.96	121.90
53	BA	205	G	N1-C6-O6	-5.63	116.52	119.90
53	BA	979	A	C4-C5-C6	-5.63	114.19	117.00
53	BA	1412	U	N3-C2-O2	-5.63	118.26	122.20
53	BA	1971	U	C5-C6-N1	-5.63	119.89	122.70
53	BA	2388	A	C5'-C4'-O4'	5.63	115.85	109.10
53	BA	2873	A	C5-C6-N1	5.63	120.51	117.70
54	BB	12	C	N1-C2-O2	5.63	122.28	118.90
21	AA	184	G	O4'-C1'-N9	5.63	112.70	108.20
21	AA	676	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	877	G	C5-C6-N1	5.63	114.31	111.50
22	A1	3	G	N1-C6-O6	-5.63	116.52	119.90
22	A1	17	U	N3-C2-O2	-5.63	118.26	122.20
53	BA	509	C	N3-C4-N4	-5.63	114.06	118.00
53	BA	1116	G	N3-C2-N2	-5.63	115.96	119.90
53	BA	1417	C	N1-C2-O2	5.63	122.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1632	A	C5-C6-N1	5.63	120.51	117.70
53	BA	1871	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1075	U	O4'-C1'-N1	5.62	112.70	108.20
21	AA	1376	U	N1-C2-N3	5.62	118.28	114.90
53	BA	2854	G	C5-C6-N1	5.62	114.31	111.50
11	AL	49	ARG	NE-CZ-NH1	5.62	123.11	120.30
21	AA	326	G	N1-C6-O6	-5.62	116.53	119.90
21	AA	636	U	O4'-C1'-N1	5.62	112.70	108.20
53	BA	970	U	O4'-C1'-N1	5.62	112.70	108.20
53	BA	1226	A	C4-C5-C6	-5.62	114.19	117.00
53	BA	1512	C	O4'-C1'-N1	5.62	112.70	108.20
21	AA	844	G	N1-C6-O6	-5.62	116.53	119.90
53	BA	519	U	O4'-C1'-N1	5.62	112.70	108.20
53	BA	1305	C	N3-C2-O2	-5.62	117.97	121.90
9	AJ	16	ARG	NE-CZ-NH1	5.62	123.11	120.30
21	AA	360	G	O4'-C1'-N9	5.62	112.70	108.20
53	BA	1392	A	C5'-C4'-O4'	5.62	115.84	109.10
53	BA	1633	G	C8-N9-C4	-5.62	104.15	106.40
53	BA	2028	U	O4'-C1'-N1	5.62	112.70	108.20
53	BA	2307	G	N1-C6-O6	-5.62	116.53	119.90
21	AA	290	C	N3-C2-O2	-5.62	117.97	121.90
21	AA	337	G	N3-C4-C5	-5.62	125.79	128.60
21	AA	1098	C	N3-C2-O2	-5.62	117.97	121.90
22	A1	2	G	O4'-C1'-N9	5.62	112.69	108.20
53	BA	1151	A	C5-C6-N1	5.62	120.51	117.70
53	BA	1300	G	N3-C4-C5	-5.62	125.79	128.60
53	BA	1493	C	O4'-C1'-N1	5.62	112.69	108.20
53	BA	1535	A	C6-C5-N7	5.62	136.23	132.30
53	BA	1977	A	C4-C5-C6	-5.62	114.19	117.00
53	BA	2512	C	N1-C2-O2	5.62	122.27	118.90
21	AA	92	U	N1-C2-N3	5.62	118.27	114.90
21	AA	205	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	947	G	C5-C6-N1	5.62	114.31	111.50
53	BA	557	C	C4'-C3'-C2'	-5.62	96.98	102.60
53	BA	1007	C	N1-C2-O2	5.62	122.27	118.90
53	BA	2003	A	C4-C5-C6	-5.62	114.19	117.00
53	BA	2726	A	C5-C6-N1	5.62	120.51	117.70
21	AA	736	C	N3-C2-O2	-5.62	117.97	121.90
21	AA	1053	G	N3-C2-N2	-5.62	115.97	119.90
21	AA	1059	C	N1-C2-O2	5.62	122.27	118.90
21	AA	1513	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	1531	A	C4-C5-C6	-5.62	114.19	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1382	G	N3-C4-C5	-5.62	125.79	128.60
21	AA	555	U	N3-C2-O2	-5.61	118.27	122.20
21	AA	1327	C	N3-C4-C5	5.61	124.15	121.90
53	BA	757	G	N3-C2-N2	-5.61	115.97	119.90
53	BA	859	G	C5-C6-N1	5.61	114.31	111.50
21	AA	1328	C	N1-C2-O2	5.61	122.27	118.90
53	BA	7	G	C5-C6-N1	5.61	114.31	111.50
53	BA	309	A	C4-C5-C6	-5.61	114.19	117.00
53	BA	330	A	C4-C5-C6	-5.61	114.19	117.00
53	BA	2091	C	O4'-C1'-N1	5.61	112.69	108.20
53	BA	2831	G	N1-C6-O6	-5.61	116.53	119.90
21	AA	313	A	C5-C6-N1	5.61	120.50	117.70
53	BA	336	C	N1-C2-O2	5.61	122.27	118.90
21	AA	161	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	316	C	N1-C2-O2	5.61	122.27	118.90
53	BA	1459	G	C8-N9-C4	-5.61	104.16	106.40
53	BA	1853	A	C5-C6-N1	5.61	120.50	117.70
21	AA	811	C	C3'-C2'-C1'	5.61	105.98	101.50
21	AA	1089	G	C8-N9-C4	-5.61	104.16	106.40
53	BA	545	U	N1-C2-N3	5.61	118.26	114.90
53	BA	736	C	N3-C2-O2	-5.61	117.98	121.90
53	BA	2022	U	N3-C2-O2	-5.61	118.28	122.20
21	AA	132	C	N3-C2-O2	-5.60	117.98	121.90
10	AK	97	ARG	NE-CZ-NH1	5.60	123.10	120.30
21	AA	35	G	N1-C6-O6	-5.60	116.54	119.90
21	AA	387	U	O4'-C1'-N1	5.60	112.68	108.20
53	BA	1113	U	O4'-C1'-N1	5.60	112.68	108.20
53	BA	1406	U	O4'-C1'-N1	5.60	112.68	108.20
53	BA	1419	A	O4'-C1'-N9	5.60	112.68	108.20
53	BA	1453	A	C1'-O4'-C4'	-5.60	105.42	109.90
53	BA	1742	U	N1-C2-N3	5.60	118.26	114.90
53	BA	2000	C	N3-C4-C5	5.60	124.14	121.90
21	AA	157	U	O4'-C1'-N1	5.60	112.68	108.20
21	AA	948	C	N1-C2-O2	5.60	122.26	118.90
21	AA	1333	A	C4-C5-C6	-5.60	114.20	117.00
53	BA	1610	A	C2-N3-C4	5.60	113.40	110.60
53	BA	1673	G	N3-C2-N2	-5.60	115.98	119.90
53	BA	1814	G	C8-N9-C4	-5.60	104.16	106.40
53	BA	1856	U	O4'-C1'-N1	5.60	112.68	108.20
53	BA	2482	A	C4-C5-C6	-5.60	114.20	117.00
54	BB	97	C	C5'-C4'-O4'	5.60	115.82	109.10
5	AF	79	ARG	NE-CZ-NH1	5.60	123.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	826	U	O4'-C1'-N1	5.60	112.68	108.20
53	BA	900	A	C4-C5-C6	-5.60	114.20	117.00
53	BA	1002	G	N3-C4-C5	-5.60	125.80	128.60
53	BA	1100	C	N3-C2-O2	-5.60	117.98	121.90
53	BA	1318	U	C3'-C2'-C1'	5.60	105.98	101.50
53	BA	1727	C	O4'-C1'-N1	5.60	112.68	108.20
53	BA	2077	A	C4-C5-C6	-5.60	114.20	117.00
53	BA	2111	U	C5-C6-N1	-5.60	119.90	122.70
53	BA	2243	U	N1-C2-N3	5.60	118.26	114.90
53	BA	2356	U	C5'-C4'-O4'	5.60	115.82	109.10
21	AA	88	U	C5-C6-N1	-5.60	119.90	122.70
21	AA	301	G	N1-C6-O6	-5.60	116.54	119.90
53	BA	1891	G	C5-C6-N1	5.60	114.30	111.50
21	AA	47	C	N3-C2-O2	-5.59	117.98	121.90
21	AA	1047	G	C5-C6-N1	5.59	114.30	111.50
53	BA	550	C	N3-C2-O2	-5.59	117.98	121.90
53	BA	2649	C	N3-C2-O2	-5.59	117.98	121.90
21	AA	1293	C	N1-C2-O2	5.59	122.26	118.90
53	BA	1281	G	N3-C2-N2	-5.59	115.98	119.90
21	AA	80	A	C4-C5-C6	-5.59	114.20	117.00
21	AA	1029	U	C5-C6-N1	-5.59	119.90	122.70
21	AA	1128	C	N1-C2-O2	5.59	122.25	118.90
21	AA	1350	A	C4-C5-C6	-5.59	114.20	117.00
53	BA	2200	C	N3-C2-O2	-5.59	117.99	121.90
53	BA	2606	C	O4'-C1'-N1	5.59	112.67	108.20
21	AA	419	C	O4'-C1'-N1	5.59	112.67	108.20
21	AA	1410	A	C4-C5-C6	-5.59	114.21	117.00
53	BA	1405	U	N3-C2-O2	-5.59	118.29	122.20
53	BA	2399	G	N1-C6-O6	-5.59	116.55	119.90
53	BA	2512	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	846	G	C4'-C3'-C2'	-5.59	97.01	102.60
53	BA	973	A	O4'-C1'-N9	5.59	112.67	108.20
53	BA	2453	A	C4-C5-C6	-5.59	114.21	117.00
53	BA	2540	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1352	C	N3-C4-C5	5.59	124.13	121.90
53	BA	1069	A	C5-C6-N1	5.59	120.49	117.70
53	BA	1139	G	C5-N7-C8	-5.59	101.51	104.30
21	AA	940	C	N3-C4-C5	5.58	124.13	121.90
21	AA	1449	C	N1-C2-O2	5.58	122.25	118.90
53	BA	729	G	C5-C6-N1	5.58	114.29	111.50
21	AA	355	C	N3-C2-O2	-5.58	117.99	121.90
21	AA	909	A	C4-C5-C6	-5.58	114.21	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1190	G	P-O3'-C3'	5.58	126.40	119.70
53	BA	61	C	N3-C4-N4	-5.58	114.09	118.00
53	BA	815	C	N3-C2-O2	-5.58	117.99	121.90
53	BA	1326	U	O4'-C1'-N1	5.58	112.67	108.20
53	BA	2731	G	N1-C6-O6	-5.58	116.55	119.90
54	BB	52	A	C4-C5-C6	-5.58	114.21	117.00
3	AD	103	ARG	NE-CZ-NH1	5.58	123.09	120.30
21	AA	129	A	O4'-C1'-N9	5.58	112.67	108.20
35	BN	96	ARG	NE-CZ-NH1	5.58	123.09	120.30
53	BA	46	G	C5'-C4'-O4'	5.58	115.80	109.10
53	BA	211	C	N3-C2-O2	-5.58	117.99	121.90
53	BA	2313	C	N1-C2-O2	5.58	122.25	118.90
53	BA	2463	C	N1-C2-O2	5.58	122.25	118.90
53	BA	2554	U	O4'-C1'-N1	5.58	112.67	108.20
53	BA	850	U	C5-C6-N1	-5.58	119.91	122.70
53	BA	2561	U	C5-C6-N1	-5.58	119.91	122.70
21	AA	64	G	N3-C4-C5	-5.58	125.81	128.60
21	AA	1257	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	1324	A	C4-C5-C6	-5.58	114.21	117.00
35	BN	90	ARG	NE-CZ-NH2	5.58	123.09	120.30
53	BA	1918	A	O4'-C1'-N9	5.58	112.66	108.20
53	BA	2015	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	752	G	N9-C4-C5	5.58	107.63	105.40
21	AA	1359	C	N3-C2-O2	-5.58	118.00	121.90
53	BA	1467	U	N3-C2-O2	-5.58	118.30	122.20
53	BA	1628	G	N1-C6-O6	-5.58	116.55	119.90
53	BA	1925	C	C6-N1-C2	-5.58	118.07	120.30
21	AA	1310	G	N9-C4-C5	5.58	107.63	105.40
33	BL	60	ARG	NE-CZ-NH2	-5.58	117.51	120.30
53	BA	879	G	N7-C8-N9	5.58	115.89	113.10
53	BA	988	A	C4-C5-C6	-5.58	114.21	117.00
53	BA	1348	C	N3-C2-O2	-5.58	118.00	121.90
53	BA	2013	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	1028	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	1493	A	O4'-C1'-N9	5.57	112.66	108.20
53	BA	1246	A	N1-C6-N6	-5.57	115.26	118.60
53	BA	1647	U	C6-N1-C2	-5.57	117.66	121.00
53	BA	1892	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	556	C	N1-C2-O2	5.57	122.24	118.90
53	BA	243	U	C5-C6-N1	-5.57	119.91	122.70
21	AA	733	G	N3-C4-C5	-5.57	125.81	128.60
21	AA	1432	G	O4'-C1'-N9	5.57	112.66	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	540	C	N3-C4-C5	5.57	124.13	121.90
53	BA	838	C	O4'-C1'-N1	5.57	112.66	108.20
53	BA	902	C	N1-C2-O2	5.57	122.24	118.90
53	BA	1633	G	N9-C4-C5	5.57	107.63	105.40
53	BA	1952	A	C4-C5-C6	-5.57	114.22	117.00
53	BA	2538	C	N3-C2-O2	-5.57	118.00	121.90
53	BA	2776	A	O4'-C1'-N9	5.57	112.66	108.20
53	BA	334	C	N1-C2-O2	5.57	122.24	118.90
53	BA	1012	U	N3-C2-O2	-5.57	118.30	122.20
21	AA	98	A	C6-C5-N7	5.57	136.20	132.30
21	AA	893	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	1378	C	N1-C2-O2	5.57	122.24	118.90
53	BA	1505	A	C6-C5-N7	5.57	136.20	132.30
53	BA	2455	G	N7-C8-N9	5.57	115.88	113.10
54	BB	92	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	99	C	N1-C2-O2	5.57	122.24	118.90
53	BA	227	A	O4'-C1'-N9	5.57	112.65	108.20
53	BA	994	C	N1-C2-O2	5.57	122.24	118.90
53	BA	1057	A	C4-C5-C6	-5.57	114.22	117.00
53	BA	1974	C	C4'-C3'-C2'	-5.57	97.03	102.60
21	AA	232	G	C8-N9-C4	-5.56	104.17	106.40
21	AA	320	A	C6-C5-N7	5.56	136.19	132.30
21	AA	1052	U	C5-C6-N1	-5.56	119.92	122.70
53	BA	94	A	C6-C5-N7	5.56	136.19	132.30
53	BA	255	A	N1-C6-N6	-5.56	115.26	118.60
53	BA	393	C	N3-C2-O2	-5.56	118.01	121.90
53	BA	458	G	N1-C6-O6	-5.56	116.56	119.90
53	BA	487	C	N3-C2-O2	-5.56	118.01	121.90
53	BA	2062	A	C1'-O4'-C4'	-5.56	105.45	109.90
11	AL	88	ASP	CB-CG-OD1	5.56	123.31	118.30
21	AA	596	A	C5-C6-N1	5.56	120.48	117.70
21	AA	868	C	O4'-C1'-N1	5.56	112.65	108.20
53	BA	1447	C	N3-C2-O2	-5.56	118.01	121.90
53	BA	1573	G	O4'-C1'-N9	5.56	112.65	108.20
19	AT	73	ARG	NE-CZ-NH1	5.56	123.08	120.30
21	AA	40	C	O4'-C1'-N1	5.56	112.65	108.20
21	AA	104	G	C5-C6-N1	5.56	114.28	111.50
53	BA	623	C	N1-C2-O2	5.56	122.24	118.90
53	BA	640	C	N3-C4-C5	5.56	124.12	121.90
54	BB	25	U	C5-C6-N1	-5.56	119.92	122.70
21	AA	249	U	O4'-C1'-N1	5.56	112.65	108.20
53	BA	314	C	O4'-C1'-N1	5.56	112.64	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1279	G	N3-C4-C5	-5.56	125.82	128.60
21	AA	837	U	C5-C6-N1	-5.56	119.92	122.70
53	BA	1194	A	C5-C6-N1	5.56	120.48	117.70
21	AA	47	C	N1-C2-O2	5.55	122.23	118.90
22	A1	74	C	C1'-O4'-C4'	-5.55	105.46	109.90
23	A2	80	C	N1-C2-O2	5.55	122.23	118.90
53	BA	773	U	C5-C6-N1	-5.55	119.92	122.70
53	BA	777	G	C8-N9-C4	-5.55	104.18	106.40
53	BA	1403	A	C5-C6-N1	5.55	120.48	117.70
53	BA	2899	A	N1-C6-N6	-5.55	115.27	118.60
21	AA	302	G	C5-C6-N1	5.55	114.28	111.50
30	BI	87	SER	C-N-CA	5.55	133.96	122.30
21	AA	33	A	C4-C5-C6	-5.55	114.22	117.00
21	AA	42	G	C5-C6-N1	5.55	114.28	111.50
21	AA	737	C	C4'-C3'-C2'	-5.55	97.05	102.60
21	AA	1038	C	N3-C4-C5	5.55	124.12	121.90
53	BA	1172	C	N3-C2-O2	-5.55	118.01	121.90
53	BA	2497	A	C4-C5-C6	-5.55	114.22	117.00
53	BA	2509	G	C4'-C3'-C2'	-5.55	97.05	102.60
53	BA	2767	C	N1-C2-O2	5.55	122.23	118.90
21	AA	291	U	O4'-C1'-N1	5.55	112.64	108.20
53	BA	817	C	N3-C4-C5	5.55	124.12	121.90
53	BA	1308	A	C4-C5-C6	-5.55	114.22	117.00
53	BA	1333	G	N1-C6-O6	-5.55	116.57	119.90
53	BA	1654	A	C5-C6-N1	5.55	120.47	117.70
53	BA	1709	U	O4'-C1'-N1	5.55	112.64	108.20
53	BA	1889	A	C4-C5-C6	-5.55	114.23	117.00
21	AA	1325	C	O4'-C1'-N1	5.55	112.64	108.20
53	BA	311	A	O4'-C1'-N9	5.55	112.64	108.20
53	BA	518	G	N3-C4-C5	-5.55	125.83	128.60
53	BA	748	G	O4'-C1'-N9	5.55	112.64	108.20
53	BA	1722	A	C5-C6-N1	5.55	120.47	117.70
21	AA	504	C	N1-C2-O2	5.55	122.23	118.90
21	AA	894	G	C5-C6-N1	5.55	114.27	111.50
21	AA	1261	A	N1-C6-N6	-5.55	115.27	118.60
53	BA	339	U	N1-C2-N3	5.55	118.23	114.90
53	BA	1855	U	O4'-C1'-N1	5.55	112.64	108.20
53	BA	634	C	N1-C2-O2	5.54	122.23	118.90
21	AA	301	G	C8-N9-C4	-5.54	104.18	106.40
21	AA	742	G	O4'-C1'-N9	5.54	112.64	108.20
28	BG	93	TYR	CB-CG-CD2	-5.54	117.67	121.00
38	BQ	23	TYR	CB-CG-CD2	-5.54	117.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	713	G	N1-C6-O6	-5.54	116.57	119.90
53	BA	1275	A	O4'-C4'-C3'	5.54	110.53	106.10
53	BA	1288	G	N1-C6-O6	-5.54	116.57	119.90
53	BA	1471	G	N7-C8-N9	5.54	115.87	113.10
54	BB	27	C	N3-C4-C5	5.54	124.12	121.90
8	AI	123	ARG	NE-CZ-NH1	5.54	123.07	120.30
21	AA	514	C	N3-C2-O2	-5.54	118.02	121.90
53	BA	849	A	C6-C5-N7	5.54	136.18	132.30
53	BA	924	G	N3-C4-C5	-5.54	125.83	128.60
53	BA	2127	G	O4'-C1'-N9	5.54	112.63	108.20
54	BB	30	C	O4'-C1'-N1	5.54	112.63	108.20
21	AA	177	G	N3-C4-C5	-5.54	125.83	128.60
21	AA	1248	A	C4-C5-C6	-5.54	114.23	117.00
53	BA	84	A	C4-C5-C6	-5.54	114.23	117.00
53	BA	380	G	C5-C6-N1	5.54	114.27	111.50
53	BA	620	G	O4'-C1'-N9	5.54	112.63	108.20
21	AA	381	C	O4'-C1'-N1	5.54	112.63	108.20
21	AA	609	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	1398	A	C2'-C3'-O3'	5.54	122.56	113.70
21	AA	1504	G	N1-C6-O6	-5.54	116.58	119.90
53	BA	516	C	C4'-C3'-C2'	-5.54	97.06	102.60
53	BA	764	A	C5-C6-N1	5.54	120.47	117.70
53	BA	2730	C	O4'-C1'-N1	5.54	112.63	108.20
53	BA	2787	C	N1-C2-O2	5.54	122.22	118.90
21	AA	1348	U	C5-C6-N1	-5.54	119.93	122.70
53	BA	1894	C	N3-C4-C5	5.54	124.11	121.90
53	BA	2071	A	C6-C5-N7	5.54	136.18	132.30
21	AA	772	U	C5-C6-N1	-5.54	119.93	122.70
53	BA	252	G	C5-C6-N1	5.54	114.27	111.50
53	BA	1542	U	O4'-C1'-N1	5.54	112.63	108.20
53	BA	1616	A	C4-C5-C6	-5.54	114.23	117.00
53	BA	1750	G	C5-C6-N1	5.54	114.27	111.50
21	AA	395	C	N1-C2-O2	5.53	122.22	118.90
29	BH	116	ARG	NE-CZ-NH1	5.53	123.07	120.30
53	BA	2029	G	O4'-C1'-N9	5.53	112.63	108.20
53	BA	2525	G	O4'-C1'-N9	5.53	112.63	108.20
53	BA	1235	G	N7-C8-N9	5.53	115.87	113.10
21	AA	211	G	C5-C6-N1	5.53	114.27	111.50
21	AA	459	A	C5-C6-N1	5.53	120.47	117.70
21	AA	1320	C	N3-C2-O2	-5.53	118.03	121.90
53	BA	1021	A	C4-C5-C6	-5.53	114.23	117.00
53	BA	1039	A	C6-C5-N7	5.53	136.17	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1246	A	C5-C6-N1	5.53	120.47	117.70
53	BA	1661	G	C5-C6-N1	5.53	114.27	111.50
53	BA	1857	G	O4'-C1'-N9	5.53	112.62	108.20
53	BA	2305	U	C4-C5-C6	5.53	123.02	119.70
21	AA	412	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	767	A	C6-C5-N7	5.53	136.17	132.30
53	BA	691	C	N1-C2-O2	5.53	122.22	118.90
53	BA	2264	C	N3-C2-O2	-5.53	118.03	121.90
21	AA	153	C	O4'-C1'-N1	5.53	112.62	108.20
21	AA	879	C	N3-C2-O2	-5.53	118.03	121.90
53	BA	944	C	O4'-C1'-N1	5.53	112.62	108.20
53	BA	1392	A	C4-C5-C6	-5.53	114.24	117.00
53	BA	2226	C	N3-C2-O2	-5.53	118.03	121.90
53	BA	2636	C	N3-C2-O2	-5.53	118.03	121.90
21	AA	300	A	N1-C6-N6	-5.53	115.28	118.60
53	BA	1819	A	C5-C6-N1	5.53	120.46	117.70
53	BA	1880	U	O4'-C1'-N1	5.53	112.62	108.20
54	BB	30	C	N3-C2-O2	-5.53	118.03	121.90
21	AA	720	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	1123	U	O4'-C1'-N1	5.52	112.62	108.20
53	BA	85	G	C5-C6-N1	5.52	114.26	111.50
53	BA	1420	A	C5-C6-N1	5.52	120.46	117.70
53	BA	1463	C	N3-C2-O2	-5.52	118.03	121.90
53	BA	1531	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	1486	G	O4'-C1'-N9	5.52	112.62	108.20
53	BA	869	G	N3-C4-C5	-5.52	125.84	128.60
53	BA	1488	C	O4'-C1'-N1	5.52	112.62	108.20
53	BA	1895	C	N3-C2-O2	-5.52	118.03	121.90
53	BA	2848	G	O4'-C1'-N9	5.52	112.62	108.20
21	AA	623	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	1342	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	757	U	O4'-C1'-N1	5.52	112.61	108.20
22	A1	51	C	N3-C2-O2	-5.52	118.04	121.90
53	BA	1176	U	C5-C6-N1	-5.52	119.94	122.70
53	BA	338	G	C8-N9-C4	-5.52	104.19	106.40
53	BA	553	G	N9-C4-C5	5.52	107.61	105.40
53	BA	1932	A	O4'-C1'-N9	5.52	112.61	108.20
53	BA	2175	C	N3-C2-O2	-5.52	118.04	121.90
53	BA	2244	U	O4'-C1'-N1	5.52	112.61	108.20
53	BA	2451	A	C4'-C3'-C2'	-5.52	97.08	102.60
53	BA	2834	G	N3-C4-C5	-5.52	125.84	128.60
53	BA	1284	A	C4-C5-C6	-5.52	114.24	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2826	A	C4-C5-C6	-5.52	114.24	117.00
54	BB	46	A	C6-C5-N7	5.52	136.16	132.30
53	BA	142	A	C4-C5-C6	-5.51	114.24	117.00
53	BA	407	G	O4'-C1'-N9	5.51	112.61	108.20
53	BA	1309	G	C5-C6-N1	5.51	114.26	111.50
53	BA	1639	C	O4'-C1'-N1	5.51	112.61	108.20
53	BA	1708	C	O4'-C1'-N1	5.51	112.61	108.20
21	AA	779	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	944	G	N1-C6-O6	-5.51	116.59	119.90
53	BA	48	G	C5-C6-N1	5.51	114.26	111.50
53	BA	500	G	N1-C6-O6	-5.51	116.59	119.90
53	BA	699	A	C4-C5-C6	-5.51	114.24	117.00
53	BA	2116	G	N3-C2-N2	-5.51	116.04	119.90
53	BA	2796	U	O4'-C1'-N1	5.51	112.61	108.20
21	AA	456	A	C4-C5-C6	-5.51	114.24	117.00
21	AA	496	A	C4-C5-C6	-5.51	114.24	117.00
21	AA	756	C	N3-C4-C5	5.51	124.11	121.90
21	AA	972	C	N3-C2-O2	-5.51	118.04	121.90
53	BA	274	C	O4'-C1'-N1	5.51	112.61	108.20
53	BA	971	G	C5-C6-N1	5.51	114.26	111.50
53	BA	1140	C	P-O3'-C3'	5.51	126.31	119.70
53	BA	2196	C	N3-C2-O2	-5.51	118.04	121.90
53	BA	2403	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	214	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	1371	G	C5-C6-N1	5.51	114.25	111.50
53	BA	952	G	N1-C6-O6	-5.51	116.59	119.90
53	BA	1690	A	C4-C5-C6	-5.51	114.25	117.00
53	BA	2237	G	C5-C6-N1	5.51	114.25	111.50
21	AA	634	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	641	U	C5-C6-N1	-5.51	119.95	122.70
21	AA	848	C	N3-C2-O2	-5.51	118.04	121.90
53	BA	616	A	C4-C5-C6	-5.51	114.25	117.00
21	AA	522	C	N3-C2-O2	-5.51	118.05	121.90
21	AA	823	C	O4'-C1'-N1	5.51	112.61	108.20
21	AA	854	U	O4'-C1'-N1	5.51	112.61	108.20
21	AA	1473	G	N1-C6-O6	-5.51	116.60	119.90
53	BA	1010	A	C4-C5-C6	-5.51	114.25	117.00
53	BA	1346	G	N1-C6-O6	-5.51	116.60	119.90
53	BA	2239	G	C5-C6-N1	5.51	114.25	111.50
53	BA	2311	A	C4-C5-C6	-5.51	114.25	117.00
53	BA	2645	G	O4'-C1'-N9	5.51	112.61	108.20
21	AA	1072	G	N1-C6-O6	-5.50	116.60	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	501	A	C5-C6-N1	5.50	120.45	117.70
53	BA	632	A	C4-C5-C6	-5.50	114.25	117.00
53	BA	645	C	N3-C2-O2	-5.50	118.05	121.90
8	AI	17	ARG	NE-CZ-NH1	5.50	123.05	120.30
21	AA	534	U	O4'-C1'-N1	5.50	112.60	108.20
53	BA	201	C	N1-C2-O2	5.50	122.20	118.90
53	BA	362	A	O4'-C1'-N9	5.50	112.60	108.20
53	BA	1210	G	N1-C6-O6	-5.50	116.60	119.90
53	BA	2478	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	1309	G	C8-N9-C4	-5.50	104.20	106.40
21	AA	1488	G	N1-C6-O6	-5.50	116.60	119.90
21	AA	1493	A	C2-N3-C4	5.50	113.35	110.60
53	BA	2270	A	C5-N7-C8	-5.50	101.15	103.90
21	AA	175	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	1081	A	C4-C5-C6	-5.50	114.25	117.00
53	BA	155	A	C4'-C3'-C2'	-5.50	97.10	102.60
53	BA	930	G	C5-C6-N1	5.50	114.25	111.50
53	BA	1025	G	C8-N9-C4	-5.50	104.20	106.40
53	BA	2525	G	C8-N9-C4	-5.50	104.20	106.40
21	AA	1204	A	C5-C6-N1	5.50	120.45	117.70
53	BA	62	U	C1'-O4'-C4'	-5.50	105.50	109.90
53	BA	2827	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	333	U	O4'-C1'-N1	5.50	112.60	108.20
53	BA	224	U	C5-C6-N1	-5.50	119.95	122.70
53	BA	1280	G	C5-C6-N1	5.50	114.25	111.50
53	BA	2895	G	C8-N9-C4	-5.50	104.20	106.40
21	AA	879	C	N1-C2-O2	5.50	122.20	118.90
21	AA	1114	C	O4'-C1'-N1	5.50	112.60	108.20
21	AA	732	C	N1-C2-O2	5.49	122.20	118.90
21	AA	919	A	N1-C6-N6	-5.49	115.30	118.60
21	AA	1190	G	C5-C6-N1	5.49	114.25	111.50
21	AA	1308	U	C1'-O4'-C4'	-5.49	105.50	109.90
21	AA	1399	C	N3-C4-C5	5.49	124.10	121.90
53	BA	1327	A	C4-C5-C6	-5.49	114.25	117.00
53	BA	1836	C	O4'-C1'-N1	5.49	112.60	108.20
53	BA	1910	G	C5-C6-N1	5.49	114.25	111.50
53	BA	2243	U	N3-C2-O2	-5.49	118.36	122.20
53	BA	2832	U	C5-C6-N1	-5.49	119.95	122.70
54	BB	56	G	C5-C6-N1	5.49	114.25	111.50
21	AA	282	A	C6-C5-N7	5.49	136.14	132.30
53	BA	12	U	C5-C6-N1	-5.49	119.95	122.70
53	BA	1121	C	N1-C2-O2	5.49	122.19	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1939	U	N1-C2-N3	5.49	118.19	114.90
21	AA	353	A	O4'-C1'-N9	5.49	112.59	108.20
21	AA	501	C	N1-C2-O2	5.49	122.19	118.90
53	BA	1559	U	N1-C2-N3	5.49	118.19	114.90
53	BA	1691	C	N1-C2-O2	5.49	122.19	118.90
21	AA	1203	C	O4'-C1'-N1	5.49	112.59	108.20
53	BA	407	G	N3-C4-C5	-5.49	125.86	128.60
53	BA	1439	A	C4-C5-C6	-5.49	114.25	117.00
53	BA	1738	G	C5-C6-N1	5.49	114.24	111.50
53	BA	1871	A	C2-N3-C4	5.49	113.34	110.60
53	BA	2733	A	C4-C5-C6	-5.49	114.25	117.00
54	BB	90	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	961	U	N3-C2-O2	-5.49	118.36	122.20
22	A1	30	C	O4'-C1'-N1	5.49	112.59	108.20
22	A1	35	A	C5-C6-N1	5.49	120.44	117.70
49	B1	27	ARG	NE-CZ-NH2	5.49	123.04	120.30
53	BA	779	U	N3-C2-O2	-5.49	118.36	122.20
53	BA	1179	G	N7-C8-N9	5.49	115.84	113.10
53	BA	2001	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	504	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	970	C	N3-C4-C5	5.49	124.09	121.90
53	BA	1603	A	C6-C5-N7	5.49	136.14	132.30
53	BA	2098	U	O4'-C1'-N1	5.49	112.59	108.20
53	BA	2536	G	N9-C4-C5	5.49	107.59	105.40
53	BA	2752	C	O4'-C1'-N1	5.49	112.59	108.20
53	BA	905	A	C5-C6-N1	5.48	120.44	117.70
53	BA	1231	U	N3-C2-O2	-5.48	118.36	122.20
53	BA	2481	G	N3-C4-C5	-5.48	125.86	128.60
21	AA	867	G	O4'-C1'-N9	5.48	112.58	108.20
32	BK	30	ARG	NE-CZ-NH2	-5.48	117.56	120.30
53	BA	2212	A	C8-N9-C4	-5.48	103.61	105.80
53	BA	2457	U	C5-C6-N1	-5.48	119.96	122.70
21	AA	74	A	C4-C5-C6	-5.48	114.26	117.00
53	BA	130	C	N3-C2-O2	-5.48	118.06	121.90
53	BA	2629	U	N3-C2-O2	-5.48	118.36	122.20
53	BA	2726	A	C4-C5-C6	-5.48	114.26	117.00
53	BA	2900	A	C5-C6-N1	5.48	120.44	117.70
21	AA	1170	A	C4-C5-C6	-5.48	114.26	117.00
53	BA	1883	U	O4'-C1'-N1	5.48	112.58	108.20
48	B0	15	ARG	NE-CZ-NH1	5.48	123.04	120.30
53	BA	99	U	N3-C2-O2	-5.48	118.36	122.20
53	BA	502	A	C4-C5-C6	-5.48	114.26	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1008	A	C5-C6-N1	5.48	120.44	117.70
53	BA	1167	C	O4'-C1'-N1	5.48	112.58	108.20
53	BA	1294	U	O4'-C1'-N1	5.48	112.58	108.20
53	BA	1769	U	C4'-C3'-C2'	-5.48	97.12	102.60
53	BA	1842	G	N9-C4-C5	5.48	107.59	105.40
53	BA	2073	C	N3-C2-O2	-5.48	118.07	121.90
53	BA	2505	G	C5-C6-N1	5.48	114.24	111.50
53	BA	2643	G	N1-C6-O6	-5.48	116.61	119.90
54	BB	55	U	O4'-C1'-N1	5.48	112.58	108.20
53	BA	748	G	N3-C2-N2	-5.48	116.07	119.90
53	BA	2063	C	N3-C2-O2	-5.48	118.07	121.90
21	AA	1045	C	C6-N1-C2	-5.47	118.11	120.30
28	BG	148	ARG	NE-CZ-NH1	5.47	123.04	120.30
53	BA	33	C	N3-C2-O2	-5.47	118.07	121.90
53	BA	620	G	N3-C2-N2	-5.47	116.07	119.90
53	BA	1542	U	C5-C6-N1	-5.47	119.96	122.70
53	BA	1904	G	N1-C6-O6	-5.47	116.61	119.90
53	BA	1924	C	N3-C2-O2	-5.47	118.07	121.90
53	BA	2009	A	C6-C5-N7	5.47	136.13	132.30
53	BA	2629	U	O4'-C1'-N1	5.47	112.58	108.20
54	BB	4	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	117	G	N9-C4-C5	5.47	107.59	105.40
21	AA	1326	U	N3-C2-O2	-5.47	118.37	122.20
53	BA	990	A	C5'-C4'-O4'	5.47	115.67	109.10
53	BA	1532	A	C4-C5-C6	-5.47	114.26	117.00
53	BA	1655	A	C5-C6-N1	5.47	120.44	117.70
53	BA	2115	G	N1-C6-O6	-5.47	116.62	119.90
14	AO	62	ARG	NE-CZ-NH1	5.47	123.04	120.30
53	BA	1944	U	O4'-C1'-N1	5.47	112.58	108.20
21	AA	261	U	N1-C2-N3	5.47	118.18	114.90
21	AA	1180	A	C4-C5-C6	-5.47	114.27	117.00
45	BX	56	ARG	NE-CZ-NH1	5.47	123.03	120.30
48	B0	49	ARG	NH1-CZ-NH2	-5.47	113.38	119.40
53	BA	353	C	N1-C2-O2	5.47	122.18	118.90
53	BA	870	U	N3-C2-O2	-5.47	118.37	122.20
53	BA	1153	C	O4'-C1'-N1	5.47	112.58	108.20
53	BA	1461	C	N1-C2-O2	5.47	122.18	118.90
53	BA	2863	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	415	A	C4-C5-C6	-5.47	114.27	117.00
53	BA	1376	C	N3-C2-O2	-5.47	118.07	121.90
53	BA	1566	A	C4-C5-C6	-5.47	114.27	117.00
53	BA	2704	C	O4'-C1'-N1	5.47	112.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2787	C	N3-C4-C5	5.47	124.09	121.90
53	BA	2788	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	585	G	C8-N9-C4	-5.47	104.21	106.40
21	AA	772	U	O4'-C1'-N1	5.47	112.57	108.20
33	BL	59	ARG	NE-CZ-NH1	5.47	123.03	120.30
53	BA	167	A	C4-C5-C6	-5.47	114.27	117.00
53	BA	401	A	O4'-C1'-N9	5.47	112.57	108.20
53	BA	480	A	C4-C5-C6	-5.47	114.27	117.00
53	BA	1620	G	C5-C6-N1	5.47	114.23	111.50
53	BA	1918	A	C3'-C2'-C1'	5.47	105.87	101.50
53	BA	2351	G	O4'-C1'-N9	5.47	112.57	108.20
53	BA	2714	G	C5-C6-N1	5.47	114.23	111.50
21	AA	339	C	N1-C2-O2	5.46	122.18	118.90
21	AA	747	A	C4-C5-C6	-5.46	114.27	117.00
23	A2	82	A	C6-C5-N7	5.46	136.12	132.30
53	BA	356	G	N1-C6-O6	-5.46	116.62	119.90
53	BA	2392	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	620	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	663	A	C6-C5-N7	5.46	136.12	132.30
53	BA	894	U	O4'-C1'-N1	5.46	112.57	108.20
53	BA	1296	G	N1-C6-O6	-5.46	116.62	119.90
53	BA	1408	G	N7-C8-N9	5.46	115.83	113.10
54	BB	88	C	N3-C4-C5	5.46	124.08	121.90
21	AA	1204	A	C4-C5-C6	-5.46	114.27	117.00
35	BN	8	ARG	NE-CZ-NH1	5.46	123.03	120.30
53	BA	682	G	O4'-C1'-N9	5.46	112.57	108.20
53	BA	2058	A	C6-C5-N7	5.46	136.12	132.30
53	BA	2409	G	C5-C6-N1	5.46	114.23	111.50
53	BA	2834	G	N1-C6-O6	-5.46	116.62	119.90
53	BA	907	G	N3-C4-C5	-5.46	125.87	128.60
22	A1	35	A	C4-C5-C6	-5.46	114.27	117.00
51	B3	41	ARG	NE-CZ-NH1	5.46	123.03	120.30
53	BA	39	G	C5-C6-N1	5.46	114.23	111.50
53	BA	198	C	N3-C2-O2	-5.46	118.08	121.90
53	BA	1102	C	N3-C2-O2	-5.46	118.08	121.90
53	BA	2322	A	C4-C5-C6	-5.46	114.27	117.00
53	BA	2655	G	C3'-C2'-C1'	-5.46	97.13	101.50
21	AA	506	G	N3-C2-N2	-5.46	116.08	119.90
21	AA	662	U	O4'-C1'-N1	5.46	112.56	108.20
53	BA	106	C	O4'-C1'-N1	5.46	112.56	108.20
53	BA	305	C	N3-C2-O2	-5.46	118.08	121.90
53	BA	381	G	C5-C6-N1	5.46	114.23	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	717	C	C1'-O4'-C4'	-5.46	105.53	109.90
53	BA	1212	G	C5-C6-N1	5.46	114.23	111.50
53	BA	1697	G	C5-C6-N1	5.46	114.23	111.50
53	BA	2715	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	609	A	O4'-C1'-N9	5.45	112.56	108.20
21	AA	1003	G	O4'-C1'-N9	5.45	112.56	108.20
53	BA	57	C	N3-C4-C5	5.45	124.08	121.90
53	BA	75	G	C5-C6-N1	5.45	114.23	111.50
53	BA	127	A	C4-C5-C6	-5.45	114.27	117.00
53	BA	2001	C	N1-C2-O2	5.45	122.17	118.90
53	BA	2502	G	N3-C4-C5	-5.45	125.87	128.60
53	BA	2535	G	C8-N9-C4	-5.45	104.22	106.40
53	BA	2867	G	N3-C4-C5	-5.45	125.87	128.60
21	AA	207	C	N1-C2-O2	5.45	122.17	118.90
21	AA	350	G	C8-N9-C4	-5.45	104.22	106.40
36	BO	7	ARG	NE-CZ-NH1	5.45	123.03	120.30
53	BA	17	G	C5-C6-N1	5.45	114.23	111.50
53	BA	1578	U	C4-C5-C6	5.45	122.97	119.70
53	BA	2888	C	N1-C2-O2	5.45	122.17	118.90
21	AA	382	A	C4-C5-C6	-5.45	114.27	117.00
53	BA	534	U	C5-C6-N1	-5.45	119.97	122.70
53	BA	860	U	C5-C6-N1	-5.45	119.97	122.70
53	BA	1696	G	N1-C6-O6	-5.45	116.63	119.90
54	BB	118	C	N3-C2-O2	-5.45	118.08	121.90
21	AA	286	C	N1-C2-O2	5.45	122.17	118.90
21	AA	454	G	C5-C6-N1	5.45	114.22	111.50
53	BA	264	C	N3-C4-C5	5.45	124.08	121.90
53	BA	1276	A	C4-C5-C6	-5.45	114.28	117.00
53	BA	1605	C	N3-C2-O2	-5.45	118.09	121.90
53	BA	2675	A	C6-C5-N7	5.45	136.11	132.30
53	BA	2794	C	N3-C2-O2	-5.45	118.09	121.90
21	AA	1233	G	N1-C6-O6	-5.45	116.63	119.90
21	AA	1499	A	C4-C5-C6	-5.45	114.28	117.00
53	BA	1342	A	N1-C6-N6	-5.45	115.33	118.60
21	AA	241	G	N3-C4-C5	-5.45	125.88	128.60
21	AA	349	A	C4-C5-C6	-5.45	114.28	117.00
53	BA	970	U	N3-C2-O2	-5.45	118.39	122.20
53	BA	1735	A	N1-C6-N6	-5.45	115.33	118.60
53	BA	1794	A	C6-C5-N7	5.45	136.11	132.30
53	BA	2582	G	N3-C4-C5	-5.45	125.88	128.60
21	AA	832	G	C5-C6-N1	5.44	114.22	111.50
53	BA	250	G	N3-C2-N2	-5.44	116.09	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2272	U	N1-C2-N3	5.44	118.17	114.90
53	BA	2838	G	N7-C8-N9	5.44	115.82	113.10
21	AA	996	A	N1-C6-N6	-5.44	115.33	118.60
21	AA	1360	A	O4'-C1'-N9	5.44	112.55	108.20
21	AA	1380	U	C5-C6-N1	-5.44	119.98	122.70
53	BA	7	G	N1-C6-O6	-5.44	116.63	119.90
53	BA	174	U	C5-C6-N1	-5.44	119.98	122.70
53	BA	388	G	N3-C2-N2	-5.44	116.09	119.90
53	BA	582	A	C6-C5-N7	5.44	136.11	132.30
53	BA	834	G	N3-C4-C5	-5.44	125.88	128.60
53	BA	1153	C	N3-C4-C5	5.44	124.08	121.90
53	BA	2738	A	C6-C5-N7	5.44	136.11	132.30
21	AA	835	U	O4'-C1'-N1	5.44	112.55	108.20
53	BA	556	A	C6-C5-N7	5.44	136.11	132.30
53	BA	1102	C	O4'-C1'-N1	5.44	112.55	108.20
53	BA	1934	C	O4'-C1'-N1	5.44	112.55	108.20
53	BA	2743	U	N1-C2-N3	5.44	118.17	114.90
22	A1	40	G	N9-C4-C5	5.44	107.58	105.40
53	BA	187	G	C8-N9-C4	-5.44	104.22	106.40
53	BA	492	A	C4-C5-C6	-5.44	114.28	117.00
53	BA	777	G	C4'-C3'-C2'	-5.44	97.16	102.60
53	BA	1749	A	C6-C5-N7	5.44	136.11	132.30
53	BA	1837	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	1178	G	N7-C8-N9	5.44	115.82	113.10
21	AA	1293	C	N3-C4-C5	5.44	124.08	121.90
53	BA	1	G	C5-C6-N1	5.44	114.22	111.50
53	BA	551	G	N7-C8-N9	5.44	115.82	113.10
53	BA	1122	G	C5-C6-N1	5.44	114.22	111.50
53	BA	2032	G	N3-C4-C5	-5.44	125.88	128.60
53	BA	2333	A	C6-C5-N7	5.44	136.11	132.30
53	BA	2378	A	C4-C5-C6	-5.44	114.28	117.00
53	BA	2756	U	N1-C1'-C2'	5.44	121.07	114.00
21	AA	912	C	N3-C4-C5	5.44	124.08	121.90
21	AA	957	U	C5-C6-N1	-5.44	119.98	122.70
53	BA	2114	A	C6-C5-N7	5.44	136.10	132.30
53	BA	2238	G	O4'-C1'-N9	5.44	112.55	108.20
21	AA	207	C	N3-C4-C5	5.43	124.07	121.90
21	AA	327	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	897	C	N3-C2-O2	-5.43	118.10	121.90
53	BA	634	C	N3-C4-C5	5.43	124.07	121.90
53	BA	744	U	C5-C6-N1	-5.43	119.98	122.70
53	BA	972	A	N1-C6-N6	-5.43	115.34	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1816	C	P-O3'-C3'	5.43	126.22	119.70
53	BA	2593	U	O4'-C1'-N1	5.43	112.55	108.20
53	BA	2820	A	C4-C5-C6	-5.43	114.28	117.00
54	BB	8	C	O4'-C1'-N1	5.43	112.55	108.20
21	AA	776	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	1268	G	C5-C6-N1	5.43	114.22	111.50
21	AA	1465	A	C6-C5-N7	5.43	136.10	132.30
27	BF	147	ARG	NE-CZ-NH1	5.43	123.02	120.30
53	BA	968	C	C4'-C3'-C2'	-5.43	97.17	102.60
53	BA	1986	C	N3-C2-O2	-5.43	118.10	121.90
21	AA	635	A	C6-C5-N7	5.43	136.10	132.30
21	AA	1032	G	P-O3'-C3'	5.43	126.22	119.70
21	AA	1183	U	N3-C2-O2	-5.43	118.40	122.20
53	BA	2282	G	O4'-C1'-N9	5.43	112.55	108.20
53	BA	2282	G	C1'-O4'-C4'	-5.43	105.56	109.90
21	AA	44	A	C5-C6-N1	5.43	120.42	117.70
21	AA	582	C	O4'-C1'-N1	5.43	112.54	108.20
21	AA	1333	A	O4'-C1'-N9	5.43	112.54	108.20
53	BA	914	G	C8-N9-C4	-5.43	104.23	106.40
53	BA	1145	C	O4'-C1'-N1	5.43	112.54	108.20
53	BA	1785	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	585	G	N7-C8-N9	5.43	115.81	113.10
21	AA	921	U	O4'-C1'-N1	5.43	112.54	108.20
27	BF	114	ARG	NE-CZ-NH2	5.43	123.01	120.30
53	BA	723	C	N1-C2-O2	5.43	122.16	118.90
53	BA	2221	G	N3-C2-N2	-5.43	116.10	119.90
13	AN	85	ARG	NE-CZ-NH2	-5.43	117.59	120.30
21	AA	278	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	502	A	O4'-C1'-N9	5.43	112.54	108.20
21	AA	1341	U	O4'-C1'-N1	5.43	112.54	108.20
30	BI	87	SER	CA-C-N	5.43	127.06	116.20
53	BA	302	C	N3-C2-O2	-5.43	118.10	121.90
53	BA	1051	G	N1-C6-O6	-5.43	116.64	119.90
53	BA	1186	G	C5-C6-N1	5.43	114.21	111.50
53	BA	1271	G	N3-C4-C5	-5.43	125.89	128.60
53	BA	1300	G	N1-C6-O6	-5.43	116.64	119.90
53	BA	1774	C	O4'-C1'-N1	5.43	112.54	108.20
53	BA	2734	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	1347	G	N1-C6-O6	-5.42	116.64	119.90
53	BA	301	G	N3-C4-C5	-5.42	125.89	128.60
53	BA	2143	C	N3-C2-O2	-5.42	118.10	121.90
53	BA	2646	C	N3-C4-C5	5.42	124.07	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	268	C	N1-C2-O2	5.42	122.15	118.90
53	BA	880	G	C8-N9-C4	-5.42	104.23	106.40
53	BA	1683	U	N3-C2-O2	-5.42	118.40	122.20
21	AA	696	A	O4'-C1'-N9	5.42	112.54	108.20
21	AA	1281	C	N3-C4-C5	5.42	124.07	121.90
22	A1	9	A	C5-C6-N1	5.42	120.41	117.70
38	BQ	10	ARG	NE-CZ-NH1	5.42	123.01	120.30
53	BA	729	G	N1-C6-O6	-5.42	116.65	119.90
53	BA	898	C	N3-C2-O2	-5.42	118.11	121.90
53	BA	1654	A	C4-C5-C6	-5.42	114.29	117.00
53	BA	2348	U	O4'-C1'-N1	5.42	112.54	108.20
53	BA	2793	C	N3-C2-O2	-5.42	118.11	121.90
53	BA	1236	G	N9-C4-C5	5.42	107.57	105.40
53	BA	2203	U	N3-C2-O2	-5.42	118.41	122.20
53	BA	2328	A	C6-C5-N7	5.42	136.09	132.30
21	AA	176	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	882	C	O4'-C1'-N1	5.42	112.53	108.20
21	AA	1112	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	1195	C	N3-C2-O2	-5.42	118.11	121.90
53	BA	119	A	C6-C5-N7	5.42	136.09	132.30
53	BA	282	A	C4-C5-C6	-5.42	114.29	117.00
53	BA	1064	C	N3-C4-C5	5.42	124.07	121.90
53	BA	2689	U	N3-C2-O2	-5.42	118.41	122.20
21	AA	613	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	883	C	C2-N3-C4	-5.42	117.19	119.90
21	AA	1033	G	C5-C6-N1	5.42	114.21	111.50
21	AA	1213	A	C6-C5-N7	5.42	136.09	132.30
21	AA	1332	A	C5-C6-N1	5.42	120.41	117.70
21	AA	1348	U	N3-C2-O2	-5.42	118.41	122.20
21	AA	1403	C	N3-C4-C5	5.42	124.07	121.90
53	BA	112	U	N1-C2-N3	5.42	118.15	114.90
53	BA	2198	A	C5-C6-N1	5.42	120.41	117.70
21	AA	1262	C	O4'-C1'-N1	5.42	112.53	108.20
21	AA	1310	G	O4'-C1'-N9	5.42	112.53	108.20
53	BA	350	G	N1-C6-O6	-5.42	116.65	119.90
53	BA	1295	C	N3-C2-O2	-5.42	118.11	121.90
53	BA	2514	U	O4'-C1'-N1	5.42	112.53	108.20
21	AA	246	A	C5-C6-N1	5.41	120.41	117.70
21	AA	255	G	N1-C6-O6	-5.41	116.65	119.90
21	AA	608	A	N1-C6-N6	-5.41	115.35	118.60
21	AA	1239	A	C5-C6-N1	5.41	120.41	117.70
53	BA	225	C	N1-C2-O2	5.41	122.15	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	759	G	C5-C6-N1	5.41	114.21	111.50
53	BA	1030	C	C6-N1-C2	-5.41	118.13	120.30
53	BA	2420	C	N3-C2-O2	-5.41	118.11	121.90
21	AA	499	A	C6-C5-N7	5.41	136.09	132.30
21	AA	841	C	N3-C4-N4	-5.41	114.21	118.00
21	AA	1510	C	N1-C2-O2	5.41	122.15	118.90
53	BA	1115	G	O4'-C1'-N9	5.41	112.53	108.20
53	BA	2888	C	C3'-C2'-C1'	5.41	105.83	101.50
21	AA	893	C	O4'-C1'-N1	5.41	112.53	108.20
21	AA	1033	G	N1-C6-O6	-5.41	116.65	119.90
21	AA	1322	C	O4'-C1'-N1	5.41	112.53	108.20
53	BA	128	C	N1-C2-O2	5.41	122.15	118.90
53	BA	306	U	N1-C2-N3	5.41	118.15	114.90
53	BA	482	A	C4-C5-C6	-5.41	114.30	117.00
53	BA	1288	G	C5-C6-N1	5.41	114.20	111.50
53	BA	1402	U	O4'-C1'-N1	5.41	112.53	108.20
53	BA	2155	U	N1-C2-N3	5.41	118.15	114.90
53	BA	2517	C	N3-C4-C5	5.41	124.06	121.90
21	AA	24	U	O4'-C1'-N1	5.41	112.53	108.20
21	AA	416	G	N3-C2-N2	-5.41	116.11	119.90
21	AA	467	U	C3'-C2'-C1'	5.41	105.83	101.50
21	AA	616	G	C5-C6-N1	5.41	114.20	111.50
21	AA	978	A	C3'-C2'-C1'	5.41	105.83	101.50
21	AA	1254	A	C5-C6-N1	5.41	120.40	117.70
21	AA	1408	A	C4-C5-C6	-5.41	114.30	117.00
22	A1	73	A	O4'-C1'-N9	5.41	112.53	108.20
53	BA	232	G	C5-C6-N1	5.41	114.20	111.50
53	BA	1352	U	N1-C2-N3	5.41	118.14	114.90
53	BA	1529	G	N3-C4-C5	-5.41	125.90	128.60
53	BA	2060	A	C4-C5-C6	-5.41	114.30	117.00
53	BA	1881	C	N3-C2-O2	-5.41	118.11	121.90
21	AA	311	C	N3-C4-C5	5.41	124.06	121.90
21	AA	1388	C	N3-C2-O2	-5.41	118.11	121.90
53	BA	446	G	O4'-C1'-N9	5.41	112.53	108.20
53	BA	480	A	C5'-C4'-O4'	5.41	115.59	109.10
53	BA	704	G	C8-N9-C4	-5.41	104.24	106.40
53	BA	1108	U	N3-C2-O2	-5.41	118.42	122.20
53	BA	2134	A	C4-C5-C6	-5.41	114.30	117.00
53	BA	2444	G	C8-N9-C4	-5.41	104.24	106.40
53	BA	670	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	7	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	62	U	C3'-C2'-C1'	5.40	105.82	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	343	U	C5-C6-N1	-5.40	120.00	122.70
21	AA	704	A	C6-C5-N7	5.40	136.08	132.30
25	BD	184	ARG	NE-CZ-NH2	5.40	123.00	120.30
53	BA	709	U	C5-C6-N1	-5.40	120.00	122.70
53	BA	995	C	N1-C2-O2	5.40	122.14	118.90
53	BA	1242	U	O4'-C1'-N1	5.40	112.52	108.20
53	BA	1741	C	O4'-C1'-N1	5.40	112.52	108.20
53	BA	1985	C	N1-C2-O2	5.40	122.14	118.90
53	BA	2515	C	C6-N1-C2	-5.40	118.14	120.30
53	BA	2606	C	N1-C2-O2	5.40	122.14	118.90
21	AA	1051	C	N3-C2-O2	-5.40	118.12	121.90
53	BA	785	G	C5'-C4'-C3'	-5.40	107.36	116.00
53	BA	786	C	N3-C4-C5	5.40	124.06	121.90
53	BA	873	C	N3-C2-O2	-5.40	118.12	121.90
53	BA	1388	G	N3-C4-C5	-5.40	125.90	128.60
53	BA	1575	C	N1-C2-O2	5.40	122.14	118.90
53	BA	2628	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	431	A	C4-C5-C6	-5.40	114.30	117.00
53	BA	2080	A	C5-C6-N1	5.40	120.40	117.70
53	BA	2650	U	C5-C6-N1	-5.40	120.00	122.70
21	AA	314	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	609	A	C5-C6-N1	5.40	120.40	117.70
21	AA	1008	U	N3-C2-O2	-5.40	118.42	122.20
21	AA	1303	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	1424	U	O4'-C1'-N1	5.40	112.52	108.20
53	BA	225	C	N3-C4-C5	5.40	124.06	121.90
53	BA	351	C	O4'-C1'-N1	5.40	112.52	108.20
53	BA	425	G	C5-C6-N1	5.40	114.20	111.50
53	BA	717	C	N3-C2-O2	-5.40	118.12	121.90
53	BA	999	U	N3-C2-O2	-5.40	118.42	122.20
53	BA	1303	G	C5-C6-N1	5.40	114.20	111.50
53	BA	1957	C	N1-C2-O2	5.40	122.14	118.90
21	AA	1201	A	C4-C5-C6	-5.40	114.30	117.00
53	BA	401	A	C6-C5-N7	5.40	136.08	132.30
53	BA	833	A	C5-C6-N1	5.40	120.40	117.70
21	AA	1243	C	C6-N1-C2	-5.39	118.14	120.30
22	A1	61	C	N3-C2-O2	-5.39	118.12	121.90
53	BA	156	A	C4-C5-C6	-5.39	114.30	117.00
53	BA	659	G	N1-C6-O6	-5.39	116.66	119.90
53	BA	1649	G	C5-C6-N1	5.39	114.20	111.50
53	BA	1924	C	N1-C2-O2	5.39	122.14	118.90
53	BA	2225	A	C4-C5-C6	-5.39	114.30	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2502	G	O4'-C1'-N9	5.39	112.52	108.20
53	BA	175	G	C5-C6-N1	5.39	114.20	111.50
53	BA	721	A	C6-C5-N7	5.39	136.07	132.30
53	BA	1253	A	C4-C5-C6	-5.39	114.30	117.00
53	BA	2089	C	N3-C2-O2	-5.39	118.12	121.90
53	BA	2277	G	N7-C8-N9	5.39	115.80	113.10
53	BA	2683	C	N3-C2-O2	-5.39	118.12	121.90
21	AA	99	C	N3-C4-C5	5.39	124.06	121.90
21	AA	699	C	N3-C2-O2	-5.39	118.13	121.90
21	AA	934	C	P-O3'-C3'	5.39	126.17	119.70
53	BA	1419	A	C5-C6-N1	5.39	120.40	117.70
53	BA	2902	C	O4'-C1'-N1	5.39	112.51	108.20
21	AA	939	G	C5-C6-N1	5.39	114.19	111.50
22	A1	67	U	C5'-C4'-O4'	5.39	115.57	109.10
53	BA	110	G	C8-N9-C4	-5.39	104.24	106.40
53	BA	462	C	N3-C2-O2	-5.39	118.13	121.90
53	BA	1314	C	C6-N1-C2	-5.39	118.14	120.30
53	BA	1349	C	N3-C2-O2	-5.39	118.13	121.90
53	BA	2632	A	C4-C5-C6	-5.39	114.31	117.00
21	AA	558	G	C8-N9-C4	-5.39	104.25	106.40
21	AA	575	G	N7-C8-N9	5.39	115.79	113.10
21	AA	716	A	C4-C5-C6	-5.39	114.31	117.00
21	AA	851	G	C5-C6-N1	5.39	114.19	111.50
53	BA	209	C	N3-C2-O2	-5.39	118.13	121.90
53	BA	584	C	N1-C2-O2	5.39	122.13	118.90
53	BA	1536	C	N3-C4-C5	5.39	124.06	121.90
53	BA	2027	G	C5-C6-N1	5.39	114.19	111.50
53	BA	2131	U	C5-C6-N1	-5.39	120.01	122.70
21	AA	628	G	C8-N9-C4	-5.39	104.25	106.40
21	AA	1315	U	O4'-C1'-N1	5.39	112.51	108.20
53	BA	294	A	C4-C5-C6	-5.39	114.31	117.00
53	BA	822	G	N3-C4-C5	-5.39	125.91	128.60
53	BA	1498	C	N3-C2-O2	-5.39	118.13	121.90
53	BA	2050	C	N3-C2-O2	-5.39	118.13	121.90
9	AJ	31	ARG	NE-CZ-NH1	5.38	122.99	120.30
21	AA	223	A	C6-C5-N7	5.38	136.07	132.30
21	AA	1006	G	N3-C2-N2	-5.38	116.13	119.90
21	AA	1534	A	O4'-C1'-N9	5.38	112.51	108.20
22	A1	28	C	N3-C2-O2	-5.38	118.13	121.90
53	BA	683	U	C5-C6-N1	-5.38	120.01	122.70
53	BA	1506	U	C5-C6-N1	-5.38	120.01	122.70
53	BA	1986	C	C4'-C3'-C2'	-5.38	97.22	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2416	C	O4'-C1'-N1	5.38	112.51	108.20
53	BA	2639	A	C6-C5-N7	5.38	136.07	132.30
21	AA	750	C	N1-C2-O2	5.38	122.13	118.90
21	AA	841	C	N1-C2-O2	5.38	122.13	118.90
21	AA	1218	C	N1-C2-O2	5.38	122.13	118.90
53	BA	672	C	N1-C2-O2	5.38	122.13	118.90
53	BA	1141	U	N3-C2-O2	-5.38	118.43	122.20
53	BA	1668	A	O4'-C1'-N9	5.38	112.51	108.20
53	BA	2803	G	N1-C6-O6	-5.38	116.67	119.90
21	AA	676	A	N1-C6-N6	-5.38	115.37	118.60
53	BA	78	U	N1-C2-N3	5.38	118.13	114.90
53	BA	508	A	C6-C5-N7	5.38	136.07	132.30
53	BA	891	G	C5-C6-N1	5.38	114.19	111.50
53	BA	922	C	C4'-C3'-C2'	-5.38	97.22	102.60
53	BA	1507	C	N1-C2-O2	5.38	122.13	118.90
53	BA	2467	C	N3-C4-N4	-5.38	114.23	118.00
53	BA	2715	C	N1-C2-O2	5.38	122.13	118.90
21	AA	312	C	N3-C2-O2	-5.38	118.13	121.90
22	A1	75	C	N1-C2-O2	5.38	122.13	118.90
53	BA	928	A	C4-C5-C6	-5.38	114.31	117.00
53	BA	1112	G	C5-C6-N1	5.38	114.19	111.50
53	BA	2457	U	N3-C2-O2	-5.38	118.43	122.20
21	AA	1027	C	N3-C2-O2	-5.38	118.14	121.90
22	A1	32	C	N3-C2-O2	-5.38	118.14	121.90
53	BA	88	G	C5-C6-N1	5.38	114.19	111.50
53	BA	864	G	C5-C6-N1	5.38	114.19	111.50
53	BA	1226	A	C5-C6-N1	5.38	120.39	117.70
53	BA	1633	G	N1-C6-O6	-5.38	116.67	119.90
53	BA	2886	A	C2-N3-C4	5.38	113.29	110.60
54	BB	59	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	758	C	N3-C2-O2	-5.38	118.14	121.90
53	BA	655	A	C4-C5-C6	-5.38	114.31	117.00
53	BA	976	G	C3'-C2'-C1'	5.38	105.80	101.50
53	BA	1215	G	N9-C4-C5	5.38	107.55	105.40
53	BA	1772	A	C5-C6-N1	5.38	120.39	117.70
21	AA	1347	G	O4'-C1'-N9	5.38	112.50	108.20
53	BA	2006	C	N3-C2-O2	-5.38	118.14	121.90
53	BA	2164	C	N3-C4-C5	5.38	124.05	121.90
53	BA	2484	G	C5-C6-N1	5.38	114.19	111.50
21	AA	277	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	1390	U	N3-C2-O2	-5.37	118.44	122.20
53	BA	609	A	C4-C5-C6	-5.37	114.31	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	876	C	O4'-C1'-N1	5.37	112.50	108.20
53	BA	1335	C	N3-C2-O2	-5.37	118.14	121.90
53	BA	2559	C	C4'-C3'-C2'	-5.37	97.23	102.60
53	BA	2611	C	N1-C2-O2	5.37	122.12	118.90
53	BA	2772	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	1351	U	N3-C2-O2	-5.37	118.44	122.20
53	BA	1981	A	C4-C5-C6	-5.37	114.31	117.00
53	BA	2544	G	C5-C6-N1	5.37	114.19	111.50
53	BA	2028	U	C5-C6-N1	-5.37	120.02	122.70
21	AA	1105	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	1326	U	C5-C6-N1	-5.37	120.02	122.70
21	AA	1471	U	O4'-C1'-N1	5.37	112.50	108.20
22	A1	21	A	C5-C6-N1	5.37	120.38	117.70
53	BA	121	G	C3'-C2'-C1'	5.37	105.80	101.50
53	BA	362	A	C4-C5-C6	-5.37	114.31	117.00
53	BA	2583	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	1460	C	N3-C2-O2	-5.37	118.14	121.90
53	BA	416	U	O4'-C1'-N1	5.37	112.49	108.20
53	BA	1068	G	N3-C4-C5	-5.37	125.92	128.60
53	BA	1591	A	O4'-C1'-N9	5.37	112.49	108.20
21	AA	578	C	N1-C2-O2	5.37	122.12	118.90
21	AA	624	C	O4'-C1'-N1	5.37	112.49	108.20
21	AA	667	G	N3-C2-N2	-5.37	116.14	119.90
21	AA	969	A	O4'-C1'-N9	5.37	112.49	108.20
53	BA	247	G	N1-C6-O6	-5.37	116.68	119.90
53	BA	344	A	C6-C5-N7	5.37	136.06	132.30
53	BA	451	U	O4'-C1'-N1	5.37	112.49	108.20
53	BA	803	U	O4'-C1'-N1	5.37	112.49	108.20
53	BA	1006	C	O4'-C1'-N1	5.37	112.49	108.20
53	BA	1859	U	C5-C6-N1	-5.37	120.02	122.70
53	BA	1983	G	C5-C6-N1	5.37	114.18	111.50
53	BA	2846	G	C5-C6-N1	5.37	114.18	111.50
21	AA	177	G	C8-N9-C4	-5.36	104.25	106.40
21	AA	699	C	N1-C2-O2	5.36	122.12	118.90
53	BA	23	G	C5-C6-N1	5.36	114.18	111.50
53	BA	671	C	O4'-C1'-N1	5.36	112.49	108.20
53	BA	1920	C	O4'-C1'-N1	5.36	112.49	108.20
53	BA	2575	C	N3-C2-O2	-5.36	118.14	121.90
53	BA	2690	U	C5-C6-N1	-5.36	120.02	122.70
53	BA	2749	A	C4-C5-C6	-5.36	114.32	117.00
53	BA	2897	U	C5-C6-N1	-5.36	120.02	122.70
21	AA	598	U	C5'-C4'-O4'	5.36	115.53	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	5	A	C5-C6-N1	5.36	120.38	117.70
53	BA	1054	A	C5-C6-N1	5.36	120.38	117.70
53	BA	2275	C	O4'-C4'-C3'	5.36	110.39	106.10
53	BA	2403	C	O4'-C1'-N1	5.36	112.49	108.20
21	AA	81	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	155	A	C6-C5-N7	5.36	136.05	132.30
21	AA	582	C	N3-C2-O2	-5.36	118.15	121.90
21	AA	600	A	C4-C5-C6	-5.36	114.32	117.00
53	BA	518	G	C5-C6-N1	5.36	114.18	111.50
53	BA	765	C	N3-C2-O2	-5.36	118.15	121.90
53	BA	921	C	N3-C2-O2	-5.36	118.15	121.90
53	BA	1710	G	N1-C6-O6	-5.36	116.68	119.90
53	BA	1732	C	O4'-C1'-N1	5.36	112.49	108.20
53	BA	2441	U	N3-C2-O2	-5.36	118.45	122.20
21	AA	1129	C	N1-C2-O2	5.36	122.11	118.90
37	BP	108	ARG	NE-CZ-NH1	5.36	122.98	120.30
53	BA	1108	U	N1-C2-N3	5.36	118.11	114.90
53	BA	1370	C	O4'-C1'-N1	5.36	112.49	108.20
54	BB	62	C	N1-C2-O2	5.36	122.12	118.90
21	AA	1373	G	C8-N9-C4	-5.36	104.26	106.40
21	AA	1493	A	C3'-C2'-C1'	5.36	105.79	101.50
22	A1	58	A	C4-C5-C6	-5.36	114.32	117.00
24	BC	13	ARG	NE-CZ-NH1	5.36	122.98	120.30
53	BA	366	C	O4'-C1'-N1	5.36	112.49	108.20
53	BA	1195	G	C8-N9-C4	-5.36	104.26	106.40
53	BA	1392	A	C5-C6-N1	5.36	120.38	117.70
11	AL	94	TYR	CB-CG-CD2	-5.36	117.79	121.00
33	BL	48	ARG	NE-CZ-NH2	-5.36	117.62	120.30
53	BA	546	U	N3-C2-O2	-5.36	118.45	122.20
53	BA	1599	U	C5-C6-N1	-5.36	120.02	122.70
53	BA	1920	C	C6-N1-C2	-5.36	118.16	120.30
53	BA	2704	C	N3-C2-O2	-5.36	118.15	121.90
54	BB	27	C	N3-C2-O2	-5.36	118.15	121.90
53	BA	814	C	O4'-C1'-N1	5.35	112.48	108.20
21	AA	1055	A	C6-C5-N7	5.35	136.05	132.30
53	BA	851	C	N3-C2-O2	-5.35	118.15	121.90
53	BA	1476	U	O4'-C1'-N1	5.35	112.48	108.20
53	BA	1637	A	O4'-C1'-N9	5.35	112.48	108.20
53	BA	2254	C	N3-C2-O2	-5.35	118.15	121.90
21	AA	739	C	N3-C4-C5	5.35	124.04	121.90
53	BA	2278	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	38	G	C5'-C4'-O4'	5.35	115.52	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	705	A	C4-C5-C6	-5.35	114.33	117.00
53	BA	2015	A	N1-C6-N6	-5.35	115.39	118.60
53	BA	2139	U	O4'-C1'-N1	5.35	112.48	108.20
53	BA	2280	G	C5-C6-N1	5.35	114.17	111.50
53	BA	2310	C	C3'-C2'-C1'	5.35	105.78	101.50
53	BA	2601	C	N1-C2-O2	5.35	122.11	118.90
21	AA	554	A	C6-C5-N7	5.35	136.04	132.30
21	AA	1282	C	N1-C2-O2	5.35	122.11	118.90
21	AA	1391	U	N3-C2-O2	-5.35	118.46	122.20
53	BA	369	U	C5-C6-N1	-5.35	120.03	122.70
53	BA	1023	U	O4'-C1'-C2'	-5.35	100.45	105.80
53	BA	1357	C	O4'-C1'-N1	5.35	112.48	108.20
53	BA	1882	U	N1-C2-N3	5.35	118.11	114.90
53	BA	2438	U	N3-C2-O2	-5.35	118.46	122.20
53	BA	2813	A	C6-C5-N7	5.35	136.04	132.30
53	BA	2849	U	N1-C2-N3	5.35	118.11	114.90
21	AA	1148	U	N3-C2-O2	-5.35	118.46	122.20
53	BA	258	G	C5-C6-N1	5.35	114.17	111.50
53	BA	1382	G	N1-C6-O6	-5.35	116.69	119.90
53	BA	1667	G	C5-C6-N1	5.35	114.17	111.50
53	BA	2292	U	C5-C6-N1	-5.35	120.03	122.70
53	BA	2521	C	O4'-C1'-N1	5.35	112.48	108.20
53	BA	2659	G	C5-C6-N1	5.35	114.17	111.50
4	AE	68	ARG	NE-CZ-NH2	-5.34	117.63	120.30
21	AA	93	U	N3-C2-O2	-5.34	118.46	122.20
21	AA	887	G	N1-C6-O6	-5.34	116.69	119.90
53	BA	1235	G	C8-N9-C4	-5.34	104.26	106.40
53	BA	1630	A	C6-C5-N7	5.34	136.04	132.30
53	BA	2113	U	O4'-C1'-N1	5.34	112.48	108.20
53	BA	2755	C	N3-C4-C5	5.34	124.04	121.90
54	BB	14	U	O4'-C1'-N1	5.34	112.47	108.20
52	B4	24	ARG	NE-CZ-NH2	-5.34	117.63	120.30
53	BA	2850	A	C6-C5-N7	5.34	136.04	132.30
53	BA	2864	G	O4'-C1'-N9	5.34	112.47	108.20
54	BB	67	G	C5-C6-N1	5.34	114.17	111.50
21	AA	343	U	N3-C2-O2	-5.34	118.46	122.20
21	AA	1463	U	O4'-C1'-N1	5.34	112.47	108.20
53	BA	473	G	C5-C6-N1	5.34	114.17	111.50
53	BA	923	G	N3-C4-C5	-5.34	125.93	128.60
53	BA	2538	C	O4'-C1'-N1	5.34	112.47	108.20
21	AA	429	U	C5-C6-N1	-5.34	120.03	122.70
21	AA	890	G	N1-C6-O6	-5.34	116.70	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1312	G	C5-C6-N1	5.34	114.17	111.50
21	AA	1382	C	N3-C2-O2	-5.34	118.16	121.90
53	BA	859	G	N3-C4-C5	-5.34	125.93	128.60
53	BA	1024	G	C5-C6-N1	5.34	114.17	111.50
53	BA	1574	C	N3-C4-C5	5.34	124.04	121.90
53	BA	1634	A	C4-C5-C6	-5.34	114.33	117.00
53	BA	2404	U	C5-C6-N1	-5.34	120.03	122.70
21	AA	467	U	N1-C2-N3	5.34	118.10	114.90
53	BA	1227	G	C5-C6-N1	5.34	114.17	111.50
54	BB	57	A	C4-C5-C6	-5.34	114.33	117.00
22	A1	70	C	O4'-C1'-N1	5.34	112.47	108.20
53	BA	834	G	N1-C6-O6	-5.34	116.70	119.90
53	BA	1242	U	N3-C2-O2	-5.34	118.46	122.20
53	BA	2092	U	N3-C2-O2	-5.34	118.47	122.20
53	BA	1147	A	C6-C5-N7	5.33	136.03	132.30
53	BA	2131	U	N3-C2-O2	-5.33	118.47	122.20
53	BA	2805	C	O4'-C1'-N1	5.33	112.47	108.20
21	AA	18	C	O4'-C1'-N1	5.33	112.47	108.20
21	AA	260	G	O4'-C1'-N9	5.33	112.47	108.20
53	BA	1055	G	C8-N9-C4	-5.33	104.27	106.40
53	BA	1182	G	N1-C6-O6	-5.33	116.70	119.90
53	BA	1301	A	C4-C5-C6	-5.33	114.33	117.00
53	BA	1964	G	O4'-C1'-N9	5.33	112.47	108.20
53	BA	2073	C	C4'-C3'-C2'	-5.33	97.27	102.60
53	BA	2728	U	C5-C6-N1	-5.33	120.03	122.70
21	AA	1358	U	N3-C2-O2	-5.33	118.47	122.20
53	BA	51	G	N1-C6-O6	-5.33	116.70	119.90
53	BA	451	U	N3-C2-O2	-5.33	118.47	122.20
53	BA	620	G	N3-C4-C5	-5.33	125.94	128.60
53	BA	1135	C	N1-C2-O2	5.33	122.10	118.90
53	BA	2016	U	O4'-C1'-N1	5.33	112.47	108.20
53	BA	2454	G	N7-C8-N9	5.33	115.77	113.10
53	BA	895	U	C5-C6-N1	-5.33	120.03	122.70
53	BA	1176	U	O4'-C1'-N1	5.33	112.46	108.20
53	BA	2476	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	408	A	C6-C5-N7	5.33	136.03	132.30
21	AA	1007	U	O4'-C1'-N1	5.33	112.46	108.20
21	AA	1053	G	C5-C6-N1	5.33	114.16	111.50
21	AA	1096	C	N3-C4-N4	-5.33	114.27	118.00
22	A1	30	C	N3-C4-C5	5.33	124.03	121.90
53	BA	379	G	N1-C6-O6	-5.33	116.70	119.90
53	BA	799	G	N3-C4-C5	-5.33	125.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1053	C	N3-C2-O2	-5.33	118.17	121.90
53	BA	1627	G	N3-C4-C5	-5.33	125.94	128.60
53	BA	1681	G	N3-C2-N2	-5.33	116.17	119.90
53	BA	1715	G	C8-N9-C4	-5.33	104.27	106.40
53	BA	2162	G	N3-C2-N2	-5.33	116.17	119.90
53	BA	2707	U	O4'-C1'-N1	5.33	112.46	108.20
54	BB	63	C	N1-C2-O2	5.33	122.10	118.90
53	BA	346	A	C4-C5-C6	-5.33	114.34	117.00
53	BA	1044	C	N1-C2-O2	5.33	122.10	118.90
53	BA	1205	A	C4-C5-C6	-5.33	114.34	117.00
21	AA	102	G	N7-C8-N9	5.33	115.76	113.10
21	AA	490	C	N1-C2-O2	5.33	122.09	118.90
21	AA	1121	U	O4'-C1'-N1	5.33	112.46	108.20
53	BA	66	C	N3-C4-C5	5.33	124.03	121.90
53	BA	293	U	N3-C2-O2	-5.33	118.47	122.20
53	BA	1299	G	N7-C8-N9	5.33	115.76	113.10
53	BA	1471	G	C8-N9-C4	-5.33	104.27	106.40
53	BA	2652	C	N1-C2-O2	5.33	122.10	118.90
53	BA	2832	U	O4'-C1'-N1	5.33	112.46	108.20
21	AA	46	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	93	U	C5-C6-N1	-5.32	120.04	122.70
21	AA	576	C	N1-C2-O2	5.32	122.09	118.90
21	AA	738	C	O4'-C1'-N1	5.32	112.46	108.20
21	AA	859	G	C8-N9-C4	-5.32	104.27	106.40
21	AA	1497	G	N9-C4-C5	5.32	107.53	105.40
53	BA	935	C	O4'-C1'-N1	5.32	112.46	108.20
53	BA	1410	G	N9-C4-C5	5.32	107.53	105.40
53	BA	2568	U	C5-C6-N1	-5.32	120.04	122.70
53	BA	2685	G	N1-C6-O6	-5.32	116.71	119.90
53	BA	2865	U	C5-C6-N1	-5.32	120.04	122.70
54	BB	88	C	N1-C2-O2	5.32	122.09	118.90
54	BB	54	G	C8-N9-C4	-5.32	104.27	106.40
48	B0	49	ARG	NE-CZ-NH1	5.32	122.96	120.30
53	BA	248	G	N7-C8-N9	5.32	115.76	113.10
53	BA	2138	G	N3-C2-N2	-5.32	116.18	119.90
53	BA	2462	C	N1-C2-O2	5.32	122.09	118.90
53	BA	2629	U	C5-C6-N1	-5.32	120.04	122.70
53	BA	2690	U	N1-C2-N3	5.32	118.09	114.90
53	BA	2030	A	O4'-C1'-N9	5.32	112.45	108.20
21	AA	48	C	N3-C4-C5	5.32	124.03	121.90
21	AA	1211	U	N1-C2-N3	5.32	118.09	114.90
21	AA	1427	C	N3-C2-O2	-5.32	118.18	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1708	C	C4'-C3'-C2'	-5.32	97.28	102.60
53	BA	2004	G	N1-C6-O6	-5.32	116.71	119.90
53	BA	2494	G	N3-C4-C5	-5.32	125.94	128.60
21	AA	1278	G	C5-C6-N1	5.32	114.16	111.50
21	AA	1351	U	C5-C6-N1	-5.32	120.04	122.70
53	BA	531	C	N1-C2-O2	5.32	122.09	118.90
53	BA	683	U	N1-C2-N3	5.32	118.09	114.90
53	BA	970	U	N1-C2-N3	5.32	118.09	114.90
53	BA	1480	C	N3-C4-C5	5.32	124.03	121.90
53	BA	1773	A	C5-C6-N1	5.32	120.36	117.70
53	BA	2209	G	C8-N9-C4	-5.32	104.27	106.40
53	BA	2658	C	O4'-C1'-N1	5.32	112.45	108.20
21	AA	647	C	O4'-C1'-N1	5.31	112.45	108.20
21	AA	1229	A	C4-C5-C6	-5.31	114.34	117.00
34	BM	66	ARG	NE-CZ-NH1	5.31	122.96	120.30
21	AA	222	C	N3-C2-O2	-5.31	118.18	121.90
21	AA	1381	U	N3-C2-O2	-5.31	118.48	122.20
53	BA	342	A	O4'-C1'-N9	5.31	112.45	108.20
53	BA	364	C	N1-C2-O2	5.31	122.09	118.90
53	BA	1518	C	N1-C2-O2	5.31	122.09	118.90
53	BA	1988	G	O4'-C1'-N9	5.31	112.45	108.20
53	BA	2043	C	N3-C4-C5	5.31	124.03	121.90
54	BB	30	C	N1-C2-O2	5.31	122.09	118.90
21	AA	1038	C	O4'-C1'-N1	5.31	112.45	108.20
53	BA	331	C	O4'-C1'-N1	5.31	112.45	108.20
53	BA	964	C	C6-N1-C2	-5.31	118.18	120.30
53	BA	2581	G	N3-C4-C5	-5.31	125.94	128.60
54	BB	87	U	O4'-C1'-N1	5.31	112.45	108.20
21	AA	696	A	C5-C6-N1	5.31	120.36	117.70
21	AA	1281	C	N1-C2-O2	5.31	122.09	118.90
53	BA	596	U	O4'-C1'-N1	5.31	112.45	108.20
53	BA	1637	A	C4'-C3'-C2'	-5.31	97.29	102.60
21	AA	726	C	N3-C4-C5	5.31	124.02	121.90
21	AA	1343	G	N1-C6-O6	-5.31	116.72	119.90
21	AA	1453	G	N3-C4-C5	-5.31	125.95	128.60
53	BA	1934	C	N1-C2-O2	5.31	122.08	118.90
53	BA	2141	G	C5-C6-N1	5.31	114.15	111.50
21	AA	1296	C	C3'-C2'-C1'	5.31	105.75	101.50
53	BA	215	G	N1-C6-O6	-5.31	116.72	119.90
53	BA	744	U	O4'-C1'-N1	5.31	112.44	108.20
2	AC	131	ARG	NE-CZ-NH2	-5.30	117.65	120.30
21	AA	711	G	N1-C6-O6	-5.30	116.72	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	33	U	C5-C6-N1	-5.30	120.05	122.70
22	A1	70	C	N3-C2-O2	-5.30	118.19	121.90
53	BA	838	C	C5'-C4'-O4'	5.30	115.47	109.10
53	BA	875	G	N1-C6-O6	-5.30	116.72	119.90
53	BA	996	A	C4-C5-C6	-5.30	114.35	117.00
53	BA	2399	G	C5-C6-N1	5.30	114.15	111.50
53	BA	2756	U	N3-C2-O2	-5.30	118.49	122.20
53	BA	2844	G	N3-C4-C5	-5.30	125.95	128.60
53	BA	678	C	N1-C2-O2	5.30	122.08	118.90
53	BA	1403	A	O4'-C1'-N9	5.30	112.44	108.20
53	BA	1917	U	O4'-C1'-N1	5.30	112.44	108.20
53	BA	2183	A	C6-C5-N7	5.30	136.01	132.30
54	BB	89	U	N3-C2-O2	-5.30	118.49	122.20
21	AA	289	G	N7-C8-N9	5.30	115.75	113.10
53	BA	147	C	N1-C2-O2	5.30	122.08	118.90
53	BA	375	G	N3-C4-C5	-5.30	125.95	128.60
53	BA	2408	U	O4'-C1'-N1	5.30	112.44	108.20
53	BA	2452	C	N1-C2-O2	5.30	122.08	118.90
53	BA	2500	U	N3-C2-O2	-5.30	118.49	122.20
53	BA	208	C	N3-C4-C5	5.30	124.02	121.90
53	BA	886	A	C6-C5-N7	5.30	136.01	132.30
53	BA	1924	C	O4'-C1'-N1	5.30	112.44	108.20
53	BA	2456	C	O4'-C1'-N1	5.30	112.44	108.20
54	BB	43	C	N3-C4-C5	5.30	124.02	121.90
53	BA	283	G	N1-C6-O6	-5.30	116.72	119.90
53	BA	917	A	N1-C6-N6	-5.30	115.42	118.60
53	BA	2417	C	N1-C2-O2	5.30	122.08	118.90
21	AA	144	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	1322	C	N1-C2-O2	5.30	122.08	118.90
21	AA	1401	G	C8-N9-C4	-5.30	104.28	106.40
21	AA	1446	A	C5-C6-N1	5.30	120.35	117.70
21	AA	1508	A	C4'-C3'-C2'	-5.30	97.30	102.60
53	BA	491	G	C5-C6-N1	5.30	114.15	111.50
53	BA	639	U	N3-C2-O2	-5.30	118.49	122.20
53	BA	882	G	C5-C6-N1	5.30	114.15	111.50
53	BA	929	U	C5-C6-N1	-5.30	120.05	122.70
53	BA	996	A	C5-C6-N1	5.30	120.35	117.70
53	BA	1258	U	O4'-C1'-N1	5.30	112.44	108.20
53	BA	1737	G	C5-C6-N1	5.30	114.15	111.50
53	BA	2159	G	C5'-C4'-O4'	5.30	115.46	109.10
53	BA	2318	G	C5-C6-N1	5.30	114.15	111.50
53	BA	2362	C	N1-C2-O2	5.30	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2599	G	N1-C6-O6	-5.30	116.72	119.90
53	BA	2634	A	C6-C5-N7	5.30	136.01	132.30
53	BA	2777	G	O4'-C1'-N9	5.30	112.44	108.20
53	BA	1350	C	N1-C2-O2	5.29	122.08	118.90
53	BA	1832	C	N1-C2-O2	5.29	122.08	118.90
53	BA	2258	C	N1-C2-O2	5.29	122.08	118.90
53	BA	2569	G	C5-C6-N1	5.29	114.15	111.50
21	AA	647	C	N1-C2-O2	5.29	122.08	118.90
37	BP	88	ARG	NE-CZ-NH1	5.29	122.95	120.30
53	BA	232	G	N1-C6-O6	-5.29	116.72	119.90
53	BA	1316	U	C5-C6-N1	-5.29	120.05	122.70
53	BA	1472	C	O4'-C1'-N1	5.29	112.44	108.20
53	BA	1682	G	N1-C6-O6	-5.29	116.72	119.90
53	BA	1773	A	C4-C5-C6	-5.29	114.35	117.00
53	BA	2300	C	N3-C2-O2	-5.29	118.19	121.90
53	BA	2428	G	N1-C6-O6	-5.29	116.72	119.90
53	BA	2567	G	N9-C4-C5	5.29	107.52	105.40
54	BB	56	G	N3-C4-C5	-5.29	125.95	128.60
11	AL	113	ARG	NE-CZ-NH2	-5.29	117.65	120.30
21	AA	174	A	C6-C5-N7	5.29	136.00	132.30
21	AA	895	G	N3-C4-C5	-5.29	125.95	128.60
53	BA	353	C	N3-C2-O2	-5.29	118.20	121.90
53	BA	1261	C	N3-C2-O2	-5.29	118.20	121.90
53	BA	1672	A	C6-C5-N7	5.29	136.00	132.30
53	BA	1922	G	C5-C6-N1	5.29	114.15	111.50
53	BA	2222	C	O4'-C1'-N1	5.29	112.43	108.20
53	BA	2366	A	C4-C5-C6	-5.29	114.35	117.00
53	BA	2463	C	N3-C4-C5	5.29	124.02	121.90
53	BA	2575	C	O4'-C1'-N1	5.29	112.43	108.20
53	BA	1897	G	N3-C4-C5	-5.29	125.95	128.60
53	BA	2494	G	N1-C6-O6	-5.29	116.73	119.90
21	AA	738	C	N3-C4-C5	5.29	124.02	121.90
21	AA	1288	A	C6-C5-N7	5.29	136.00	132.30
53	BA	25	U	C3'-C2'-C1'	5.29	105.73	101.50
53	BA	601	C	O4'-C1'-N1	5.29	112.43	108.20
53	BA	1073	A	O4'-C1'-N9	5.29	112.43	108.20
53	BA	2331	G	N3-C4-C5	-5.29	125.95	128.60
21	AA	1071	C	N3-C2-O2	-5.29	118.20	121.90
21	AA	231	U	O4'-C1'-N1	5.29	112.43	108.20
21	AA	922	G	N3-C4-C5	-5.29	125.96	128.60
53	BA	233	A	C5-C6-N1	5.29	120.34	117.70
53	BA	441	U	N3-C2-O2	-5.29	118.50	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	713	G	O4'-C1'-N9	5.29	112.43	108.20
53	BA	1095	A	C6-C5-N7	5.29	136.00	132.30
53	BA	1118	C	N1-C2-O2	5.29	122.07	118.90
53	BA	1311	G	O4'-C1'-N9	5.29	112.43	108.20
53	BA	2497	A	O4'-C1'-N9	5.29	112.43	108.20
14	AO	63	ARG	NE-CZ-NH1	5.28	122.94	120.30
21	AA	513	C	N3-C2-O2	-5.28	118.20	121.90
21	AA	735	C	C4'-C3'-C2'	-5.28	97.32	102.60
53	BA	91	A	C4-C5-C6	-5.28	114.36	117.00
53	BA	268	C	N3-C4-N4	-5.28	114.30	118.00
53	BA	1083	U	C4-C5-C6	5.28	122.87	119.70
53	BA	1329	U	N1-C2-N3	5.28	118.07	114.90
53	BA	1533	C	N3-C2-O2	-5.28	118.20	121.90
53	BA	2033	A	C1'-O4'-C4'	-5.28	105.67	109.90
21	AA	252	U	N3-C2-O2	-5.28	118.50	122.20
21	AA	370	C	N1-C2-O2	5.28	122.07	118.90
21	AA	1532	U	N3-C2-O2	-5.28	118.50	122.20
53	BA	1614	A	C4-C5-C6	-5.28	114.36	117.00
53	BA	1816	C	N3-C2-O2	-5.28	118.20	121.90
21	AA	183	C	C6-N1-C2	-5.28	118.19	120.30
21	AA	532	A	O4'-C1'-N9	5.28	112.42	108.20
21	AA	904	U	O4'-C1'-N1	5.28	112.42	108.20
21	AA	1520	C	O4'-C1'-N1	5.28	112.42	108.20
53	BA	666	A	C6-C5-N7	5.28	136.00	132.30
53	BA	2021	C	O4'-C1'-N1	5.28	112.42	108.20
53	BA	2261	C	N1-C2-O2	5.28	122.07	118.90
21	AA	255	G	O4'-C1'-N9	5.28	112.42	108.20
21	AA	674	G	N1-C6-O6	-5.28	116.73	119.90
21	AA	1345	U	N3-C2-O2	-5.28	118.50	122.20
53	BA	88	G	N3-C4-C5	-5.28	125.96	128.60
53	BA	1322	A	C6-C5-N7	5.28	136.00	132.30
53	BA	1460	U	O4'-C1'-N1	5.28	112.42	108.20
53	BA	1682	G	N9-C4-C5	5.28	107.51	105.40
53	BA	1898	U	N3-C2-O2	-5.28	118.50	122.20
21	AA	71	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	236	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	1437	A	C4-C5-C6	-5.28	114.36	117.00
32	BK	78	ARG	NE-CZ-NH1	5.28	122.94	120.30
53	BA	1016	G	C5-C6-N1	5.28	114.14	111.50
53	BA	2858	C	N1-C2-O2	5.28	122.07	118.90
21	AA	221	C	N3-C2-O2	-5.28	118.21	121.90
21	AA	1360	A	C6-C5-N7	5.28	135.99	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	37	C	C4'-C3'-C2'	-5.28	97.32	102.60
53	BA	55	G	N1-C6-O6	-5.28	116.73	119.90
53	BA	1003	G	N1-C6-O6	-5.28	116.73	119.90
53	BA	1484	U	N3-C2-O2	-5.28	118.51	122.20
53	BA	1905	C	N3-C4-C5	5.28	124.01	121.90
53	BA	2250	G	N9-C4-C5	5.28	107.51	105.40
53	BA	2301	C	N3-C2-O2	-5.28	118.21	121.90
53	BA	560	C	N1-C2-O2	5.27	122.06	118.90
53	BA	2645	G	C3'-C2'-C1'	5.27	105.72	101.50
21	AA	149	A	C5-C6-N1	5.27	120.34	117.70
21	AA	1011	C	N3-C2-O2	-5.27	118.21	121.90
53	BA	69	C	O4'-C1'-N1	5.27	112.42	108.20
53	BA	731	C	N3-C2-O2	-5.27	118.21	121.90
53	BA	1093	G	C5-C6-N1	5.27	114.14	111.50
53	BA	1236	G	N3-C2-N2	-5.27	116.21	119.90
53	BA	1564	C	N1-C2-O2	5.27	122.06	118.90
53	BA	2014	A	C4-C5-C6	-5.27	114.36	117.00
53	BA	2445	G	N1-C6-O6	-5.27	116.74	119.90
20	AU	33	ARG	NE-CZ-NH1	5.27	122.94	120.30
53	BA	80	G	N1-C6-O6	-5.27	116.74	119.90
53	BA	289	G	C5-C6-N1	5.27	114.14	111.50
53	BA	2033	A	C2-N3-C4	5.27	113.24	110.60
21	AA	108	G	C5-C6-N1	5.27	114.13	111.50
21	AA	229	U	O4'-C1'-N1	5.27	112.42	108.20
21	AA	1336	C	N3-C4-C5	5.27	124.01	121.90
21	AA	1377	A	C2-N3-C4	5.27	113.23	110.60
53	BA	314	C	C6-N1-C2	-5.27	118.19	120.30
53	BA	486	C	N3-C2-O2	-5.27	118.21	121.90
53	BA	2282	G	C5-C6-N1	5.27	114.14	111.50
53	BA	2767	C	N3-C4-C5	5.27	124.01	121.90
53	BA	2778	A	O4'-C1'-N9	5.27	112.42	108.20
54	BB	114	C	N1-C2-O2	5.27	122.06	118.90
21	AA	1205	U	C5-C6-N1	-5.27	120.07	122.70
34	BM	51	ARG	NE-CZ-NH1	5.27	122.93	120.30
53	BA	178	G	C5-C6-N1	5.27	114.13	111.50
53	BA	439	A	C4-C5-C6	-5.27	114.37	117.00
53	BA	861	A	C6-C5-N7	5.27	135.99	132.30
53	BA	2206	C	O4'-C1'-N1	5.27	112.42	108.20
21	AA	559	A	C4-C5-C6	-5.27	114.37	117.00
21	AA	335	C	N1-C2-O2	5.26	122.06	118.90
52	B4	19	ARG	NE-CZ-NH2	-5.26	117.67	120.30
53	BA	996	A	C5'-C4'-C3'	-5.26	107.58	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1504	A	C4-C5-C6	-5.26	114.37	117.00
53	BA	2590	A	C6-C5-N7	5.26	135.99	132.30
53	BA	2658	C	C5'-C4'-O4'	5.26	115.42	109.10
53	BA	2740	A	C4-C5-C6	-5.26	114.37	117.00
54	BB	74	U	O4'-C1'-N1	5.26	112.41	108.20
21	AA	55	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	637	C	N3-C4-C5	5.26	124.00	121.90
21	AA	1363	A	C4-C5-C6	-5.26	114.37	117.00
53	BA	1421	G	C5-C6-N1	5.26	114.13	111.50
53	BA	1902	C	N3-C2-O2	-5.26	118.22	121.90
53	BA	2272	U	N3-C2-O2	-5.26	118.52	122.20
21	AA	603	U	N3-C2-O2	-5.26	118.52	122.20
21	AA	944	G	O4'-C1'-N9	5.26	112.41	108.20
53	BA	1294	U	C4'-C3'-C2'	-5.26	97.34	102.60
53	BA	1416	G	C5-C6-N1	5.26	114.13	111.50
53	BA	1592	C	O4'-C1'-N1	5.26	112.41	108.20
53	BA	1669	A	C2-N3-C4	5.26	113.23	110.60
53	BA	2033	A	C5'-C4'-O4'	5.26	115.41	109.10
21	AA	556	C	N3-C4-C5	5.26	124.00	121.90
21	AA	771	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	1497	G	O4'-C1'-N9	5.26	112.41	108.20
53	BA	63	A	C6-C5-N7	5.26	135.98	132.30
53	BA	1116	G	C8-N9-C4	-5.26	104.30	106.40
21	AA	218	U	O4'-C1'-N1	5.26	112.41	108.20
53	BA	242	G	N3-C4-C5	-5.26	125.97	128.60
53	BA	592	A	C6-C5-N7	5.26	135.98	132.30
53	BA	1507	C	O4'-C1'-N1	5.26	112.41	108.20
53	BA	2797	U	C5-C6-N1	-5.26	120.07	122.70
21	AA	372	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	737	C	O4'-C1'-N1	5.26	112.41	108.20
21	AA	782	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	1379	G	N3-C4-C5	-5.26	125.97	128.60
22	A1	39	G	C8-N9-C4	-5.26	104.30	106.40
53	BA	2593	U	C5-C6-N1	-5.26	120.07	122.70
54	BB	11	C	N3-C4-C5	5.26	124.00	121.90
21	AA	886	G	N9-C4-C5	5.25	107.50	105.40
22	A1	66	A	C4-C5-C6	-5.25	114.37	117.00
53	BA	419	U	N3-C2-O2	-5.25	118.52	122.20
53	BA	528	A	C4-C5-C6	-5.25	114.37	117.00
53	BA	614	A	N9-C1'-C2'	-5.25	106.22	112.00
53	BA	2489	U	N3-C2-O2	-5.25	118.52	122.20
21	AA	697	U	C4-C5-C6	5.25	122.85	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	776	G	N3-C2-N2	-5.25	116.22	119.90
53	BA	785	G	N3-C4-C5	-5.25	125.97	128.60
53	BA	930	G	N1-C6-O6	-5.25	116.75	119.90
53	BA	1081	U	O4'-C1'-N1	5.25	112.40	108.20
53	BA	1933	G	C5-C6-N1	5.25	114.13	111.50
53	BA	2378	A	O4'-C1'-N9	5.25	112.40	108.20
53	BA	2817	U	C5-C6-N1	-5.25	120.07	122.70
21	AA	36	C	N3-C4-C5	5.25	124.00	121.90
21	AA	373	A	C4-C5-C6	-5.25	114.37	117.00
21	AA	1158	C	N3-C4-N4	-5.25	114.32	118.00
53	BA	379	G	O4'-C1'-N9	5.25	112.40	108.20
53	BA	424	G	C5'-C4'-O4'	5.25	115.40	109.10
53	BA	486	C	O4'-C1'-N1	5.25	112.40	108.20
53	BA	914	G	O4'-C1'-N9	5.25	112.40	108.20
53	BA	917	A	C5-C6-N1	5.25	120.33	117.70
28	BG	169	ARG	NE-CZ-NH2	5.25	122.92	120.30
53	BA	1224	U	O4'-C1'-N1	5.25	112.40	108.20
21	AA	911	U	N3-C2-O2	-5.25	118.53	122.20
21	AA	1147	C	O4'-C1'-N1	5.25	112.40	108.20
53	BA	243	U	O4'-C1'-N1	5.25	112.40	108.20
53	BA	539	G	N3-C4-C5	-5.25	125.98	128.60
53	BA	898	C	N3-C4-C5	5.25	124.00	121.90
53	BA	1104	C	N1-C2-O2	5.25	122.05	118.90
53	BA	1197	G	O4'-C1'-N9	5.25	112.40	108.20
53	BA	1797	G	N7-C8-N9	5.25	115.72	113.10
53	BA	2094	A	C4-C5-C6	-5.25	114.38	117.00
53	BA	2103	C	N3-C2-O2	-5.25	118.23	121.90
53	BA	2403	C	C4'-C3'-C2'	-5.25	97.35	102.60
54	BB	66	A	O4'-C1'-N9	5.25	112.40	108.20
21	AA	83	C	N3-C4-C5	5.25	124.00	121.90
21	AA	512	U	C5'-C4'-O4'	5.25	115.40	109.10
21	AA	1045	C	O4'-C1'-N1	5.25	112.40	108.20
53	BA	316	C	O4'-C1'-N1	5.25	112.40	108.20
53	BA	424	G	N1-C6-O6	-5.25	116.75	119.90
53	BA	457	A	C4-C5-C6	-5.25	114.38	117.00
53	BA	1400	U	C5-C6-N1	-5.25	120.08	122.70
53	BA	2424	C	N1-C2-O2	5.25	122.05	118.90
24	BC	86	ARG	CD-NE-CZ	5.25	130.94	123.60
53	BA	1204	A	C4-C5-C6	-5.25	114.38	117.00
53	BA	1778	U	N3-C2-O2	-5.25	118.53	122.20
53	BA	2784	U	O4'-C1'-N1	5.25	112.40	108.20
21	AA	595	A	C5-C6-N1	5.24	120.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	269	C	N1-C2-O2	5.24	122.05	118.90
53	BA	694	U	N3-C2-O2	-5.24	118.53	122.20
53	BA	1034	G	N1-C6-O6	-5.24	116.75	119.90
53	BA	1637	A	C4-C5-C6	-5.24	114.38	117.00
53	BA	1820	U	N3-C2-O2	-5.24	118.53	122.20
53	BA	2723	C	N1-C2-O2	5.24	122.05	118.90
53	BA	2853	C	C2-N3-C4	-5.24	117.28	119.90
21	AA	1400	C	N1-C2-O2	5.24	122.05	118.90
53	BA	382	A	N1-C6-N6	-5.24	115.45	118.60
53	BA	1905	C	N1-C2-O2	5.24	122.05	118.90
21	AA	89	U	N1-C2-N3	5.24	118.05	114.90
21	AA	376	G	C5-C6-N1	5.24	114.12	111.50
21	AA	1235	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	1344	C	N1-C2-O2	5.24	122.04	118.90
38	BQ	63	ARG	NE-CZ-NH1	5.24	122.92	120.30
50	B2	28	ARG	NH1-CZ-NH2	-5.24	113.64	119.40
53	BA	268	C	N3-C4-C5	5.24	124.00	121.90
53	BA	1840	G	N7-C8-N9	5.24	115.72	113.10
21	AA	571	U	C5-C6-N1	-5.24	120.08	122.70
21	AA	769	G	C8-N9-C4	-5.24	104.31	106.40
53	BA	516	C	O4'-C1'-N1	5.24	112.39	108.20
53	BA	980	A	C4-C5-C6	-5.24	114.38	117.00
53	BA	1795	C	N3-C4-C5	5.24	124.00	121.90
53	BA	2473	U	N3-C2-O2	-5.24	118.53	122.20
54	BB	17	C	O4'-C1'-N1	5.24	112.39	108.20
54	BB	32	U	N3-C2-O2	-5.24	118.53	122.20
3	AD	134	TYR	CB-CG-CD2	-5.24	117.86	121.00
21	AA	82	G	C5-C6-N1	5.24	114.12	111.50
53	BA	379	G	N9-C4-C5	5.24	107.50	105.40
53	BA	900	A	C4'-C3'-C2'	-5.24	97.36	102.60
53	BA	1067	A	C4-C5-C6	-5.24	114.38	117.00
53	BA	1655	A	N1-C6-N6	-5.24	115.46	118.60
53	BA	2155	U	C5-C6-N1	-5.24	120.08	122.70
53	BA	2627	G	C5-C6-N1	5.24	114.12	111.50
21	AA	1263	C	N3-C4-C5	5.24	124.00	121.90
21	AA	1506	U	O4'-C1'-N1	5.24	112.39	108.20
44	BW	24	ARG	NE-CZ-NH2	5.24	122.92	120.30
53	BA	1	G	N1-C6-O6	-5.24	116.76	119.90
53	BA	407	G	C5-C6-N1	5.24	114.12	111.50
53	BA	428	A	N1-C6-N6	-5.24	115.46	118.60
53	BA	1126	A	P-O3'-C3'	5.24	125.98	119.70
53	BA	1129	A	C6-C5-N7	5.24	135.97	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1158	C	C4'-C3'-C2'	-5.24	97.36	102.60
53	BA	1251	C	N3-C2-O2	-5.24	118.23	121.90
53	BA	1660	G	N3-C4-C5	-5.24	125.98	128.60
53	BA	1666	G	N9-C4-C5	5.24	107.49	105.40
53	BA	1799	G	N7-C8-N9	5.24	115.72	113.10
53	BA	91	A	O4'-C1'-N9	5.23	112.39	108.20
53	BA	435	C	C2-N3-C4	-5.23	117.28	119.90
53	BA	1443	U	O4'-C1'-N1	5.23	112.39	108.20
53	BA	1469	A	C2-N3-C4	5.23	113.22	110.60
53	BA	1859	U	O4'-C1'-N1	5.23	112.39	108.20
53	BA	1960	A	O4'-C1'-N9	5.23	112.39	108.20
53	BA	2617	U	C4'-C3'-C2'	-5.23	97.37	102.60
53	BA	2674	G	N3-C4-C5	-5.23	125.98	128.60
21	AA	1197	A	C5-C6-N1	5.23	120.32	117.70
53	BA	228	C	N1-C2-O2	5.23	122.04	118.90
53	BA	1302	A	C4-C5-C6	-5.23	114.38	117.00
53	BA	1454	C	O4'-C1'-N1	5.23	112.39	108.20
53	BA	1676	A	O4'-C1'-N9	5.23	112.39	108.20
53	BA	2149	U	O4'-C1'-N1	5.23	112.39	108.20
21	AA	550	G	C5-C6-N1	5.23	114.12	111.50
21	AA	1090	U	N3-C2-O2	-5.23	118.54	122.20
53	BA	138	U	O4'-C1'-N1	5.23	112.38	108.20
53	BA	195	A	C5'-C4'-O4'	5.23	115.38	109.10
53	BA	459	U	C5-C6-N1	-5.23	120.08	122.70
53	BA	1236	G	C8-N9-C4	-5.23	104.31	106.40
53	BA	2047	C	N1-C2-O2	5.23	122.04	118.90
53	BA	2172	U	C5-C6-N1	-5.23	120.08	122.70
54	BB	77	U	O4'-C1'-N1	5.23	112.39	108.20
21	AA	699	C	N3-C4-C5	5.23	123.99	121.90
21	AA	1360	A	C4'-C3'-C2'	-5.23	97.37	102.60
53	BA	325	G	O4'-C1'-N9	5.23	112.38	108.20
53	BA	616	A	O4'-C1'-N9	5.23	112.38	108.20
53	BA	966	G	C5-C6-N1	5.23	114.11	111.50
53	BA	1403	A	C4-C5-C6	-5.23	114.39	117.00
53	BA	1804	C	N3-C2-O2	-5.23	118.24	121.90
53	BA	2472	G	N3-C4-C5	-5.23	125.98	128.60
21	AA	466	A	O4'-C1'-N9	5.23	112.38	108.20
21	AA	1436	U	O4'-C1'-N1	5.23	112.38	108.20
53	BA	855	G	C5-C6-N1	5.23	114.11	111.50
53	BA	871	U	C5-C6-N1	-5.23	120.09	122.70
53	BA	1995	U	O4'-C1'-N1	5.23	112.38	108.20
53	BA	2072	C	N3-C4-C5	5.23	123.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	302	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	1407	C	O4'-C1'-N1	5.23	112.38	108.20
53	BA	944	C	C1'-O4'-C4'	-5.23	105.72	109.90
53	BA	1612	C	N1-C2-O2	5.23	122.03	118.90
53	BA	1808	A	C4-C5-C6	-5.23	114.39	117.00
53	BA	2682	A	C6-C5-N7	5.23	135.96	132.30
21	AA	381	C	N3-C4-C5	5.22	123.99	121.90
21	AA	930	C	O4'-C1'-N1	5.22	112.38	108.20
53	BA	98	G	N3-C4-C5	-5.22	125.99	128.60
53	BA	395	U	N3-C2-O2	-5.22	118.54	122.20
53	BA	442	G	C5-C6-N1	5.22	114.11	111.50
53	BA	783	A	C5-C6-N1	5.22	120.31	117.70
53	BA	1315	C	N3-C4-C5	5.22	123.99	121.90
53	BA	1791	A	C6-C5-N7	5.22	135.96	132.30
53	BA	2438	U	C5-C6-N1	-5.22	120.09	122.70
53	BA	2510	C	O4'-C1'-N1	5.22	112.38	108.20
53	BA	2843	G	O4'-C1'-N9	5.22	112.38	108.20
21	AA	217	C	O4'-C1'-N1	5.22	112.38	108.20
53	BA	355	U	O4'-C1'-N1	5.22	112.38	108.20
53	BA	1844	C	N1-C2-O2	5.22	122.03	118.90
53	BA	2447	G	N3-C4-C5	-5.22	125.99	128.60
53	BA	2551	C	C6-N1-C2	-5.22	118.21	120.30
53	BA	2785	C	O4'-C1'-N1	5.22	112.38	108.20
21	AA	206	C	N3-C4-C5	5.22	123.99	121.90
53	BA	2812	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	73	C	N1-C2-O2	5.22	122.03	118.90
21	AA	494	G	C5-C6-N1	5.22	114.11	111.50
21	AA	722	G	N3-C4-C5	-5.22	125.99	128.60
21	AA	858	G	C8-N9-C4	-5.22	104.31	106.40
21	AA	1200	C	N1-C2-O2	5.22	122.03	118.90
53	BA	837	C	N3-C2-O2	-5.22	118.25	121.90
53	BA	1332	G	N7-C8-N9	5.22	115.71	113.10
53	BA	2069	G	N3-C2-N2	-5.22	116.25	119.90
53	BA	1798	U	O4'-C1'-N1	5.22	112.37	108.20
53	BA	2567	G	N3-C2-N2	-5.22	116.25	119.90
53	BA	2859	G	N1-C6-O6	-5.22	116.77	119.90
53	BA	1839	G	C5-C6-N1	5.22	114.11	111.50
53	BA	1864	U	O4'-C1'-N1	5.22	112.37	108.20
53	BA	1868	C	C5'-C4'-O4'	5.22	115.36	109.10
53	BA	2227	A	C4'-C3'-C2'	-5.22	97.38	102.60
21	AA	298	A	C6-C5-N7	5.21	135.95	132.30
53	BA	939	G	N3-C4-C5	-5.21	125.99	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1640	A	C2-N3-C4	5.21	113.21	110.60
53	BA	2286	G	C5-C6-N1	5.21	114.11	111.50
21	AA	938	A	C4-C5-C6	-5.21	114.39	117.00
21	AA	199	A	C6-C5-N7	5.21	135.95	132.30
21	AA	1324	A	C5-C6-N1	5.21	120.31	117.70
53	BA	713	G	N9-C4-C5	5.21	107.48	105.40
53	BA	2524	G	N7-C8-N9	5.21	115.71	113.10
53	BA	2633	G	C5-C6-N1	5.21	114.11	111.50
21	AA	280	C	N3-C2-O2	-5.21	118.25	121.90
53	BA	1203	U	N3-C2-O2	-5.21	118.55	122.20
21	AA	570	G	C8-N9-C4	-5.21	104.32	106.40
21	AA	629	A	C4-C5-C6	-5.21	114.40	117.00
21	AA	1069	C	O4'-C1'-N1	5.21	112.37	108.20
21	AA	1500	A	C6-C5-N7	5.21	135.95	132.30
25	BD	59	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
53	BA	221	A	C4-C5-C6	-5.21	114.40	117.00
53	BA	1783	A	C5-C6-N1	5.21	120.31	117.70
53	BA	2752	C	N3-C2-O2	-5.21	118.25	121.90
21	AA	867	G	C4'-C3'-C2'	-5.21	97.39	102.60
21	AA	919	A	C4-C5-C6	-5.21	114.40	117.00
53	BA	104	A	C4'-C3'-C2'	-5.21	97.39	102.60
53	BA	595	C	N3-C2-O2	-5.21	118.26	121.90
53	BA	740	C	C5'-C4'-O4'	5.21	115.35	109.10
39	BR	84	ARG	NE-CZ-NH1	5.21	122.90	120.30
53	BA	590	A	C4-C5-C6	-5.21	114.40	117.00
21	AA	10	A	O4'-C1'-N9	5.20	112.36	108.20
21	AA	153	C	N3-C2-O2	-5.20	118.26	121.90
21	AA	175	C	N1-C2-O2	5.20	122.02	118.90
21	AA	472	U	O4'-C1'-N1	5.20	112.36	108.20
21	AA	521	G	N3-C2-N2	-5.20	116.26	119.90
21	AA	781	A	C5-C6-N1	5.20	120.30	117.70
53	BA	315	G	N1-C6-O6	-5.20	116.78	119.90
53	BA	713	G	N3-C2-N2	-5.20	116.26	119.90
53	BA	1069	A	C8-N9-C4	-5.20	103.72	105.80
53	BA	1658	C	N3-C2-O2	-5.20	118.26	121.90
53	BA	2167	U	O4'-C1'-N1	5.20	112.36	108.20
53	BA	2207	C	N3-C2-O2	-5.20	118.26	121.90
53	BA	2326	C	N1-C2-O2	5.20	122.02	118.90
53	BA	2600	A	C6-C5-N7	5.20	135.94	132.30
53	BA	2870	C	O4'-C1'-N1	5.20	112.36	108.20
54	BB	42	C	N1-C2-O2	5.20	122.02	118.90
17	AR	42	ARG	NE-CZ-NH1	5.20	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	562	U	C5-C6-N1	-5.20	120.10	122.70
53	BA	1688	U	N1-C2-N3	5.20	118.02	114.90
21	AA	646	G	C8-N9-C4	-5.20	104.32	106.40
21	AA	697	U	N1-C2-N3	5.20	118.02	114.90
21	AA	956	U	C5-C6-N1	-5.20	120.10	122.70
21	AA	1416	G	N9-C4-C5	5.20	107.48	105.40
31	BJ	116	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
53	BA	11	C	N3-C2-O2	-5.20	118.26	121.90
53	BA	519	U	C5-C6-N1	-5.20	120.10	122.70
53	BA	801	G	O4'-C4'-C3'	5.20	110.26	106.10
53	BA	1289	C	C6-N1-C2	-5.20	118.22	120.30
53	BA	1453	A	C6-C5-N7	5.20	135.94	132.30
53	BA	2155	U	N3-C2-O2	-5.20	118.56	122.20
54	BB	44	G	N1-C6-O6	-5.20	116.78	119.90
21	AA	60	A	C5-C6-N1	5.20	120.30	117.70
21	AA	108	G	N3-C4-C5	-5.20	126.00	128.60
53	BA	78	U	C4-C5-C6	5.20	122.82	119.70
53	BA	654	A	C4-C5-C6	-5.20	114.40	117.00
53	BA	695	G	C5-C6-N1	5.20	114.10	111.50
53	BA	1660	G	C5'-C4'-C3'	-5.20	107.68	116.00
53	BA	1825	U	C5-C6-N1	-5.20	120.10	122.70
53	BA	2045	C	O4'-C1'-N1	5.20	112.36	108.20
53	BA	2090	A	C5-C6-N1	5.20	120.30	117.70
53	BA	2718	G	C8-N9-C4	-5.20	104.32	106.40
21	AA	715	A	C4-C5-C6	-5.20	114.40	117.00
53	BA	375	G	N1-C6-O6	-5.20	116.78	119.90
53	BA	2203	U	N1-C2-N3	5.20	118.02	114.90
21	AA	549	C	N3-C4-C5	5.20	123.98	121.90
21	AA	549	C	O4'-C1'-N1	5.20	112.36	108.20
53	BA	70	G	N3-C4-C5	-5.20	126.00	128.60
53	BA	262	A	C4-C5-C6	-5.20	114.40	117.00
53	BA	1091	G	C8-N9-C4	-5.20	104.32	106.40
53	BA	1556	C	O4'-C1'-N1	5.20	112.36	108.20
53	BA	1992	G	N3-C4-C5	-5.20	126.00	128.60
53	BA	2305	U	N3-C2-O2	-5.20	118.56	122.20
53	BA	2840	C	O4'-C1'-N1	5.20	112.36	108.20
21	AA	1281	C	C2-N3-C4	-5.19	117.30	119.90
53	BA	426	C	N3-C4-C5	5.19	123.98	121.90
53	BA	1638	C	C4'-C3'-C2'	-5.19	97.41	102.60
53	BA	1842	G	N1-C6-O6	-5.19	116.78	119.90
21	AA	350	G	N9-C4-C5	5.19	107.48	105.40
21	AA	1396	A	C6-C5-N7	5.19	135.94	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	800	A	C6-C5-N7	5.19	135.94	132.30
53	BA	1500	G	N3-C4-C5	-5.19	126.00	128.60
53	BA	2167	U	N1-C2-N3	5.19	118.02	114.90
53	BA	2305	U	N1-C2-N3	5.19	118.02	114.90
53	BA	2817	U	N3-C2-O2	-5.19	118.57	122.20
21	AA	216	U	N1-C2-N3	5.19	118.01	114.90
21	AA	534	U	C3'-C2'-C1'	5.19	105.65	101.50
21	AA	770	C	C6-N1-C2	-5.19	118.22	120.30
53	BA	56	A	C6-C5-N7	5.19	135.93	132.30
53	BA	674	G	C5-C6-N1	5.19	114.10	111.50
53	BA	753	A	C6-C5-N7	5.19	135.93	132.30
53	BA	1328	A	C6-C5-N7	5.19	135.93	132.30
53	BA	1423	G	C8-N9-C4	-5.19	104.32	106.40
53	BA	1863	G	N1-C6-O6	-5.19	116.79	119.90
53	BA	2211	A	C6-C5-N7	5.19	135.93	132.30
53	BA	2468	A	C2-N3-C4	5.19	113.20	110.60
54	BB	107	G	N3-C4-C5	-5.19	126.00	128.60
21	AA	1200	C	N3-C4-C5	5.19	123.98	121.90
53	BA	1817	G	N3-C2-N2	-5.19	116.27	119.90
53	BA	2056	G	N3-C4-C5	-5.19	126.00	128.60
53	BA	2718	G	N1-C6-O6	-5.19	116.79	119.90
21	AA	251	G	C2-N3-C4	5.19	114.49	111.90
21	AA	654	G	N1-C6-O6	-5.19	116.79	119.90
21	AA	852	G	N3-C2-N2	-5.19	116.27	119.90
21	AA	985	C	N3-C2-O2	-5.19	118.27	121.90
21	AA	1036	A	C5-C6-N1	5.19	120.29	117.70
22	A1	74	C	N3-C4-C5	5.19	123.97	121.90
53	BA	42	A	C5-C6-N1	5.19	120.29	117.70
53	BA	188	G	N1-C6-O6	-5.19	116.79	119.90
53	BA	215	G	C5-C6-N1	5.19	114.09	111.50
53	BA	606	U	N3-C2-O2	-5.19	118.57	122.20
53	BA	767	U	N3-C2-O2	-5.19	118.57	122.20
53	BA	1010	A	C6-C5-N7	5.19	135.93	132.30
53	BA	1473	G	N9-C4-C5	5.19	107.47	105.40
53	BA	1695	G	C5-C6-N1	5.19	114.09	111.50
53	BA	2869	G	N3-C2-N2	-5.19	116.27	119.90
21	AA	562	U	C5-C6-N1	-5.18	120.11	122.70
53	BA	673	C	N1-C2-O2	5.18	122.01	118.90
53	BA	940	G	N3-C4-C5	-5.18	126.01	128.60
53	BA	948	C	N3-C2-O2	-5.18	118.27	121.90
53	BA	962	G	N3-C2-N2	-5.18	116.27	119.90
53	BA	1031	G	N1-C6-O6	-5.18	116.79	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1331	G	C8-N9-C4	-5.18	104.33	106.40
53	BA	1502	A	C6-C5-N7	5.18	135.93	132.30
53	BA	2578	G	P-O3'-C3'	5.18	125.92	119.70
21	AA	160	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	344	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	421	U	O4'-C1'-N1	5.18	112.35	108.20
53	BA	889	C	C6-N1-C2	-5.18	118.23	120.30
53	BA	1718	G	C5'-C4'-O4'	5.18	115.32	109.10
53	BA	2369	A	C6-C5-N7	5.18	135.93	132.30
53	BA	2730	C	N3-C2-O2	-5.18	118.27	121.90
54	BB	108	A	C4-C5-C6	-5.18	114.41	117.00
22	A1	48	C	N3-C4-C5	5.18	123.97	121.90
53	BA	418	C	N3-C2-O2	-5.18	118.27	121.90
21	AA	148	G	C1'-O4'-C4'	-5.18	105.76	109.90
21	AA	862	C	N1-C2-O2	5.18	122.01	118.90
53	BA	78	U	O4'-C1'-N1	5.18	112.34	108.20
53	BA	726	G	C5-C6-N1	5.18	114.09	111.50
53	BA	1192	G	N1-C6-O6	-5.18	116.79	119.90
53	BA	1825	U	N3-C2-O2	-5.18	118.57	122.20
53	BA	2117	A	C2-N3-C4	5.18	113.19	110.60
21	AA	945	G	N3-C2-N2	-5.18	116.28	119.90
53	BA	37	C	N3-C2-O2	-5.18	118.28	121.90
53	BA	718	A	C4-C5-C6	-5.18	114.41	117.00
6	AG	78	ARG	NE-CZ-NH1	5.18	122.89	120.30
21	AA	826	C	N3-C2-O2	-5.18	118.28	121.90
21	AA	939	G	N1-C6-O6	-5.18	116.79	119.90
53	BA	613	A	C2-N3-C4	5.18	113.19	110.60
53	BA	827	U	C5-C6-N1	-5.18	120.11	122.70
53	BA	2297	A	C5-C6-N1	5.18	120.29	117.70
53	BA	2840	C	N1-C2-O2	5.18	122.01	118.90
21	AA	301	G	N3-C4-C5	-5.17	126.01	128.60
53	BA	361	G	C5-C6-N1	5.17	114.09	111.50
53	BA	1784	A	O4'-C1'-N9	5.17	112.34	108.20
53	BA	2168	G	N3-C4-C5	-5.17	126.01	128.60
53	BA	2195	U	O4'-C1'-N1	5.17	112.34	108.20
53	BA	2540	C	O4'-C1'-N1	5.17	112.34	108.20
28	BG	34	ARG	NE-CZ-NH1	5.17	122.89	120.30
53	BA	1232	G	N3-C4-C5	-5.17	126.01	128.60
53	BA	1340	U	C5-C6-N1	-5.17	120.11	122.70
53	BA	1640	A	C6-C5-N7	5.17	135.92	132.30
21	AA	396	C	O4'-C1'-N1	5.17	112.34	108.20
21	AA	744	C	N3-C4-C5	5.17	123.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1172	C	N1-C2-O2	5.17	122.00	118.90
21	AA	1347	G	C5-C6-N1	5.17	114.09	111.50
21	AA	1438	G	N1-C6-O6	-5.17	116.80	119.90
32	BK	31	ARG	NE-CZ-NH1	5.17	122.89	120.30
53	BA	62	U	C5-C6-N1	-5.17	120.11	122.70
53	BA	80	G	N3-C4-C5	-5.17	126.02	128.60
53	BA	1929	G	N3-C2-N2	-5.17	116.28	119.90
53	BA	1965	C	O4'-C1'-N1	5.17	112.34	108.20
53	BA	2265	U	N1-C2-N3	5.17	118.00	114.90
53	BA	2711	A	C6-C5-N7	5.17	135.92	132.30
53	BA	673	C	C2-N3-C4	-5.17	117.31	119.90
53	BA	1189	A	C5-C6-N1	5.17	120.28	117.70
21	AA	342	C	O4'-C1'-N1	5.17	112.33	108.20
21	AA	867	G	C8-N9-C4	-5.17	104.33	106.40
53	BA	622	G	C5-C6-N1	5.17	114.08	111.50
53	BA	1003	G	C5-C6-N1	5.17	114.08	111.50
53	BA	1428	C	O4'-C1'-N1	5.17	112.33	108.20
53	BA	2287	A	C5-C6-N1	5.17	120.28	117.70
53	BA	2532	G	N3-C4-C5	-5.17	126.02	128.60
53	BA	2567	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	124	C	N3-C4-N4	-5.17	114.38	118.00
21	AA	266	G	C5-C6-N1	5.17	114.08	111.50
21	AA	1059	C	N3-C4-C5	5.17	123.97	121.90
21	AA	1185	G	N3-C4-C5	-5.17	126.02	128.60
53	BA	45	G	C5-C6-N1	5.17	114.08	111.50
53	BA	650	C	N3-C4-C5	5.17	123.97	121.90
53	BA	680	C	N1-C2-O2	5.17	122.00	118.90
53	BA	893	C	N3-C2-O2	-5.17	118.28	121.90
53	BA	1271	G	N1-C6-O6	-5.17	116.80	119.90
53	BA	1350	C	O4'-C1'-N1	5.17	112.33	108.20
53	BA	2415	G	N3-C2-N2	-5.17	116.28	119.90
21	AA	242	G	O4'-C1'-N9	5.17	112.33	108.20
21	AA	586	C	O4'-C1'-N1	5.17	112.33	108.20
29	BH	68	ARG	NE-CZ-NH1	5.17	122.88	120.30
53	BA	2137	U	O4'-C1'-C2'	-5.17	100.64	105.80
53	BA	2261	C	N3-C4-C5	5.17	123.97	121.90
53	BA	2607	G	C5-C6-N1	5.17	114.08	111.50
20	AU	32	ARG	NE-CZ-NH2	5.16	122.88	120.30
21	AA	535	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	820	U	N3-C2-O2	-5.16	118.59	122.20
21	AA	1299	A	C5-C6-N1	5.16	120.28	117.70
53	BA	1203	U	C5-C6-N1	-5.16	120.12	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1939	U	C4-C5-C6	5.16	122.80	119.70
53	BA	1984	G	C5-C6-N1	5.16	114.08	111.50
53	BA	2873	A	C4-C5-C6	-5.16	114.42	117.00
53	BA	2877	G	N3-C4-C5	-5.16	126.02	128.60
21	AA	63	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	1331	G	C4-C5-N7	-5.16	108.73	110.80
53	BA	810	U	N3-C2-O2	-5.16	118.59	122.20
21	AA	566	G	N3-C2-N2	-5.16	116.29	119.90
21	AA	1192	C	N3-C4-C5	5.16	123.96	121.90
21	AA	1339	A	C6-C5-N7	5.16	135.91	132.30
53	BA	583	G	N1-C6-O6	-5.16	116.80	119.90
53	BA	764	A	C4-C5-C6	-5.16	114.42	117.00
53	BA	791	C	N1-C2-O2	5.16	122.00	118.90
53	BA	1292	G	N3-C4-C5	-5.16	126.02	128.60
53	BA	1653	G	N3-C4-C5	-5.16	126.02	128.60
53	BA	2023	C	N3-C4-C5	5.16	123.97	121.90
53	BA	2465	C	N3-C2-O2	-5.16	118.29	121.90
21	AA	1365	G	C5-C6-N1	5.16	114.08	111.50
53	BA	339	U	O4'-C1'-N1	5.16	112.33	108.20
53	BA	2237	G	N3-C4-C5	-5.16	126.02	128.60
53	BA	2471	A	C4-C5-C6	-5.16	114.42	117.00
53	BA	2832	U	N3-C2-O2	-5.16	118.59	122.20
53	BA	2871	U	C5-C6-N1	-5.16	120.12	122.70
21	AA	315	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	1209	C	N3-C2-O2	-5.16	118.29	121.90
53	BA	395	U	C5-C6-N1	-5.16	120.12	122.70
53	BA	881	G	N3-C4-C5	-5.16	126.02	128.60
53	BA	2689	U	O4'-C1'-N1	5.16	112.33	108.20
2	AC	130	ARG	NE-CZ-NH2	5.16	122.88	120.30
21	AA	84	U	C5-C6-N1	-5.16	120.12	122.70
21	AA	459	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	970	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	1041	G	N1-C6-O6	-5.16	116.81	119.90
21	AA	1446	A	C1'-O4'-C4'	-5.16	105.78	109.90
53	BA	665	U	O4'-C1'-N1	5.16	112.33	108.20
53	BA	844	A	C6-C5-N7	5.16	135.91	132.30
53	BA	1150	C	N3-C2-O2	-5.16	118.29	121.90
21	AA	764	C	O4'-C1'-N1	5.15	112.32	108.20
22	A1	5	G	N1-C6-O6	-5.15	116.81	119.90
53	BA	444	C	N1-C2-O2	5.15	121.99	118.90
53	BA	723	C	O4'-C1'-N1	5.15	112.32	108.20
53	BA	2076	U	N1-C2-N3	5.15	117.99	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2145	C	N1-C2-O2	5.15	121.99	118.90
21	AA	597	G	C4-C5-N7	-5.15	108.74	110.80
21	AA	1025	U	O4'-C4'-C3'	5.15	110.22	106.10
21	AA	1290	G	C5-N7-C8	-5.15	101.72	104.30
22	A1	8	U	N1-C2-N3	5.15	117.99	114.90
53	BA	2	G	N1-C6-O6	-5.15	116.81	119.90
53	BA	117	G	N3-C4-C5	-5.15	126.02	128.60
53	BA	1773	A	C4'-C3'-C2'	-5.15	97.45	102.60
53	BA	2760	C	N1-C2-O2	5.15	121.99	118.90
53	BA	2886	A	C6-C5-N7	5.15	135.91	132.30
55	B5	164	ARG	NE-CZ-NH1	5.15	122.88	120.30
21	AA	435	A	C6-C5-N7	5.15	135.91	132.30
21	AA	610	U	N3-C2-O2	-5.15	118.59	122.20
21	AA	964	A	C4-C5-C6	-5.15	114.42	117.00
21	AA	1248	A	N1-C6-N6	-5.15	115.51	118.60
21	AA	1284	C	C6-N1-C2	-5.15	118.24	120.30
53	BA	43	G	N9-C4-C5	5.15	107.46	105.40
53	BA	1367	A	C4-C5-C6	-5.15	114.42	117.00
53	BA	1415	U	N1-C2-N3	5.15	117.99	114.90
53	BA	1867	G	O4'-C1'-N9	5.15	112.32	108.20
53	BA	2871	U	N1-C2-N3	5.15	117.99	114.90
21	AA	1108	G	N1-C6-O6	-5.15	116.81	119.90
21	AA	1411	C	N1-C2-O2	5.15	121.99	118.90
53	BA	2279	G	N1-C6-O6	-5.15	116.81	119.90
21	AA	402	G	N3-C4-C5	-5.15	126.03	128.60
21	AA	748	G	O4'-C1'-N9	5.15	112.32	108.20
21	AA	1249	C	O4'-C1'-N1	5.15	112.32	108.20
53	BA	1308	A	C6-C5-N7	5.15	135.90	132.30
53	BA	2247	A	C5-C6-N1	5.15	120.27	117.70
53	BA	89	A	C6-C5-N7	5.15	135.90	132.30
53	BA	691	C	N3-C4-C5	5.15	123.96	121.90
53	BA	1085	A	C5-C6-N1	5.15	120.27	117.70
53	BA	1108	U	C4-C5-C6	5.15	122.79	119.70
21	AA	520	A	C6-C5-N7	5.14	135.90	132.30
21	AA	1263	C	O4'-C1'-N1	5.14	112.31	108.20
23	A2	79	A	C2-N3-C4	5.14	113.17	110.60
53	BA	112	U	N3-C2-O2	-5.14	118.60	122.20
53	BA	271	G	N7-C8-N9	5.14	115.67	113.10
53	BA	334	C	O4'-C1'-N1	5.14	112.31	108.20
53	BA	895	U	N3-C2-O2	-5.14	118.60	122.20
53	BA	1178	C	N1-C2-O2	5.14	121.99	118.90
53	BA	1335	C	C6-N1-C2	-5.14	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1531	C	N1-C2-O2	5.14	121.99	118.90
53	BA	1694	C	N1-C2-O2	5.14	121.99	118.90
53	BA	2072	C	C4'-C3'-C2'	-5.14	97.46	102.60
53	BA	2204	G	C5-C6-N1	5.14	114.07	111.50
53	BA	2686	G	N3-C4-C5	-5.14	126.03	128.60
53	BA	2795	C	O4'-C1'-N1	5.14	112.32	108.20
53	BA	2813	A	O4'-C1'-N9	5.14	112.31	108.20
54	BB	34	A	O4'-C1'-N9	5.14	112.32	108.20
22	A1	42	G	C5-C6-N1	5.14	114.07	111.50
53	BA	1628	G	C5-C6-N1	5.14	114.07	111.50
53	BA	1941	C	O4'-C1'-N1	5.14	112.31	108.20
53	BA	2728	U	N3-C2-O2	-5.14	118.60	122.20
27	BF	91	ARG	NE-CZ-NH1	5.14	122.87	120.30
53	BA	1078	U	O4'-C1'-N1	5.14	112.31	108.20
21	AA	68	G	N3-C2-N2	-5.14	116.30	119.90
21	AA	95	C	N1-C2-O2	5.14	121.98	118.90
21	AA	98	A	O4'-C1'-N9	5.14	112.31	108.20
21	AA	266	G	N3-C4-C5	-5.14	126.03	128.60
21	AA	639	G	N7-C8-N9	5.14	115.67	113.10
21	AA	1498	U	C5-C6-N1	-5.14	120.13	122.70
53	BA	45	G	P-O3'-C3'	5.14	125.87	119.70
53	BA	785	G	N1-C6-O6	-5.14	116.82	119.90
53	BA	1190	G	N3-C4-C5	-5.14	126.03	128.60
53	BA	1554	U	N3-C2-O2	-5.14	118.60	122.20
53	BA	1697	G	N3-C4-C5	-5.14	126.03	128.60
53	BA	1772	A	C4'-C3'-C2'	-5.14	97.46	102.60
53	BA	2065	C	N3-C4-C5	5.14	123.96	121.90
53	BA	2085	U	N1-C2-N3	5.14	117.98	114.90
53	BA	2278	A	C6-C5-N7	5.14	135.90	132.30
53	BA	2576	G	C5-C6-N1	5.14	114.07	111.50
53	BA	2853	C	N3-C4-C5	5.14	123.96	121.90
54	BB	95	U	N3-C2-O2	-5.14	118.60	122.20
21	AA	1260	G	N3-C4-C5	-5.14	126.03	128.60
53	BA	1638	C	O4'-C1'-N1	5.14	112.31	108.20
53	BA	2520	C	N3-C2-O2	-5.14	118.30	121.90
21	AA	69	G	N3-C4-C5	-5.14	126.03	128.60
21	AA	365	U	N3-C2-O2	-5.14	118.61	122.20
21	AA	971	G	C5-C6-N1	5.14	114.07	111.50
21	AA	1395	C	N1-C2-O2	5.14	121.98	118.90
53	BA	430	A	C4-C5-C6	-5.14	114.43	117.00
53	BA	491	G	N3-C4-C5	-5.14	126.03	128.60
53	BA	1401	G	N3-C2-N2	-5.14	116.30	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2189	U	C5-C6-N1	-5.14	120.13	122.70
53	BA	2291	U	N1-C2-N3	5.14	117.98	114.90
21	AA	10	A	C6-C5-N7	5.13	135.89	132.30
21	AA	1462	C	O4'-C1'-N1	5.13	112.31	108.20
53	BA	222	A	C4-C5-C6	-5.13	114.43	117.00
53	BA	527	C	O4'-C1'-N1	5.13	112.31	108.20
53	BA	1138	G	C5-C6-N1	5.13	114.07	111.50
53	BA	1540	G	C8-N9-C4	-5.13	104.35	106.40
53	BA	2317	A	O4'-C1'-N9	5.13	112.31	108.20
53	BA	2429	G	N7-C8-N9	5.13	115.67	113.10
53	BA	762	U	C5-C6-N1	-5.13	120.13	122.70
53	BA	788	A	C4-C5-C6	-5.13	114.43	117.00
53	BA	2347	C	N1-C2-O2	5.13	121.98	118.90
21	AA	102	G	N3-C4-C5	-5.13	126.03	128.60
21	AA	130	A	C6-C5-N7	5.13	135.89	132.30
21	AA	1173	U	O4'-C1'-N1	5.13	112.31	108.20
21	AA	1266	G	C8-N9-C4	-5.13	104.35	106.40
53	BA	283	G	O4'-C1'-N9	5.13	112.31	108.20
53	BA	1117	C	N1-C2-O2	5.13	121.98	118.90
53	BA	1310	G	C4'-C3'-C2'	-5.13	97.47	102.60
53	BA	1769	U	C5-C6-N1	-5.13	120.13	122.70
53	BA	1972	G	C5-C6-N1	5.13	114.07	111.50
54	BB	28	C	N1-C2-O2	5.13	121.98	118.90
21	AA	545	C	N3-C4-C5	5.13	123.95	121.90
21	AA	977	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	1401	G	N3-C4-C5	-5.13	126.03	128.60
53	BA	150	U	C4'-C3'-C2'	-5.13	97.47	102.60
53	BA	192	C	N3-C4-C5	5.13	123.95	121.90
53	BA	217	A	C4-C5-C6	-5.13	114.44	117.00
53	BA	1189	A	C4-C5-C6	-5.13	114.44	117.00
54	BB	28	C	C2-N3-C4	-5.13	117.33	119.90
21	AA	907	A	C4-C5-C6	-5.13	114.44	117.00
22	A1	13	C	C4'-C3'-C2'	-5.13	97.47	102.60
53	BA	137	U	N3-C2-O2	-5.13	118.61	122.20
53	BA	1405	U	N1-C2-N3	5.13	117.98	114.90
53	BA	1898	U	O4'-C1'-N1	5.13	112.30	108.20
21	AA	213	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	374	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	794	A	C6-C5-N7	5.13	135.89	132.30
21	AA	1160	G	C8-N9-C4	-5.13	104.35	106.40
21	AA	1356	G	C8-N9-C4	-5.13	104.35	106.40
53	BA	370	G	C8-N9-C4	-5.13	104.35	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	968	C	N1-C2-O2	5.13	121.98	118.90
53	BA	1356	G	O4'-C1'-N9	5.13	112.30	108.20
53	BA	1501	G	N1-C6-O6	-5.13	116.82	119.90
53	BA	2185	U	O4'-C1'-N1	5.13	112.30	108.20
54	BB	63	C	O4'-C1'-N1	5.13	112.30	108.20
22	A1	22	G	O4'-C1'-N9	5.12	112.30	108.20
43	BV	19	ARG	NE-CZ-NH2	5.12	122.86	120.30
53	BA	197	A	C6-C5-N7	5.12	135.89	132.30
53	BA	800	A	C5-C6-N6	5.12	127.80	123.70
53	BA	1320	C	N1-C2-O2	5.12	121.97	118.90
53	BA	2267	A	C4-C5-C6	-5.12	114.44	117.00
53	BA	2509	G	C5'-C4'-O4'	5.12	115.25	109.10
53	BA	2703	C	N3-C2-O2	-5.12	118.31	121.90
53	BA	2845	U	N3-C2-O2	-5.12	118.61	122.20
21	AA	262	A	N1-C2-N3	-5.12	126.74	129.30
21	AA	603	U	O4'-C1'-N1	5.12	112.30	108.20
21	AA	1124	G	N1-C6-O6	-5.12	116.83	119.90
53	BA	133	U	C5-C6-N1	-5.12	120.14	122.70
53	BA	1443	U	N3-C2-O2	-5.12	118.61	122.20
53	BA	1668	A	C4-C5-C6	-5.12	114.44	117.00
53	BA	1939	U	C5-C6-N1	-5.12	120.14	122.70
53	BA	2231	U	O4'-C1'-N1	5.12	112.30	108.20
53	BA	2333	A	C3'-C2'-C1'	5.12	105.60	101.50
53	BA	2665	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	728	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	856	C	N1-C2-O2	5.12	121.97	118.90
21	AA	1303	C	N1-C2-O2	5.12	121.97	118.90
53	BA	349	U	N3-C2-O2	-5.12	118.61	122.20
53	BA	1584	U	C4-C5-C6	5.12	122.77	119.70
53	BA	2086	U	C4-C5-C6	5.12	122.77	119.70
53	BA	2469	A	C6-C5-N7	5.12	135.88	132.30
53	BA	2687	U	N3-C2-O2	-5.12	118.61	122.20
21	AA	669	G	C5-C6-N1	5.12	114.06	111.50
53	BA	825	A	C6-C5-N7	5.12	135.88	132.30
21	AA	423	G	O4'-C1'-N9	5.12	112.30	108.20
21	AA	829	G	O4'-C1'-N9	5.12	112.30	108.20
21	AA	887	G	C5-C6-N1	5.12	114.06	111.50
21	AA	969	A	C6-C5-N7	5.12	135.88	132.30
21	AA	988	G	O4'-C1'-N9	5.12	112.29	108.20
21	AA	1191	A	C5'-C4'-O4'	5.12	115.24	109.10
53	BA	1319	C	C6-N1-C2	-5.12	118.25	120.30
53	BA	1448	G	O4'-C1'-N9	5.12	112.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2122	U	O4'-C1'-N1	5.12	112.30	108.20
53	BA	2411	A	C4-C5-C6	-5.12	114.44	117.00
53	BA	2864	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	69	G	N9-C4-C5	5.12	107.45	105.40
21	AA	406	G	C5-C6-N1	5.12	114.06	111.50
53	BA	2509	G	C8-N9-C4	-5.12	104.35	106.40
21	AA	679	C	O4'-C1'-N1	5.12	112.29	108.20
21	AA	849	G	N9-C4-C5	5.12	107.45	105.40
21	AA	1117	A	C5'-C4'-O4'	5.12	115.24	109.10
21	AA	1338	G	N9-C4-C5	5.12	107.45	105.40
53	BA	458	G	N3-C4-C5	-5.12	126.04	128.60
53	BA	2323	G	N3-C4-C5	-5.12	126.04	128.60
21	AA	835	U	N1-C2-N3	5.11	117.97	114.90
21	AA	1157	A	C6-C5-N7	5.11	135.88	132.30
21	AA	1340	A	C6-C5-N7	5.11	135.88	132.30
53	BA	813	U	O4'-C1'-N1	5.11	112.29	108.20
53	BA	1200	C	N3-C2-O2	-5.11	118.32	121.90
53	BA	1561	C	N1-C2-O2	5.11	121.97	118.90
53	BA	2583	G	N3-C2-N2	-5.11	116.32	119.90
53	BA	84	A	O4'-C1'-N9	5.11	112.29	108.20
53	BA	533	G	N3-C4-C5	-5.11	126.04	128.60
53	BA	987	C	N3-C2-O2	-5.11	118.32	121.90
53	BA	2618	G	N3-C2-N2	-5.11	116.32	119.90
21	AA	288	A	C4-C5-C6	-5.11	114.44	117.00
21	AA	319	G	N3-C4-C5	-5.11	126.05	128.60
21	AA	717	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	1404	C	O4'-C1'-N1	5.11	112.29	108.20
53	BA	461	C	N3-C2-O2	-5.11	118.32	121.90
53	BA	692	C	N1-C2-O2	5.11	121.97	118.90
53	BA	977	G	N7-C8-N9	5.11	115.66	113.10
53	BA	1542	U	C4-C5-C6	5.11	122.77	119.70
53	BA	1649	G	N1-C6-O6	-5.11	116.83	119.90
53	BA	1731	G	N7-C8-N9	5.11	115.66	113.10
53	BA	2209	G	N7-C8-N9	5.11	115.66	113.10
53	BA	2533	U	C5-C6-N1	-5.11	120.14	122.70
53	BA	2573	C	N3-C4-C5	5.11	123.94	121.90
53	BA	2719	G	N1-C6-O6	-5.11	116.83	119.90
21	AA	73	C	N3-C4-C5	5.11	123.94	121.90
21	AA	575	G	C8-N9-C4	-5.11	104.36	106.40
21	AA	578	C	C4'-C3'-C2'	-5.11	97.49	102.60
53	BA	607	U	C5-C6-N1	-5.11	120.14	122.70
53	BA	913	U	N3-C2-O2	-5.11	118.62	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BB	28	C	N3-C4-C5	5.11	123.94	121.90
21	AA	66	A	C2-N3-C4	5.11	113.15	110.60
21	AA	965	U	C5-C6-N1	-5.11	120.15	122.70
53	BA	234	U	C4-C5-C6	5.11	122.76	119.70
53	BA	567	U	O4'-C1'-N1	5.11	112.29	108.20
53	BA	656	G	C5-C6-N1	5.11	114.05	111.50
53	BA	1478	G	N3-C4-C5	-5.11	126.05	128.60
53	BA	1605	C	C6-N1-C2	-5.11	118.26	120.30
53	BA	1685	C	N1-C2-O2	5.11	121.97	118.90
53	BA	2480	C	N3-C2-O2	-5.11	118.33	121.90
21	AA	351	G	N1-C6-O6	-5.11	116.84	119.90
21	AA	1190	G	N1-C6-O6	-5.11	116.84	119.90
21	AA	1376	U	C4-C5-C6	5.11	122.76	119.70
21	AA	1514	G	C8-N9-C4	-5.11	104.36	106.40
53	BA	1741	C	C4'-C3'-C2'	-5.11	97.49	102.60
53	BA	2032	G	C5-C6-N1	5.11	114.05	111.50
53	BA	2524	G	C8-N9-C4	-5.11	104.36	106.40
21	AA	266	G	N9-C4-C5	5.10	107.44	105.40
53	BA	231	A	C6-C5-N7	5.10	135.87	132.30
53	BA	2133	G	N3-C4-C5	-5.10	126.05	128.60
53	BA	2617	U	C5-C6-N1	-5.10	120.15	122.70
53	BA	2865	U	O4'-C1'-N1	5.10	112.28	108.20
21	AA	390	U	N1-C2-N3	5.10	117.96	114.90
21	AA	956	U	N1-C2-N3	5.10	117.96	114.90
53	BA	752	A	C4-C5-C6	-5.10	114.45	117.00
53	BA	757	G	N7-C8-N9	5.10	115.65	113.10
53	BA	1202	G	N9-C4-C5	5.10	107.44	105.40
53	BA	2172	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	974	A	C6-C5-N7	5.10	135.87	132.30
21	AA	1053	G	C4'-C3'-O3'	5.10	123.20	113.00
21	AA	1245	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1325	C	C4'-C3'-C2'	-5.10	97.50	102.60
53	BA	488	G	N9-C4-C5	5.10	107.44	105.40
53	BA	1999	C	N1-C2-O2	5.10	121.96	118.90
53	BA	2662	A	C8-N9-C4	-5.10	103.76	105.80
21	AA	43	C	N3-C2-O2	-5.10	118.33	121.90
21	AA	297	G	C5-C6-N1	5.10	114.05	111.50
21	AA	776	G	C5-C6-N1	5.10	114.05	111.50
21	AA	1438	G	C5-C6-N1	5.10	114.05	111.50
53	BA	290	U	C5-C6-N1	-5.10	120.15	122.70
53	BA	698	C	N3-C2-O2	-5.10	118.33	121.90
53	BA	2181	U	O4'-C1'-N1	5.10	112.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2483	C	N1-C2-O2	5.10	121.96	118.90
21	AA	618	C	N3-C4-C5	5.10	123.94	121.90
21	AA	777	A	C6-C5-N7	5.10	135.87	132.30
21	AA	1507	A	C4-C5-C6	-5.10	114.45	117.00
53	BA	139	U	N3-C2-O2	-5.10	118.63	122.20
53	BA	378	C	N3-C2-O2	-5.10	118.33	121.90
53	BA	560	C	N3-C4-C5	5.10	123.94	121.90
53	BA	1299	G	N3-C2-N2	-5.10	116.33	119.90
53	BA	1526	C	N3-C4-C5	5.10	123.94	121.90
53	BA	1726	C	C4'-C3'-C2'	-5.10	97.50	102.60
53	BA	1730	C	C2-N3-C4	-5.10	117.35	119.90
53	BA	2881	U	O4'-C1'-N1	5.10	112.28	108.20
54	BB	13	G	N1-C6-O6	-5.10	116.84	119.90
21	AA	939	G	N3-C4-C5	-5.10	126.05	128.60
21	AA	1296	C	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1314	C	N3-C2-O2	-5.10	118.33	121.90
53	BA	1682	G	C8-N9-C4	-5.10	104.36	106.40
53	BA	2507	C	N3-C2-O2	-5.10	118.33	121.90
53	BA	2901	C	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1102	A	C5'-C4'-C3'	-5.09	107.85	116.00
21	AA	1400	C	N3-C4-C5	5.09	123.94	121.90
45	BX	10	ARG	NE-CZ-NH1	5.09	122.85	120.30
53	BA	704	G	N9-C4-C5	5.09	107.44	105.40
53	BA	1015	U	O4'-C1'-N1	5.09	112.28	108.20
53	BA	1768	C	O4'-C1'-N1	5.09	112.28	108.20
53	BA	1822	C	C6-N1-C2	-5.09	118.26	120.30
53	BA	2296	U	O3'-P-O5'	-5.09	94.32	104.00
53	BA	2489	U	C5-C6-N1	-5.09	120.15	122.70
21	AA	469	C	N1-C2-O2	5.09	121.96	118.90
21	AA	1001	C	N3-C2-O2	-5.09	118.33	121.90
53	BA	355	U	N1-C2-N3	5.09	117.96	114.90
53	BA	472	A	C4-C5-C6	-5.09	114.45	117.00
11	AL	82	ARG	NE-CZ-NH2	-5.09	117.75	120.30
21	AA	1211	U	N3-C2-O2	-5.09	118.64	122.20
21	AA	1485	U	O4'-C1'-N1	5.09	112.27	108.20
53	BA	1585	C	N3-C2-O2	-5.09	118.33	121.90
53	BA	2287	A	C8-N9-C4	-5.09	103.76	105.80
53	BA	2346	A	C4-C5-C6	-5.09	114.45	117.00
15	AP	14	ARG	NE-CZ-NH1	5.09	122.84	120.30
21	AA	103	U	N1-C2-N3	5.09	117.95	114.90
21	AA	214	C	C4'-C3'-C2'	-5.09	97.51	102.60
21	AA	443	C	O4'-C1'-N1	5.09	112.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	999	C	C2-N3-C4	-5.09	117.36	119.90
53	BA	27	G	C5-C6-N1	5.09	114.05	111.50
53	BA	337	C	N1-C2-O2	5.09	121.95	118.90
53	BA	1026	G	O4'-C1'-N9	5.09	112.27	108.20
53	BA	1406	U	N3-C2-O2	-5.09	118.64	122.20
53	BA	1535	A	C2-N3-C4	5.09	113.14	110.60
53	BA	2592	G	C8-N9-C4	-5.09	104.36	106.40
39	BR	21	ARG	NE-CZ-NH1	5.09	122.84	120.30
53	BA	157	C	O4'-C1'-N1	5.09	112.27	108.20
53	BA	471	A	N1-C6-N6	-5.09	115.55	118.60
53	BA	1435	G	N1-C6-O6	-5.09	116.85	119.90
53	BA	1760	C	N3-C4-C5	5.09	123.94	121.90
53	BA	2472	G	C5-C6-N1	5.09	114.04	111.50
53	BA	2839	G	N7-C8-N9	5.09	115.64	113.10
21	AA	545	C	O4'-C1'-N1	5.09	112.27	108.20
21	AA	856	C	N3-C4-C5	5.09	123.93	121.90
21	AA	928	G	O4'-C1'-N9	5.09	112.27	108.20
21	AA	1472	U	C5'-C4'-O4'	5.09	115.20	109.10
24	BC	270	ARG	NE-CZ-NH2	5.09	122.84	120.30
53	BA	2581	G	O4'-C1'-N9	5.09	112.27	108.20
21	AA	1366	C	N3-C4-C5	5.08	123.93	121.90
53	BA	334	C	N3-C4-C5	5.08	123.93	121.90
53	BA	399	U	N3-C2-O2	-5.08	118.64	122.20
53	BA	827	U	C3'-C2'-C1'	5.08	105.57	101.50
53	BA	881	G	C5-C6-N1	5.08	114.04	111.50
53	BA	970	U	C5-C6-N1	-5.08	120.16	122.70
53	BA	1379	U	O4'-C1'-N1	5.08	112.27	108.20
53	BA	2365	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	585	G	N3-C4-C5	-5.08	126.06	128.60
21	AA	616	G	O4'-C1'-N9	5.08	112.27	108.20
21	AA	1042	A	C6-C5-N7	5.08	135.86	132.30
21	AA	1279	G	N3-C4-C5	-5.08	126.06	128.60
21	AA	1460	C	O4'-C1'-N1	5.08	112.27	108.20
53	BA	142	A	O4'-C1'-N9	5.08	112.27	108.20
53	BA	727	A	C4-C5-C6	-5.08	114.46	117.00
53	BA	922	C	C6-N1-C2	-5.08	118.27	120.30
21	AA	5	U	N3-C2-O2	-5.08	118.64	122.20
21	AA	811	C	N3-C2-O2	-5.08	118.34	121.90
21	AA	1352	C	C2-N3-C4	-5.08	117.36	119.90
53	BA	1101	U	N1-C2-N3	5.08	117.95	114.90
53	BA	1761	C	N3-C4-C5	5.08	123.93	121.90
53	BA	1972	G	C3'-C2'-C1'	5.08	105.56	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2051	A	C4-C5-C6	-5.08	114.46	117.00
53	BA	2436	G	C8-N9-C4	-5.08	104.37	106.40
54	BB	94	A	C6-C5-N7	5.08	135.86	132.30
21	AA	574	A	C6-C5-N7	5.08	135.86	132.30
22	A1	24	G	N3-C4-C5	-5.08	126.06	128.60
53	BA	2146	C	N3-C4-C5	5.08	123.93	121.90
53	BA	2501	C	N1-C2-O2	5.08	121.95	118.90
53	BA	2879	A	C2-N3-C4	5.08	113.14	110.60
21	AA	427	U	O4'-C1'-N1	5.08	112.26	108.20
21	AA	1210	C	C6-N1-C2	-5.08	118.27	120.30
53	BA	637	A	C6-C5-N7	5.08	135.85	132.30
53	BA	1313	U	N1-C2-N3	5.08	117.95	114.90
53	BA	1683	U	O4'-C1'-N1	5.08	112.26	108.20
53	BA	1868	C	O4'-C1'-N1	5.08	112.26	108.20
53	BA	2147	A	O4'-C1'-N9	5.08	112.26	108.20
53	BA	2405	G	C5-C6-N1	5.08	114.04	111.50
53	BA	2564	A	C5'-C4'-O4'	5.08	115.19	109.10
22	A1	14	A	N1-C6-N6	-5.08	115.55	118.60
53	BA	273	G	N1-C6-O6	-5.08	116.85	119.90
53	BA	1043	C	N3-C2-O2	-5.08	118.35	121.90
53	BA	1135	C	C5'-C4'-C3'	-5.08	107.88	116.00
53	BA	1586	A	C4-C5-C6	-5.08	114.46	117.00
1	AB	221	ARG	NE-CZ-NH1	5.08	122.84	120.30
21	AA	570	G	N9-C4-C5	5.08	107.43	105.40
21	AA	756	C	O4'-C1'-N1	5.08	112.26	108.20
25	BD	179	ARG	NE-CZ-NH1	5.08	122.84	120.30
53	BA	629	G	C5-C6-N1	5.08	114.04	111.50
53	BA	719	C	N3-C2-O2	-5.08	118.35	121.90
53	BA	1002	G	O4'-C1'-N9	5.08	112.26	108.20
53	BA	1721	G	C8-N9-C4	-5.08	104.37	106.40
53	BA	1732	C	N3-C4-C5	5.08	123.93	121.90
53	BA	2408	U	C5-C6-N1	-5.08	120.16	122.70
53	BA	2574	G	C8-N9-C4	-5.08	104.37	106.40
21	AA	152	A	C6-C5-N7	5.07	135.85	132.30
21	AA	204	G	N1-C6-O6	-5.07	116.86	119.90
21	AA	1401	G	N7-C8-N9	5.07	115.64	113.10
53	BA	720	U	O4'-C1'-N1	5.07	112.26	108.20
53	BA	919	U	N3-C2-O2	-5.07	118.65	122.20
53	BA	1076	C	N3-C4-C5	5.07	123.93	121.90
53	BA	2126	A	C4-C5-C6	-5.07	114.46	117.00
53	BA	2579	C	N1-C2-O2	5.07	121.94	118.90
54	BB	12	C	O4'-C1'-N1	5.07	112.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	238	C	C3'-C2'-C1'	5.07	105.56	101.50
53	BA	1254	A	C4-C5-C6	-5.07	114.46	117.00
21	AA	467	U	N3-C2-O2	-5.07	118.65	122.20
21	AA	1353	G	N3-C4-C5	-5.07	126.06	128.60
53	BA	387	U	N1-C2-N3	5.07	117.94	114.90
53	BA	490	C	N3-C4-C5	5.07	123.93	121.90
53	BA	1222	U	O4'-C1'-N1	5.07	112.26	108.20
53	BA	1707	G	N7-C8-N9	5.07	115.64	113.10
53	BA	2695	U	N1-C2-N3	5.07	117.94	114.90
21	AA	473	U	O4'-C1'-N1	5.07	112.25	108.20
53	BA	695	G	N1-C6-O6	-5.07	116.86	119.90
53	BA	1893	C	C6-N1-C2	-5.07	118.27	120.30
21	AA	89	U	C4-C5-C6	5.07	122.74	119.70
21	AA	1136	C	N3-C4-C5	5.07	123.93	121.90
53	BA	6	A	O4'-C1'-N9	5.07	112.25	108.20
53	BA	43	G	N3-C4-C5	-5.07	126.07	128.60
53	BA	60	G	C1'-O4'-C4'	-5.07	105.84	109.90
53	BA	446	G	O4'-C4'-C3'	5.07	110.15	106.10
53	BA	446	G	N1-C6-O6	-5.07	116.86	119.90
53	BA	693	A	C4'-C3'-C2'	-5.07	97.53	102.60
53	BA	1037	G	C5'-C4'-O4'	5.07	115.18	109.10
53	BA	1055	G	N9-C4-C5	5.07	107.43	105.40
53	BA	1775	U	N3-C2-O2	-5.07	118.65	122.20
53	BA	2317	A	C5-C6-N1	5.07	120.23	117.70
53	BA	2869	G	C8-N9-C4	-5.07	104.37	106.40
54	BB	29	A	O4'-C1'-N9	5.07	112.25	108.20
53	BA	279	A	C6-C5-N7	5.07	135.84	132.30
53	BA	344	A	O4'-C1'-N9	5.07	112.25	108.20
53	BA	1331	G	N7-C8-N9	5.07	115.63	113.10
53	BA	1551	A	C5'-C4'-O4'	5.07	115.18	109.10
53	BA	1598	A	N1-C6-N6	-5.07	115.56	118.60
53	BA	2383	G	N1-C6-O6	-5.07	116.86	119.90
53	BA	2441	U	O4'-C1'-N1	5.07	112.25	108.20
53	BA	2588	G	N1-C6-O6	-5.07	116.86	119.90
53	BA	2689	U	C5-C6-N1	-5.07	120.17	122.70
27	BF	94	ARG	NE-CZ-NH1	5.06	122.83	120.30
53	BA	1784	A	C5-C6-N1	5.06	120.23	117.70
53	BA	2475	C	C6-N1-C2	-5.06	118.27	120.30
21	AA	700	G	C5'-C4'-O4'	5.06	115.18	109.10
21	AA	1143	G	C5-C6-N1	5.06	114.03	111.50
53	BA	132	G	O4'-C1'-N9	5.06	112.25	108.20
53	BA	287	G	C8-N9-C4	-5.06	104.38	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1013	C	N3-C2-O2	-5.06	118.36	121.90
53	BA	1786	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	1091	U	C5'-C4'-O4'	5.06	115.17	109.10
21	AA	1119	C	N3-C2-O2	-5.06	118.36	121.90
26	BE	102	ARG	NE-CZ-NH1	5.06	122.83	120.30
53	BA	550	C	N3-C4-C5	5.06	123.92	121.90
53	BA	743	A	O4'-C1'-N9	5.06	112.25	108.20
21	AA	738	C	N1-C2-O2	5.06	121.94	118.90
21	AA	922	G	C5-C6-N1	5.06	114.03	111.50
21	AA	1025	U	N1-C2-N3	5.06	117.94	114.90
53	BA	138	U	N3-C2-O2	-5.06	118.66	122.20
53	BA	773	U	N3-C2-O2	-5.06	118.66	122.20
53	BA	1768	C	C4'-C3'-C2'	-5.06	97.54	102.60
53	BA	1852	U	N1-C2-N3	5.06	117.94	114.90
53	BA	2040	G	N3-C4-C5	-5.06	126.07	128.60
53	BA	2471	A	C5-C6-N1	5.06	120.23	117.70
21	AA	308	C	N3-C4-C5	5.06	123.92	121.90
21	AA	898	G	O4'-C1'-N9	5.06	112.25	108.20
21	AA	905	U	N3-C2-O2	-5.06	118.66	122.20
53	BA	97	C	O4'-C1'-N1	5.06	112.25	108.20
53	BA	512	G	N9-C4-C5	5.06	107.42	105.40
53	BA	1136	G	C8-N9-C4	-5.06	104.38	106.40
53	BA	1500	G	N1-C6-O6	-5.06	116.86	119.90
53	BA	1524	G	N3-C2-N2	-5.06	116.36	119.90
53	BA	1643	G	N3-C4-C5	-5.06	126.07	128.60
53	BA	1674	G	N7-C8-N9	5.06	115.63	113.10
53	BA	2063	C	N3-C4-C5	5.06	123.92	121.90
53	BA	2473	U	C5-C6-N1	-5.06	120.17	122.70
21	AA	1212	U	O4'-C1'-N1	5.06	112.25	108.20
22	A1	48	C	C2-N3-C4	-5.06	117.37	119.90
53	BA	1808	A	C5-C6-N1	5.06	120.23	117.70
21	AA	242	G	C5-C6-N1	5.05	114.03	111.50
21	AA	1113	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1348	U	N1-C2-N3	5.05	117.93	114.90
21	AA	1498	U	N1-C2-N3	5.05	117.93	114.90
53	BA	277	G	O4'-C1'-N9	5.05	112.24	108.20
53	BA	537	G	O4'-C1'-N9	5.05	112.24	108.20
53	BA	593	U	O4'-C1'-N1	5.05	112.24	108.20
53	BA	1183	U	C5-C6-N1	-5.05	120.17	122.70
53	BA	1323	C	N3-C4-C5	5.05	123.92	121.90
53	BA	1907	G	C8-N9-C4	-5.05	104.38	106.40
54	BB	36	C	N3-C4-C5	5.05	123.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	793	U	C3'-C2'-C1'	5.05	105.54	101.50
21	AA	1004	A	C6-C5-N7	5.05	135.84	132.30
21	AA	1316	G	N3-C4-C5	-5.05	126.07	128.60
41	BT	76	ARG	NE-CZ-NH1	5.05	122.83	120.30
53	BA	1083	U	C5-C6-N1	-5.05	120.17	122.70
53	BA	1086	A	O4'-C1'-N9	5.05	112.24	108.20
53	BA	2316	G	N7-C8-N9	5.05	115.63	113.10
53	BA	295	G	O4'-C1'-N9	5.05	112.24	108.20
53	BA	317	G	N3-C4-C5	-5.05	126.07	128.60
53	BA	1072	C	O4'-C4'-C3'	5.05	110.14	106.10
53	BA	1832	C	C3'-C2'-C1'	5.05	105.54	101.50
21	AA	411	A	O4'-C1'-N9	5.05	112.24	108.20
21	AA	802	A	O4'-C1'-N9	5.05	112.24	108.20
21	AA	900	A	C4-C5-C6	-5.05	114.47	117.00
21	AA	1395	C	O4'-C1'-N1	5.05	112.24	108.20
53	BA	69	C	C6-N1-C2	-5.05	118.28	120.30
53	BA	131	A	C4-C5-C6	-5.05	114.47	117.00
53	BA	158	U	O4'-C1'-N1	5.05	112.24	108.20
53	BA	1267	U	O4'-C1'-N1	5.05	112.24	108.20
53	BA	2165	C	N3-C2-O2	-5.05	118.36	121.90
53	BA	2226	C	O4'-C1'-N1	5.05	112.24	108.20
53	BA	2277	G	N9-C4-C5	5.05	107.42	105.40
53	BA	2338	C	N3-C2-O2	-5.05	118.36	121.90
53	BA	2448	A	C4-C5-C6	-5.05	114.47	117.00
53	BA	2582	G	N7-C8-N9	5.05	115.62	113.10
53	BA	2688	G	C4'-C3'-C2'	-5.05	97.55	102.60
53	BA	2747	G	O4'-C1'-N9	5.05	112.24	108.20
21	AA	980	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1069	C	N1-C2-O2	5.05	121.93	118.90
53	BA	116	C	N3-C2-O2	-5.05	118.37	121.90
53	BA	1542	U	N1-C2-N3	5.05	117.93	114.90
53	BA	2680	U	C5-C6-N1	-5.05	120.18	122.70
21	AA	184	G	C5-C6-N1	5.05	114.02	111.50
21	AA	272	C	N1-C2-O2	5.05	121.93	118.90
21	AA	489	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1152	A	C4-C5-C6	-5.05	114.48	117.00
53	BA	544	C	N1-C2-O2	5.05	121.93	118.90
53	BA	1987	A	C4-C5-C6	-5.05	114.48	117.00
53	BA	2495	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	681	A	C6-C5-N7	5.04	135.83	132.30
53	BA	677	A	C5'-C4'-O4'	5.04	115.15	109.10
53	BA	1116	G	N1-C6-O6	-5.04	116.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	1539	U	O4'-C1'-N1	5.04	112.24	108.20
21	AA	786	G	C5-C6-N1	5.04	114.02	111.50
47	BZ	15	ARG	CD-NE-CZ	5.04	130.66	123.60
53	BA	500	G	C5-C6-N1	5.04	114.02	111.50
53	BA	983	A	C4-C5-C6	-5.04	114.48	117.00
53	BA	1117	C	O4'-C1'-N1	5.04	112.23	108.20
53	BA	1425	G	C5-C6-N1	5.04	114.02	111.50
53	BA	1599	U	N3-C2-O2	-5.04	118.67	122.20
53	BA	2043	C	C5'-C4'-C3'	-5.04	107.93	116.00
53	BA	2356	U	O4'-C1'-N1	5.04	112.23	108.20
53	BA	2664	G	C5-C6-N1	5.04	114.02	111.50
53	BA	2811	G	O4'-C1'-N9	5.04	112.23	108.20
53	BA	2857	G	N3-C4-C5	-5.04	126.08	128.60
53	BA	2863	C	O4'-C1'-N1	5.04	112.23	108.20
21	AA	218	U	C5-C6-N1	-5.04	120.18	122.70
21	AA	561	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	655	A	N1-C6-N6	-5.04	115.58	118.60
21	AA	1131	G	N9-C4-C5	5.04	107.42	105.40
53	BA	143	C	N1-C2-O2	5.04	121.92	118.90
53	BA	451	U	C5-C6-N1	-5.04	120.18	122.70
53	BA	888	C	O4'-C1'-N1	5.04	112.23	108.20
53	BA	1206	G	C5-C6-N1	5.04	114.02	111.50
53	BA	1724	G	C5-C6-N1	5.04	114.02	111.50
53	BA	1971	U	N3-C2-O2	-5.04	118.67	122.20
53	BA	455	C	N3-C2-O2	-5.04	118.37	121.90
53	BA	799	G	C5'-C4'-O4'	5.04	115.15	109.10
53	BA	1216	G	N3-C4-C5	-5.04	126.08	128.60
53	BA	1764	C	N1-C2-O2	5.04	121.92	118.90
53	BA	1945	G	C5-C6-N1	5.04	114.02	111.50
53	BA	2208	C	O4'-C1'-N1	5.04	112.23	108.20
53	BA	2535	G	N7-C8-N9	5.04	115.62	113.10
21	AA	999	C	N3-C4-C5	5.04	123.92	121.90
21	AA	1112	C	N1-C2-O2	5.04	121.92	118.90
53	BA	12	U	N3-C2-O2	-5.04	118.67	122.20
53	BA	400	G	C5-C6-N1	5.04	114.02	111.50
53	BA	1306	C	N3-C2-O2	-5.04	118.37	121.90
53	BA	2150	C	O4'-C1'-N1	5.04	112.23	108.20
53	BA	2426	A	C6-C5-N7	5.04	135.83	132.30
53	BA	2444	G	O4'-C1'-N9	5.04	112.23	108.20
53	BA	2558	C	N3-C2-O2	-5.04	118.37	121.90
53	BA	2588	G	C5-C6-N1	5.04	114.02	111.50
21	AA	278	G	N3-C4-C5	-5.04	126.08	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1251	A	C4-C5-C6	-5.04	114.48	117.00
53	BA	210	C	N3-C2-O2	-5.04	118.37	121.90
53	BA	221	A	C2-N3-C4	5.04	113.12	110.60
53	BA	751	A	C4-C5-C6	-5.04	114.48	117.00
53	BA	940	G	C5-C6-N1	5.04	114.02	111.50
53	BA	2245	U	C5-C6-N1	-5.04	120.18	122.70
21	AA	313	A	C4-C5-C6	-5.04	114.48	117.00
21	AA	1245	C	O4'-C1'-N1	5.04	112.23	108.20
21	AA	1407	C	C6-N1-C2	-5.04	118.29	120.30
53	BA	177	G	N1-C6-O6	-5.04	116.88	119.90
53	BA	289	G	O4'-C1'-N9	5.04	112.23	108.20
53	BA	343	C	O4'-C1'-N1	5.04	112.23	108.20
53	BA	726	G	N1-C6-O6	-5.04	116.88	119.90
53	BA	1411	U	N3-C2-O2	-5.04	118.67	122.20
53	BA	1644	C	O4'-C1'-N1	5.04	112.23	108.20
53	BA	2440	C	N3-C4-C5	5.04	123.91	121.90
53	BA	2643	G	N3-C4-C5	-5.04	126.08	128.60
53	BA	2697	G	N1-C6-O6	-5.04	116.88	119.90
53	BA	2716	C	N3-C2-O2	-5.04	118.38	121.90
21	AA	97	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	562	U	N3-C2-O2	-5.03	118.68	122.20
21	AA	829	G	C8-N9-C4	-5.03	104.39	106.40
21	AA	1131	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	1230	C	N1-C2-O2	5.03	121.92	118.90
21	AA	1272	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	1348	U	C4'-C3'-C2'	-5.03	97.57	102.60
53	BA	846	U	N3-C2-O2	-5.03	118.68	122.20
53	BA	1044	C	N3-C4-N4	-5.03	114.48	118.00
53	BA	1169	A	C6-C5-N7	5.03	135.82	132.30
53	BA	2508	G	O4'-C1'-N9	5.03	112.23	108.20
21	AA	721	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	1290	G	N3-C2-N2	-5.03	116.38	119.90
53	BA	1782	U	N3-C2-O2	-5.03	118.68	122.20
54	BB	33	G	C5-C6-N1	5.03	114.02	111.50
21	AA	329	A	C6-C5-N7	5.03	135.82	132.30
21	AA	1013	G	C5-C6-N1	5.03	114.02	111.50
21	AA	1013	G	N3-C4-C5	-5.03	126.08	128.60
21	AA	1272	G	C8-N9-C4	-5.03	104.39	106.40
22	A1	27	C	N3-C2-O2	-5.03	118.38	121.90
53	BA	425	G	N1-C6-O6	-5.03	116.88	119.90
53	BA	572	A	C4-C5-C6	-5.03	114.48	117.00
53	BA	1840	G	C8-N9-C4	-5.03	104.39	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	2889	C	C6-N1-C2	-5.03	118.29	120.30
21	AA	305	G	N1-C6-O6	-5.03	116.88	119.90
54	BB	56	G	O4'-C4'-C3'	5.03	110.12	106.10
22	A1	76	A	O4'-C1'-N9	5.03	112.22	108.20
53	BA	1737	G	N3-C4-C5	-5.03	126.09	128.60
53	BA	1755	A	C6-C5-N7	5.03	135.82	132.30
53	BA	2199	A	C4-C5-C6	-5.03	114.49	117.00
53	BA	2434	A	C4-C5-C6	-5.03	114.49	117.00
21	AA	688	G	N7-C8-N9	5.03	115.61	113.10
53	BA	1194	A	C4'-C3'-C2'	-5.03	97.58	102.60
53	BA	1467	U	C5-C6-N1	-5.03	120.19	122.70
53	BA	2003	A	C5-C6-N1	5.03	120.21	117.70
53	BA	2298	A	O4'-C1'-N9	5.03	112.22	108.20
53	BA	2427	C	O4'-C4'-C3'	5.03	110.12	106.10
53	BA	2773	C	N3-C2-O2	-5.03	118.38	121.90
21	AA	958	A	C6-C5-N7	5.02	135.82	132.30
53	BA	1191	G	O4'-C1'-N9	5.02	112.22	108.20
53	BA	1723	G	O4'-C1'-N9	5.02	112.22	108.20
21	AA	169	C	N3-C2-O2	-5.02	118.38	121.90
21	AA	849	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	861	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	944	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	988	G	C5-C6-N1	5.02	114.01	111.50
22	A1	15	G	N9-C4-C5	5.02	107.41	105.40
53	BA	364	C	O4'-C1'-N1	5.02	112.22	108.20
53	BA	1524	G	O4'-C1'-N9	5.02	112.22	108.20
53	BA	1648	U	O4'-C1'-N1	5.02	112.22	108.20
53	BA	1755	A	C4-C5-C6	-5.02	114.49	117.00
53	BA	2342	C	O4'-C1'-N1	5.02	112.22	108.20
53	BA	2796	U	C5-C6-N1	-5.02	120.19	122.70
21	AA	110	C	O4'-C1'-N1	5.02	112.22	108.20
53	BA	790	U	N3-C2-O2	-5.02	118.69	122.20
21	AA	15	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	97	G	O4'-C1'-N9	5.02	112.22	108.20
21	AA	279	A	C3'-C2'-C1'	5.02	105.52	101.50
21	AA	791	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	991	U	C5-C6-N1	-5.02	120.19	122.70
53	BA	514	A	C6-C5-N7	5.02	135.81	132.30
53	BA	1063	G	C5-C6-N1	5.02	114.01	111.50
53	BA	1482	G	N3-C4-C5	-5.02	126.09	128.60
53	BA	2069	G	C8-N9-C4	-5.02	104.39	106.40
54	BB	87	U	N3-C2-O2	-5.02	118.69	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	275	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	993	G	N3-C4-N9	5.02	129.01	126.00
21	AA	1009	U	N3-C2-O2	-5.02	118.69	122.20
21	AA	1028	C	O4'-C1'-N1	5.02	112.21	108.20
21	AA	1492	A	C3'-C2'-C1'	-5.02	97.49	101.50
27	BF	6	TYR	CB-CG-CD2	-5.02	117.99	121.00
53	BA	1770	G	C5-C6-N1	5.02	114.01	111.50
53	BA	2359	C	N1-C2-O2	5.02	121.91	118.90
53	BA	2831	G	C5-C6-N1	5.02	114.01	111.50
21	AA	1379	G	O4'-C1'-N9	5.02	112.21	108.20
53	BA	182	A	C4-C5-C6	-5.02	114.49	117.00
21	AA	166	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	418	C	N1-C2-O2	5.01	121.91	118.90
21	AA	1425	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	1513	A	N1-C6-N6	-5.01	115.59	118.60
53	BA	562	U	C4-C5-C6	5.01	122.71	119.70
53	BA	962	G	N7-C8-N9	5.01	115.61	113.10
53	BA	1125	G	C8-N9-C4	-5.01	104.39	106.40
53	BA	1741	C	C6-N1-C2	-5.01	118.29	120.30
53	BA	2212	A	C5-C6-N6	5.01	127.71	123.70
53	BA	2266	A	C6-C5-N7	5.01	135.81	132.30
53	BA	2713	U	C4-C5-C6	5.01	122.71	119.70
21	AA	6	G	C5-C6-N1	5.01	114.01	111.50
21	AA	618	C	O4'-C1'-N1	5.01	112.21	108.20
53	BA	989	G	N9-C4-C5	5.01	107.41	105.40
53	BA	1522	A	O4'-C1'-N9	5.01	112.21	108.20
53	BA	2707	U	C4'-C3'-C2'	-5.01	97.59	102.60
21	AA	107	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	368	U	N3-C2-O2	-5.01	118.69	122.20
21	AA	1516	G	N1-C6-O6	-5.01	116.89	119.90
53	BA	148	U	C5-C6-N1	-5.01	120.19	122.70
53	BA	642	U	N3-C2-O2	-5.01	118.69	122.20
53	BA	802	A	C4-C5-C6	-5.01	114.49	117.00
53	BA	864	G	N3-C4-C5	-5.01	126.09	128.60
53	BA	1698	A	N1-C6-N6	-5.01	115.59	118.60
53	BA	1879	C	N3-C4-C5	5.01	123.90	121.90
53	BA	1982	U	N1-C2-N3	5.01	117.91	114.90
53	BA	2327	A	C4-C5-C6	-5.01	114.49	117.00
53	BA	2539	C	N1-C2-O2	5.01	121.91	118.90
53	BA	2548	U	C5-C6-N1	-5.01	120.19	122.70
53	BA	2663	G	O4'-C1'-N9	5.01	112.21	108.20
21	AA	292	G	C5-C6-N1	5.01	114.00	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	449	G	C8-N9-C4	-5.01	104.40	106.40
21	AA	468	A	O4'-C1'-N9	5.01	112.21	108.20
21	AA	836	G	N3-C4-C5	-5.01	126.09	128.60
21	AA	1283	U	C4-C5-C6	5.01	122.71	119.70
21	AA	1469	C	N1-C2-O2	5.01	121.91	118.90
53	BA	406	G	N1-C6-O6	-5.01	116.89	119.90
53	BA	470	A	N1-C6-N6	-5.01	115.59	118.60
53	BA	790	U	N1-C2-N3	5.01	117.91	114.90
53	BA	817	C	C4'-C3'-C2'	-5.01	97.59	102.60
53	BA	1748	C	O4'-C1'-N1	5.01	112.21	108.20
53	BA	1752	C	N3-C4-C5	5.01	123.90	121.90
53	BA	1768	C	C5'-C4'-O4'	5.01	115.11	109.10
53	BA	1062	G	C3'-C2'-C1'	5.01	105.51	101.50
4	AE	92	ARG	CD-NE-CZ	5.01	130.61	123.60
21	AA	421	U	C5-C6-N1	-5.01	120.20	122.70
21	AA	775	G	N3-C2-N2	-5.01	116.40	119.90
21	AA	1215	G	N1-C6-O6	-5.01	116.90	119.90
53	BA	1433	A	C4-C5-C6	-5.01	114.50	117.00
53	BA	1497	U	C1'-O4'-C4'	-5.01	105.89	109.90
53	BA	1675	C	O4'-C1'-N1	5.01	112.21	108.20
53	BA	2046	G	N3-C4-C5	-5.01	126.10	128.60
21	AA	975	A	C4'-C3'-C2'	-5.00	97.59	102.60
21	AA	675	A	C6-C5-N7	5.00	135.80	132.30
53	BA	287	G	C4'-C3'-C2'	-5.00	97.60	102.60
53	BA	390	U	O4'-C1'-C2'	-5.00	100.80	105.80
53	BA	612	G	N1-C6-O6	-5.00	116.90	119.90
53	BA	912	C	N1-C2-O2	5.00	121.90	118.90
53	BA	1834	U	N3-C2-O2	-5.00	118.70	122.20
53	BA	2057	G	N1-C6-O6	-5.00	116.90	119.90
53	BA	2127	G	C5'-C4'-O4'	5.00	115.10	109.10
53	BA	2404	U	N1-C2-N3	5.00	117.90	114.90
21	AA	666	G	N3-C2-N2	-5.00	116.40	119.90
21	AA	1244	G	N3-C4-C5	-5.00	126.10	128.60
53	BA	199	A	C6-C5-N7	5.00	135.80	132.30
53	BA	493	G	N1-C6-O6	-5.00	116.90	119.90
53	BA	2344	U	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (1028) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	11	C	Sidechain

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Mol	Chain	Res	Type	Group
22	A1	17	U	Sidechain
22	A1	18	G	Sidechain
22	A1	19	G	Sidechain
22	A1	20	G	Sidechain
22	A1	27	C	Sidechain
22	A1	31	C	Sidechain
22	A1	41	A	Sidechain
22	A1	44	G	Sidechain
22	A1	50	G	Sidechain
22	A1	52	G	Sidechain
22	A1	56	C	Sidechain
22	A1	6	A	Sidechain
22	A1	63	G	Sidechain
22	A1	68	C	Sidechain
22	A1	74	C	Sidechain
22	A1	75	C	Sidechain
22	A1	76	A	Sidechain
23	A2	84	G	Sidechain
23	A2	88	U	Sidechain
21	AA	100	G	Sidechain
21	AA	1010	U	Sidechain
21	AA	1019	A	Sidechain
21	AA	1025	U	Sidechain
21	AA	1026	G	Sidechain
21	AA	1038	C	Sidechain
21	AA	1040	U	Sidechain
21	AA	1044	A	Sidechain
21	AA	1049	U	Sidechain
21	AA	1051	C	Sidechain
21	AA	1054	C	Sidechain
21	AA	1055	A	Sidechain
21	AA	1056	U	Sidechain
21	AA	1060	U	Sidechain
21	AA	1064	G	Sidechain
21	AA	1071	C	Sidechain
21	AA	1072	G	Sidechain
21	AA	1077	G	Sidechain
21	AA	1078	U	Sidechain
21	AA	108	G	Sidechain
21	AA	1085	U	Sidechain
21	AA	1086	U	Sidechain
21	AA	1087	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1089	G	Sidechain
21	AA	109	A	Sidechain
21	AA	1091	U	Sidechain
21	AA	1092	A	Sidechain
21	AA	1094	G	Sidechain
21	AA	1095	U	Sidechain
21	AA	1100	C	Sidechain
21	AA	1118	U	Sidechain
21	AA	1119	C	Sidechain
21	AA	112	G	Sidechain
21	AA	1124	G	Sidechain
21	AA	1125	U	Sidechain
21	AA	1126	U	Sidechain
21	AA	1128	C	Sidechain
21	AA	1133	G	Sidechain
21	AA	1137	C	Sidechain
21	AA	1139	G	Sidechain
21	AA	1141	C	Sidechain
21	AA	1145	A	Sidechain
21	AA	1147	C	Sidechain
21	AA	1149	C	Sidechain
21	AA	116	A	Sidechain
21	AA	1160	G	Sidechain
21	AA	1162	C	Sidechain
21	AA	1166	G	Sidechain
21	AA	1168	U	Sidechain
21	AA	1169	A	Sidechain
21	AA	1170	A	Sidechain
21	AA	1172	C	Sidechain
21	AA	1176	A	Sidechain
21	AA	1178	G	Sidechain
21	AA	1179	A	Sidechain
21	AA	1189	U	Sidechain
21	AA	1190	G	Sidechain
21	AA	1191	A	Sidechain
21	AA	120	A	Sidechain
21	AA	1218	C	Sidechain
21	AA	122	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1226	C	Sidechain
21	AA	123	U	Sidechain
21	AA	1231	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1233	G	Sidechain
21	AA	1237	C	Sidechain
21	AA	1244	G	Sidechain
21	AA	1258	G	Sidechain
21	AA	1266	G	Sidechain
21	AA	1270	G	Sidechain
21	AA	1275	A	Sidechain
21	AA	1279	G	Sidechain
21	AA	128	G	Sidechain
21	AA	1282	C	Sidechain
21	AA	1285	A	Sidechain
21	AA	1295	U	Sidechain
21	AA	1298	U	Sidechain
21	AA	130	A	Sidechain
21	AA	1300	G	Sidechain
21	AA	1308	U	Sidechain
21	AA	1311	A	Sidechain
21	AA	1316	G	Sidechain
21	AA	1317	C	Sidechain
21	AA	1326	U	Sidechain
21	AA	1327	C	Sidechain
21	AA	1328	C	Sidechain
21	AA	1335	U	Sidechain
21	AA	1336	C	Sidechain
21	AA	1337	G	Sidechain
21	AA	1345	U	Sidechain
21	AA	1351	U	Sidechain
21	AA	1352	C	Sidechain
21	AA	1353	G	Sidechain
21	AA	1357	A	Sidechain
21	AA	1358	U	Sidechain
21	AA	136	C	Sidechain
21	AA	1360	A	Sidechain
21	AA	1363	A	Sidechain
21	AA	1367	C	Sidechain
21	AA	1368	A	Sidechain
21	AA	1380	U	Sidechain
21	AA	1387	G	Sidechain
21	AA	1396	A	Sidechain
21	AA	1405	G	Sidechain
21	AA	1417	G	Sidechain
21	AA	1435	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1436	U	Sidechain
21	AA	1438	G	Sidechain
21	AA	1442	G	Sidechain
21	AA	1444	U	Sidechain
21	AA	1452	C	Sidechain
21	AA	1461	G	Sidechain
21	AA	1471	U	Sidechain
21	AA	1473	G	Sidechain
21	AA	1477	U	Sidechain
21	AA	1482	G	Sidechain
21	AA	149	A	Sidechain
21	AA	1492	A	Sidechain
21	AA	1494	G	Sidechain
21	AA	1495	U	Sidechain
21	AA	1502	A	Sidechain
21	AA	151	A	Sidechain
21	AA	1510	C	Sidechain
21	AA	1519	A	Sidechain
21	AA	1521	C	Sidechain
21	AA	1525	G	Sidechain
21	AA	1527	U	Sidechain
21	AA	1528	U	Sidechain
21	AA	1529	G	Sidechain
21	AA	153	C	Sidechain
21	AA	1532	U	Sidechain
21	AA	159	G	Sidechain
21	AA	163	C	Sidechain
21	AA	165	G	Sidechain
21	AA	167	A	Sidechain
21	AA	173	U	Sidechain
21	AA	175	C	Sidechain
21	AA	179	A	Sidechain
21	AA	183	C	Sidechain
21	AA	187	G	Sidechain
21	AA	193	C	Sidechain
21	AA	194	C	Sidechain
21	AA	21	G	Sidechain
21	AA	217	C	Sidechain
21	AA	218	U	Sidechain
21	AA	223	A	Sidechain
21	AA	227	G	Sidechain
21	AA	229	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	242	G	Sidechain
21	AA	243	A	Sidechain
21	AA	250	A	Sidechain
21	AA	251	G	Sidechain
21	AA	260	G	Sidechain
21	AA	265	G	Sidechain
21	AA	274	A	Sidechain
21	AA	277	C	Sidechain
21	AA	286	C	Sidechain
21	AA	297	G	Sidechain
21	AA	300	A	Sidechain
21	AA	302	G	Sidechain
21	AA	308	C	Sidechain
21	AA	309	A	Sidechain
21	AA	310	G	Sidechain
21	AA	318	G	Sidechain
21	AA	323	U	Sidechain
21	AA	324	G	Sidechain
21	AA	326	G	Sidechain
21	AA	330	C	Sidechain
21	AA	334	C	Sidechain
21	AA	349	A	Sidechain
21	AA	35	G	Sidechain
21	AA	36	C	Sidechain
21	AA	362	G	Sidechain
21	AA	363	A	Sidechain
21	AA	368	U	Sidechain
21	AA	369	G	Sidechain
21	AA	37	U	Sidechain
21	AA	372	C	Sidechain
21	AA	378	G	Sidechain
21	AA	380	G	Sidechain
21	AA	382	A	Sidechain
21	AA	383	A	Sidechain
21	AA	388	G	Sidechain
21	AA	390	U	Sidechain
21	AA	391	G	Sidechain
21	AA	394	G	Sidechain
21	AA	399	G	Sidechain
21	AA	400	C	Sidechain
21	AA	401	C	Sidechain
21	AA	403	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	404	G	Sidechain
21	AA	406	G	Sidechain
21	AA	410	G	Sidechain
21	AA	42	G	Sidechain
21	AA	428	G	Sidechain
21	AA	429	U	Sidechain
21	AA	435	A	Sidechain
21	AA	442	G	Sidechain
21	AA	444	G	Sidechain
21	AA	452	A	Sidechain
21	AA	455	G	Sidechain
21	AA	464	U	Sidechain
21	AA	475	C	Sidechain
21	AA	478	A	Sidechain
21	AA	487	A	Sidechain
21	AA	490	C	Sidechain
21	AA	491	G	Sidechain
21	AA	494	G	Sidechain
21	AA	496	A	Sidechain
21	AA	505	G	Sidechain
21	AA	506	G	Sidechain
21	AA	509	A	Sidechain
21	AA	512	U	Sidechain
21	AA	515	G	Sidechain
21	AA	516	U	Sidechain
21	AA	517	G	Sidechain
21	AA	518	C	Sidechain
21	AA	519	C	Sidechain
21	AA	523	A	Sidechain
21	AA	526	C	Sidechain
21	AA	532	A	Sidechain
21	AA	534	U	Sidechain
21	AA	536	C	Sidechain
21	AA	538	G	Sidechain
21	AA	539	A	Sidechain
21	AA	542	G	Sidechain
21	AA	544	G	Sidechain
21	AA	547	A	Sidechain
21	AA	558	G	Sidechain
21	AA	561	U	Sidechain
21	AA	562	U	Sidechain
21	AA	564	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	579	A	Sidechain
21	AA	59	A	Sidechain
21	AA	598	U	Sidechain
21	AA	6	G	Sidechain
21	AA	606	G	Sidechain
21	AA	608	A	Sidechain
21	AA	611	C	Sidechain
21	AA	624	C	Sidechain
21	AA	63	C	Sidechain
21	AA	635	A	Sidechain
21	AA	637	C	Sidechain
21	AA	641	U	Sidechain
21	AA	642	A	Sidechain
21	AA	643	C	Sidechain
21	AA	646	G	Sidechain
21	AA	647	C	Sidechain
21	AA	652	U	Sidechain
21	AA	657	U	Sidechain
21	AA	664	G	Sidechain
21	AA	665	A	Sidechain
21	AA	666	G	Sidechain
21	AA	67	C	Sidechain
21	AA	671	G	Sidechain
21	AA	676	A	Sidechain
21	AA	68	G	Sidechain
21	AA	690	G	Sidechain
21	AA	691	G	Sidechain
21	AA	698	G	Sidechain
21	AA	703	G	Sidechain
21	AA	716	A	Sidechain
21	AA	720	C	Sidechain
21	AA	722	G	Sidechain
21	AA	729	A	Sidechain
21	AA	734	G	Sidechain
21	AA	74	A	Sidechain
21	AA	741	G	Sidechain
21	AA	752	G	Sidechain
21	AA	754	C	Sidechain
21	AA	765	G	Sidechain
21	AA	772	U	Sidechain
21	AA	774	G	Sidechain
21	AA	777	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	792	A	Sidechain
21	AA	793	U	Sidechain
21	AA	797	C	Sidechain
21	AA	808	C	Sidechain
21	AA	81	A	Sidechain
21	AA	811	C	Sidechain
21	AA	812	G	Sidechain
21	AA	815	A	Sidechain
21	AA	82	G	Sidechain
21	AA	825	A	Sidechain
21	AA	826	C	Sidechain
21	AA	836	G	Sidechain
21	AA	838	G	Sidechain
21	AA	842	U	Sidechain
21	AA	847	G	Sidechain
21	AA	849	G	Sidechain
21	AA	850	U	Sidechain
21	AA	856	C	Sidechain
21	AA	857	C	Sidechain
21	AA	858	G	Sidechain
21	AA	863	U	Sidechain
21	AA	867	G	Sidechain
21	AA	871	U	Sidechain
21	AA	874	G	Sidechain
21	AA	883	C	Sidechain
21	AA	891	U	Sidechain
21	AA	892	A	Sidechain
21	AA	894	G	Sidechain
21	AA	895	G	Sidechain
21	AA	896	C	Sidechain
21	AA	898	G	Sidechain
21	AA	901	A	Sidechain
21	AA	918	A	Sidechain
21	AA	92	U	Sidechain
21	AA	922	G	Sidechain
21	AA	926	G	Sidechain
21	AA	928	G	Sidechain
21	AA	93	U	Sidechain
21	AA	934	C	Sidechain
21	AA	946	A	Sidechain
21	AA	949	A	Sidechain
21	AA	95	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	953	G	Sidechain
21	AA	965	U	Sidechain
21	AA	972	C	Sidechain
21	AA	975	A	Sidechain
21	AA	978	A	Sidechain
21	AA	98	A	Sidechain
21	AA	984	C	Sidechain
21	AA	987	G	Sidechain
21	AA	99	C	Sidechain
21	AA	997	U	Sidechain
21	AA	999	C	Sidechain
18	AS	74	ALA	Peptide
53	BA	1001	A	Sidechain
53	BA	1013	C	Sidechain
53	BA	1014	A	Sidechain
53	BA	1016	G	Sidechain
53	BA	102	U	Sidechain
53	BA	1022	G	Sidechain
53	BA	1025	G	Sidechain
53	BA	1036	G	Sidechain
53	BA	1038	G	Sidechain
53	BA	1044	C	Sidechain
53	BA	1051	G	Sidechain
53	BA	1060	U	Sidechain
53	BA	1062	G	Sidechain
53	BA	1066	U	Sidechain
53	BA	1069	A	Sidechain
53	BA	1075	C	Sidechain
53	BA	108	G	Sidechain
53	BA	1087	G	Sidechain
53	BA	1088	A	Sidechain
53	BA	1091	G	Sidechain
53	BA	1094	U	Sidechain
53	BA	1106	G	Sidechain
53	BA	1109	C	Sidechain
53	BA	1118	C	Sidechain
53	BA	1126	A	Sidechain
53	BA	1127	A	Sidechain
53	BA	1139	G	Sidechain
53	BA	1147	A	Sidechain
53	BA	1149	G	Sidechain
53	BA	1151	A	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	1154	G	Sidechain
53	BA	1162	G	Sidechain
53	BA	1182	G	Sidechain
53	BA	1183	U	Sidechain
53	BA	1187	G	Sidechain
53	BA	1188	U	Sidechain
53	BA	1190	G	Sidechain
53	BA	1191	G	Sidechain
53	BA	1195	G	Sidechain
53	BA	1196	C	Sidechain
53	BA	1199	U	Sidechain
53	BA	1201	U	Sidechain
53	BA	1215	G	Sidechain
53	BA	1220	G	Sidechain
53	BA	1223	G	Sidechain
53	BA	1224	U	Sidechain
53	BA	1227	G	Sidechain
53	BA	1231	U	Sidechain
53	BA	1234	U	Sidechain
53	BA	1235	G	Sidechain
53	BA	1236	G	Sidechain
53	BA	1243	C	Sidechain
53	BA	1244	A	Sidechain
53	BA	125	A	Sidechain
53	BA	126	A	Sidechain
53	BA	1266	G	Sidechain
53	BA	1268	A	Sidechain
53	BA	1270	C	Sidechain
53	BA	1271	G	Sidechain
53	BA	1272	A	Sidechain
53	BA	1274	A	Sidechain
53	BA	1276	A	Sidechain
53	BA	1279	G	Sidechain
53	BA	1283	G	Sidechain
53	BA	1286	A	Sidechain
53	BA	1291	C	Sidechain
53	BA	1292	G	Sidechain
53	BA	1308	A	Sidechain
53	BA	1310	G	Sidechain
53	BA	1311	G	Sidechain
53	BA	1317	G	Sidechain
53	BA	1320	C	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	1322	A	Sidechain
53	BA	1324	G	Sidechain
53	BA	1325	U	Sidechain
53	BA	1330	C	Sidechain
53	BA	1339	G	Sidechain
53	BA	1343	G	Sidechain
53	BA	1344	U	Sidechain
53	BA	1359	A	Sidechain
53	BA	1360	G	Sidechain
53	BA	1366	A	Sidechain
53	BA	137	U	Sidechain
53	BA	1370	C	Sidechain
53	BA	1376	C	Sidechain
53	BA	1378	A	Sidechain
53	BA	1392	A	Sidechain
53	BA	1394	U	Sidechain
53	BA	1395	A	Sidechain
53	BA	1396	U	Sidechain
53	BA	1399	C	Sidechain
53	BA	1410	G	Sidechain
53	BA	1425	G	Sidechain
53	BA	1426	G	Sidechain
53	BA	1429	G	Sidechain
53	BA	143	C	Sidechain
53	BA	1439	A	Sidechain
53	BA	1441	G	Sidechain
53	BA	1444	G	Sidechain
53	BA	1445	G	Sidechain
53	BA	1459	G	Sidechain
53	BA	1460	U	Sidechain
53	BA	1469	A	Sidechain
53	BA	147	C	Sidechain
53	BA	1472	C	Sidechain
53	BA	1476	U	Sidechain
53	BA	1478	G	Sidechain
53	BA	1490	A	Sidechain
53	BA	1492	G	Sidechain
53	BA	1494	A	Sidechain
53	BA	1514	G	Sidechain
53	BA	1519	G	Sidechain
53	BA	1522	A	Sidechain
53	BA	1523	U	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	1526	C	Sidechain
53	BA	1536	C	Sidechain
53	BA	1540	G	Sidechain
53	BA	1543	G	Sidechain
53	BA	1546	G	Sidechain
53	BA	1551	A	Sidechain
53	BA	1552	A	Sidechain
53	BA	1555	G	Sidechain
53	BA	1560	G	Sidechain
53	BA	1561	C	Sidechain
53	BA	1562	U	Sidechain
53	BA	1563	U	Sidechain
53	BA	1564	C	Sidechain
53	BA	1565	C	Sidechain
53	BA	1567	G	Sidechain
53	BA	1570	A	Sidechain
53	BA	1573	G	Sidechain
53	BA	1585	C	Sidechain
53	BA	159	G	Sidechain
53	BA	1595	C	Sidechain
53	BA	1599	U	Sidechain
53	BA	160	A	Sidechain
53	BA	1600	C	Sidechain
53	BA	1601	G	Sidechain
53	BA	1602	U	Sidechain
53	BA	1604	C	Sidechain
53	BA	1605	C	Sidechain
53	BA	1606	C	Sidechain
53	BA	1614	A	Sidechain
53	BA	1619	G	Sidechain
53	BA	1624	U	Sidechain
53	BA	163	C	Sidechain
53	BA	1631	G	Sidechain
53	BA	1632	A	Sidechain
53	BA	1641	A	Sidechain
53	BA	1642	G	Sidechain
53	BA	1653	G	Sidechain
53	BA	1655	A	Sidechain
53	BA	1656	C	Sidechain
53	BA	1658	C	Sidechain
53	BA	1671	U	Sidechain
53	BA	1673	G	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	1695	G	Sidechain
53	BA	1700	A	Sidechain
53	BA	1703	G	Sidechain
53	BA	1707	G	Sidechain
53	BA	1709	U	Sidechain
53	BA	1710	G	Sidechain
53	BA	1713	A	Sidechain
53	BA	1715	G	Sidechain
53	BA	1718	G	Sidechain
53	BA	1721	G	Sidechain
53	BA	1734	G	Sidechain
53	BA	1735	A	Sidechain
53	BA	1740	G	Sidechain
53	BA	1745	A	Sidechain
53	BA	1747	U	Sidechain
53	BA	1748	C	Sidechain
53	BA	1750	G	Sidechain
53	BA	1753	G	Sidechain
53	BA	1757	A	Sidechain
53	BA	1766	G	Sidechain
53	BA	177	G	Sidechain
53	BA	1773	A	Sidechain
53	BA	1777	U	Sidechain
53	BA	1779	U	Sidechain
53	BA	178	G	Sidechain
53	BA	1784	A	Sidechain
53	BA	179	C	Sidechain
53	BA	1794	A	Sidechain
53	BA	1797	G	Sidechain
53	BA	18	U	Sidechain
53	BA	1802	A	Sidechain
53	BA	1805	A	Sidechain
53	BA	181	A	Sidechain
53	BA	1810	A	Sidechain
53	BA	1811	G	Sidechain
53	BA	1816	C	Sidechain
53	BA	1817	G	Sidechain
53	BA	182	A	Sidechain
53	BA	1820	U	Sidechain
53	BA	1826	G	Sidechain
53	BA	1827	U	Sidechain
53	BA	183	C	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	1830	C	Sidechain
53	BA	1831	G	Sidechain
53	BA	1834	U	Sidechain
53	BA	1841	U	Sidechain
53	BA	1845	G	Sidechain
53	BA	1846	G	Sidechain
53	BA	1847	A	Sidechain
53	BA	1849	G	Sidechain
53	BA	1857	G	Sidechain
53	BA	1858	A	Sidechain
53	BA	186	G	Sidechain
53	BA	1861	G	Sidechain
53	BA	1867	G	Sidechain
53	BA	1869	G	Sidechain
53	BA	187	G	Sidechain
53	BA	1877	A	Sidechain
53	BA	1883	U	Sidechain
53	BA	1885	A	Sidechain
53	BA	1886	U	Sidechain
53	BA	19	A	Sidechain
53	BA	1901	A	Sidechain
53	BA	1910	G	Sidechain
53	BA	1918	A	Sidechain
53	BA	1920	C	Sidechain
53	BA	1925	C	Sidechain
53	BA	1927	A	Sidechain
53	BA	1932	A	Sidechain
53	BA	1937	A	Sidechain
53	BA	1938	A	Sidechain
53	BA	194	G	Sidechain
53	BA	1951	U	Sidechain
53	BA	1954	G	Sidechain
53	BA	1955	U	Sidechain
53	BA	1964	G	Sidechain
53	BA	1971	U	Sidechain
53	BA	1982	U	Sidechain
53	BA	1987	A	Sidechain
53	BA	199	A	Sidechain
53	BA	1993	U	Sidechain
53	BA	1996	C	Sidechain
53	BA	2002	G	Sidechain
53	BA	2005	A	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	2006	C	Sidechain
53	BA	2009	A	Sidechain
53	BA	201	C	Sidechain
53	BA	2016	U	Sidechain
53	BA	202	U	Sidechain
53	BA	2029	G	Sidechain
53	BA	2034	U	Sidechain
53	BA	2035	G	Sidechain
53	BA	2048	G	Sidechain
53	BA	205	G	Sidechain
53	BA	2052	A	Sidechain
53	BA	2057	G	Sidechain
53	BA	2061	G	Sidechain
53	BA	2062	A	Sidechain
53	BA	2064	C	Sidechain
53	BA	207	A	Sidechain
53	BA	2078	C	Sidechain
53	BA	208	C	Sidechain
53	BA	2080	A	Sidechain
53	BA	2093	G	Sidechain
53	BA	2094	A	Sidechain
53	BA	2101	A	Sidechain
53	BA	2103	C	Sidechain
53	BA	2109	U	Sidechain
53	BA	2126	A	Sidechain
53	BA	2132	U	Sidechain
53	BA	2133	G	Sidechain
53	BA	2136	G	Sidechain
53	BA	2137	U	Sidechain
53	BA	214	G	Sidechain
53	BA	2147	A	Sidechain
53	BA	215	G	Sidechain
53	BA	2154	A	Sidechain
53	BA	2157	G	Sidechain
53	BA	2158	A	Sidechain
53	BA	2159	G	Sidechain
53	BA	2160	C	Sidechain
53	BA	2163	A	Sidechain
53	BA	2165	C	Sidechain
53	BA	2168	G	Sidechain
53	BA	2178	C	Sidechain
53	BA	2181	U	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	2196	C	Sidechain
53	BA	2197	U	Sidechain
53	BA	220	G	Sidechain
53	BA	2206	C	Sidechain
53	BA	2207	C	Sidechain
53	BA	2218	G	Sidechain
53	BA	2219	U	Sidechain
53	BA	223	A	Sidechain
53	BA	2234	G	Sidechain
53	BA	2238	G	Sidechain
53	BA	2246	G	Sidechain
53	BA	2259	U	Sidechain
53	BA	2260	C	Sidechain
53	BA	2266	A	Sidechain
53	BA	2267	A	Sidechain
53	BA	227	A	Sidechain
53	BA	2279	G	Sidechain
53	BA	2280	G	Sidechain
53	BA	2282	G	Sidechain
53	BA	2286	G	Sidechain
53	BA	2288	A	Sidechain
53	BA	2292	U	Sidechain
53	BA	2296	U	Sidechain
53	BA	2299	U	Sidechain
53	BA	2303	G	Sidechain
53	BA	2310	C	Sidechain
53	BA	2314	A	Sidechain
53	BA	2321	U	Sidechain
53	BA	2324	U	Sidechain
53	BA	2338	C	Sidechain
53	BA	2345	G	Sidechain
53	BA	2349	G	Sidechain
53	BA	235	U	Sidechain
53	BA	2357	G	Sidechain
53	BA	2361	G	Sidechain
53	BA	2375	G	Sidechain
53	BA	2379	G	Sidechain
53	BA	2380	C	Sidechain
53	BA	2385	C	Sidechain
53	BA	2387	U	Sidechain
53	BA	239	C	Sidechain
53	BA	2391	G	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	2393	U	Sidechain
53	BA	24	G	Sidechain
53	BA	2401	U	Sidechain
53	BA	2402	U	Sidechain
53	BA	2406	A	Sidechain
53	BA	241	A	Sidechain
53	BA	2410	G	Sidechain
53	BA	2413	G	Sidechain
53	BA	2416	C	Sidechain
53	BA	2421	G	Sidechain
53	BA	2425	A	Sidechain
53	BA	2428	G	Sidechain
53	BA	2429	G	Sidechain
53	BA	243	U	Sidechain
53	BA	2433	A	Sidechain
53	BA	2434	A	Sidechain
53	BA	2439	A	Sidechain
53	BA	244	A	Sidechain
53	BA	2444	G	Sidechain
53	BA	2448	A	Sidechain
53	BA	2452	C	Sidechain
53	BA	2453	A	Sidechain
53	BA	2455	G	Sidechain
53	BA	2456	C	Sidechain
53	BA	2458	G	Sidechain
53	BA	246	C	Sidechain
53	BA	2460	U	Sidechain
53	BA	2464	G	Sidechain
53	BA	2465	C	Sidechain
53	BA	2469	A	Sidechain
53	BA	2470	G	Sidechain
53	BA	2475	C	Sidechain
53	BA	2476	A	Sidechain
53	BA	2478	A	Sidechain
53	BA	2481	G	Sidechain
53	BA	2485	G	Sidechain
53	BA	2489	U	Sidechain
53	BA	2498	C	Sidechain
53	BA	250	G	Sidechain
53	BA	2502	G	Sidechain
53	BA	2506	U	Sidechain
53	BA	2507	C	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	2516	A	Sidechain
53	BA	2517	C	Sidechain
53	BA	252	G	Sidechain
53	BA	2523	G	Sidechain
53	BA	2537	U	Sidechain
53	BA	2540	C	Sidechain
53	BA	2552	U	Sidechain
53	BA	256	A	Sidechain
53	BA	2560	A	Sidechain
53	BA	2564	A	Sidechain
53	BA	2566	A	Sidechain
53	BA	2567	G	Sidechain
53	BA	2576	G	Sidechain
53	BA	2582	G	Sidechain
53	BA	2583	G	Sidechain
53	BA	2585	U	Sidechain
53	BA	2586	U	Sidechain
53	BA	2587	A	Sidechain
53	BA	2595	G	Sidechain
53	BA	26	G	Sidechain
53	BA	2603	G	Sidechain
53	BA	2606	C	Sidechain
53	BA	2607	G	Sidechain
53	BA	2608	G	Sidechain
53	BA	2613	U	Sidechain
53	BA	2618	G	Sidechain
53	BA	2636	C	Sidechain
53	BA	2638	G	Sidechain
53	BA	264	C	Sidechain
53	BA	2642	G	Sidechain
53	BA	2645	G	Sidechain
53	BA	265	A	Sidechain
53	BA	2659	G	Sidechain
53	BA	2661	G	Sidechain
53	BA	2666	C	Sidechain
53	BA	2668	G	Sidechain
53	BA	268	C	Sidechain
53	BA	2680	U	Sidechain
53	BA	2685	G	Sidechain
53	BA	2688	G	Sidechain
53	BA	27	G	Sidechain
53	BA	2700	A	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	2709	G	Sidechain
53	BA	2715	C	Sidechain
53	BA	272	A	Sidechain
53	BA	2726	A	Sidechain
53	BA	273	G	Sidechain
53	BA	2733	A	Sidechain
53	BA	2747	G	Sidechain
53	BA	275	C	Sidechain
53	BA	2753	A	Sidechain
53	BA	2755	C	Sidechain
53	BA	2756	U	Sidechain
53	BA	2757	A	Sidechain
53	BA	2763	G	Sidechain
53	BA	2765	A	Sidechain
53	BA	2767	C	Sidechain
53	BA	2771	C	Sidechain
53	BA	2773	C	Sidechain
53	BA	2797	U	Sidechain
53	BA	2798	U	Sidechain
53	BA	28	A	Sidechain
53	BA	2804	U	Sidechain
53	BA	2807	U	Sidechain
53	BA	2812	G	Sidechain
53	BA	2813	A	Sidechain
53	BA	2816	G	Sidechain
53	BA	2822	G	Sidechain
53	BA	2824	C	Sidechain
53	BA	2825	G	Sidechain
53	BA	2832	U	Sidechain
53	BA	2835	A	Sidechain
53	BA	2836	U	Sidechain
53	BA	2838	G	Sidechain
53	BA	2839	G	Sidechain
53	BA	2843	G	Sidechain
53	BA	2846	G	Sidechain
53	BA	2847	U	Sidechain
53	BA	285	G	Sidechain
53	BA	2853	C	Sidechain
53	BA	2857	G	Sidechain
53	BA	2858	C	Sidechain
53	BA	2859	G	Sidechain
53	BA	2871	U	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	2872	A	Sidechain
53	BA	2873	A	Sidechain
53	BA	2874	C	Sidechain
53	BA	2875	C	Sidechain
53	BA	2879	A	Sidechain
53	BA	2883	A	Sidechain
53	BA	2884	U	Sidechain
53	BA	2885	G	Sidechain
53	BA	2887	A	Sidechain
53	BA	2892	G	Sidechain
53	BA	2893	A	Sidechain
53	BA	2895	G	Sidechain
53	BA	2897	U	Sidechain
53	BA	293	U	Sidechain
53	BA	298	G	Sidechain
53	BA	301	G	Sidechain
53	BA	307	G	Sidechain
53	BA	308	G	Sidechain
53	BA	310	A	Sidechain
53	BA	313	G	Sidechain
53	BA	327	G	Sidechain
53	BA	330	A	Sidechain
53	BA	332	A	Sidechain
53	BA	333	G	Sidechain
53	BA	339	U	Sidechain
53	BA	345	A	Sidechain
53	BA	350	G	Sidechain
53	BA	352	A	Sidechain
53	BA	356	G	Sidechain
53	BA	357	C	Sidechain
53	BA	359	G	Sidechain
53	BA	360	U	Sidechain
53	BA	361	G	Sidechain
53	BA	362	A	Sidechain
53	BA	370	G	Sidechain
53	BA	372	G	Sidechain
53	BA	373	U	Sidechain
53	BA	374	A	Sidechain
53	BA	376	G	Sidechain
53	BA	379	G	Sidechain
53	BA	389	G	Sidechain
53	BA	390	U	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	394	C	Sidechain
53	BA	395	U	Sidechain
53	BA	397	U	Sidechain
53	BA	405	U	Sidechain
53	BA	407	G	Sidechain
53	BA	418	C	Sidechain
53	BA	422	A	Sidechain
53	BA	426	C	Sidechain
53	BA	428	A	Sidechain
53	BA	43	G	Sidechain
53	BA	432	A	Sidechain
53	BA	446	G	Sidechain
53	BA	454	A	Sidechain
53	BA	458	G	Sidechain
53	BA	461	C	Sidechain
53	BA	463	G	Sidechain
53	BA	464	U	Sidechain
53	BA	469	G	Sidechain
53	BA	474	G	Sidechain
53	BA	475	C	Sidechain
53	BA	477	A	Sidechain
53	BA	481	G	Sidechain
53	BA	484	C	Sidechain
53	BA	49	A	Sidechain
53	BA	498	G	Sidechain
53	BA	500	G	Sidechain
53	BA	501	A	Sidechain
53	BA	502	A	Sidechain
53	BA	503	A	Sidechain
53	BA	505	A	Sidechain
53	BA	506	G	Sidechain
53	BA	512	G	Sidechain
53	BA	517	C	Sidechain
53	BA	520	G	Sidechain
53	BA	521	U	Sidechain
53	BA	527	C	Sidechain
53	BA	530	G	Sidechain
53	BA	533	G	Sidechain
53	BA	536	G	Sidechain
53	BA	539	G	Sidechain
53	BA	545	U	Sidechain
53	BA	547	A	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	548	G	Sidechain
53	BA	549	G	Sidechain
53	BA	559	G	Sidechain
53	BA	56	A	Sidechain
53	BA	570	G	Sidechain
53	BA	571	U	Sidechain
53	BA	575	A	Sidechain
53	BA	576	U	Sidechain
53	BA	577	G	Sidechain
53	BA	578	G	Sidechain
53	BA	58	G	Sidechain
53	BA	587	C	Sidechain
53	BA	597	G	Sidechain
53	BA	599	A	Sidechain
53	BA	603	A	Sidechain
53	BA	606	U	Sidechain
53	BA	607	U	Sidechain
53	BA	608	A	Sidechain
53	BA	610	C	Sidechain
53	BA	611	C	Sidechain
53	BA	614	A	Sidechain
53	BA	62	U	Sidechain
53	BA	620	G	Sidechain
53	BA	621	A	Sidechain
53	BA	629	G	Sidechain
53	BA	630	G	Sidechain
53	BA	632	A	Sidechain
53	BA	633	A	Sidechain
53	BA	643	A	Sidechain
53	BA	651	G	Sidechain
53	BA	652	U	Sidechain
53	BA	654	A	Sidechain
53	BA	661	A	Sidechain
53	BA	665	U	Sidechain
53	BA	669	G	Sidechain
53	BA	672	C	Sidechain
53	BA	673	C	Sidechain
53	BA	674	G	Sidechain
53	BA	675	A	Sidechain
53	BA	68	G	Sidechain
53	BA	683	U	Sidechain
53	BA	697	G	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	699	A	Sidechain
53	BA	70	G	Sidechain
53	BA	700	G	Sidechain
53	BA	701	G	Sidechain
53	BA	704	G	Sidechain
53	BA	712	G	Sidechain
53	BA	714	U	Sidechain
53	BA	716	A	Sidechain
53	BA	718	A	Sidechain
53	BA	726	G	Sidechain
53	BA	736	C	Sidechain
53	BA	738	G	Sidechain
53	BA	749	A	Sidechain
53	BA	75	G	Sidechain
53	BA	750	A	Sidechain
53	BA	752	A	Sidechain
53	BA	753	A	Sidechain
53	BA	76	C	Sidechain
53	BA	763	G	Sidechain
53	BA	765	C	Sidechain
53	BA	772	C	Sidechain
53	BA	775	G	Sidechain
53	BA	780	G	Sidechain
53	BA	783	A	Sidechain
53	BA	784	G	Sidechain
53	BA	785	G	Sidechain
53	BA	789	A	Sidechain
53	BA	797	G	Sidechain
53	BA	798	G	Sidechain
53	BA	800	A	Sidechain
53	BA	801	G	Sidechain
53	BA	805	G	Sidechain
53	BA	806	C	Sidechain
53	BA	810	U	Sidechain
53	BA	818	G	Sidechain
53	BA	828	U	Sidechain
53	BA	831	G	Sidechain
53	BA	834	G	Sidechain
53	BA	835	C	Sidechain
53	BA	841	G	Sidechain
53	BA	848	C	Sidechain
53	BA	851	C	Sidechain

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Mol	Chain	Res	Type	Group
53	BA	852	U	Sidechain
53	BA	856	G	Sidechain
53	BA	857	G	Sidechain
53	BA	858	G	Sidechain
53	BA	86	G	Sidechain
53	BA	861	A	Sidechain
53	BA	862	G	Sidechain
53	BA	863	A	Sidechain
53	BA	882	G	Sidechain
53	BA	883	G	Sidechain
53	BA	892	A	Sidechain
53	BA	896	A	Sidechain
53	BA	897	C	Sidechain
53	BA	900	A	Sidechain
53	BA	907	G	Sidechain
53	BA	912	C	Sidechain
53	BA	916	G	Sidechain
53	BA	920	A	Sidechain
53	BA	923	G	Sidechain
53	BA	932	U	Sidechain
53	BA	934	U	Sidechain
53	BA	948	C	Sidechain
53	BA	956	G	Sidechain
53	BA	959	A	Sidechain
53	BA	964	C	Sidechain
53	BA	969	G	Sidechain
53	BA	971	G	Sidechain
53	BA	972	A	Sidechain
53	BA	976	G	Sidechain
53	BA	979	A	Sidechain
53	BA	982	C	Sidechain
53	BA	988	A	Sidechain
53	BA	989	G	Sidechain
53	BA	999	U	Sidechain
54	BB	10	G	Sidechain
54	BB	105	G	Sidechain
54	BB	107	G	Sidechain
54	BB	112	G	Sidechain
54	BB	117	G	Sidechain
54	BB	13	G	Sidechain
54	BB	14	U	Sidechain
54	BB	2	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BB	21	G	Sidechain
54	BB	25	U	Sidechain
54	BB	27	C	Sidechain
54	BB	35	C	Sidechain
54	BB	4	C	Sidechain
54	BB	40	U	Sidechain
54	BB	50	A	Sidechain
54	BB	56	G	Sidechain
54	BB	60	C	Sidechain
54	BB	61	G	Sidechain
54	BB	64	G	Sidechain
54	BB	73	A	Sidechain
54	BB	75	G	Sidechain
54	BB	80	U	Sidechain
54	BB	81	G	Sidechain
54	BB	83	G	Sidechain
54	BB	85	G	Sidechain
54	BB	89	U	Sidechain
54	BB	93	C	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	1	0
2	AC	1625	0	1699	2	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	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	AP	639	0	656	0	0
16	AQ	652	0	695	1	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16108	7	0
22	A1	1627	0	808	0	0
23	A2	309	0	158	0	0
24	BC	2083	0	2157	0	0
25	BD	1565	0	1616	0	0
26	BE	1552	0	1619	0	0
27	BF	1420	0	1460	1	0
28	BG	1323	0	1374	0	0
29	BH	1111	0	1148	0	0
30	BI	1032	0	1088	0	0
31	BJ	1129	0	1162	1	0
32	BK	939	0	1012	1	0
33	BL	1045	0	1117	2	0
34	BM	1074	0	1157	1	0
35	BN	961	0	1000	0	0
36	BO	892	0	923	0	0
37	BP	917	0	965	0	0
38	BQ	947	0	1022	0	0
39	BR	816	0	839	1	0
40	BS	857	0	922	0	0
41	BT	739	0	807	0	0
42	BU	780	0	834	0	0
43	BV	753	0	780	0	0
44	BW	599	0	614	0	0
45	BX	625	0	655	0	0
46	BY	509	0	543	0	0
47	BZ	449	0	491	1	0
48	B0	444	0	461	0	0
49	B1	413	0	444	1	0
50	B2	377	0	418	0	0
51	B3	504	0	574	1	0
52	B4	302	0	343	0	0
53	BA	62317	0	30428	10	0
54	BB	2504	0	1247	0	0
55	B5	1658	0	1751	0	0
56	A1	7	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	BA	10	0	10	1	0
All	All	146011	0	97443	27	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 (27) 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)
53:BA:2644:G:H2'	53:BA:2645:G:C8	2.46	0.51
53:BA:1287:A:H2'	53:BA:1288:G:C2	2.47	0.50
49:B1:9:LYS:HE3	49:B1:19:PHE:CD2	2.49	0.48
21:AA:292:G:C5	21:AA:293:G:H1'	2.48	0.47
33:BL:54:GLN:HE21	53:BA:2428:G:N2	2.11	0.47
53:BA:2506:U:C4'	57:BA:3001:FME:HE3	2.45	0.46
31:BJ:47:HIS:CG	53:BA:536:G:H21	2.34	0.45
32:BK:107:LEU:H	32:BK:107:LEU:HD23	1.82	0.45
53:BA:752:A:H2'	53:BA:1781:U:C5	2.52	0.44
21:AA:35:G:H2'	21:AA:36:C:C6	2.53	0.44
53:BA:1646:C:H3'	53:BA:1647:U:C5'	2.48	0.44
53:BA:1570:A:H2'	53:BA:1571:A:C8	2.52	0.44
27:BF:107:VAL:H	27:BF:108:PRO:CD	2.30	0.44
21:AA:235:C:H2'	21:AA:236:A:C8	2.54	0.43
34:BM:14:LYS:HE3	53:BA:956:G:C8	2.54	0.43
47:BZ:28:LEU:H	47:BZ:28:LEU:HD23	1.84	0.43
16:AQ:67:SER:HB2	16:AQ:70:LYS:HE2	2.01	0.42
1:AB:185:ILE:N	1:AB:185:ILE:HD12	2.34	0.42
2:AC:149:LYS:HE3	2:AC:200:TRP:CE3	2.54	0.42
2:AC:149:LYS:HE3	2:AC:200:TRP:CZ3	2.55	0.42
21:AA:989:U:H2'	21:AA:990:C:C6	2.55	0.42
21:AA:420:U:H2'	21:AA:422:C:C5	2.55	0.42
39:BR:24:LYS:HE2	39:BR:66:HIS:CG	2.55	0.42
33:BL:2:ARG:HA	33:BL:3:LEU:O	2.18	0.42
21:AA:920:U:H2'	21:AA:921:U:C6	2.55	0.41
21:AA:1053:G:H2'	21:AA:1199:U:C5	2.55	0.41
51:B3:51:LYS:HE3	53:BA:938:G:OP1	2.21	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%)	193 (88%)	24 (11%)	1 (0%)	34	77
2	AC	205/208 (99%)	186 (91%)	11 (5%)	8 (4%)	4	36
3	AD	203/206 (98%)	192 (95%)	9 (4%)	2 (1%)	19	65
4	AE	150/152 (99%)	141 (94%)	5 (3%)	4 (3%)	6	45
5	AF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	19	65
6	AG	150/152 (99%)	138 (92%)	8 (5%)	4 (3%)	6	45
7	AH	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	24	69
8	AI	126/128 (98%)	115 (91%)	9 (7%)	2 (2%)	12	56
9	AJ	98/100 (98%)	87 (89%)	8 (8%)	3 (3%)	5	42
10	AK	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	11	55
11	AL	121/124 (98%)	111 (92%)	6 (5%)	4 (3%)	5	40
12	AM	112/115 (97%)	94 (84%)	15 (13%)	3 (3%)	6	45
13	AN	98/101 (97%)	89 (91%)	7 (7%)	2 (2%)	9	51
14	AO	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
15	AP	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
16	AQ	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	15	60
17	AR	55/57 (96%)	51 (93%)	2 (4%)	2 (4%)	4	38
18	AS	79/81 (98%)	73 (92%)	3 (4%)	3 (4%)	4	37
19	AT	84/86 (98%)	74 (88%)	7 (8%)	3 (4%)	4	38
20	AU	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
24	BC	270/273 (99%)	245 (91%)	17 (6%)	8 (3%)	5	42
25	BD	207/209 (99%)	174 (84%)	21 (10%)	12 (6%)	2	27
26	BE	199/201 (99%)	182 (92%)	13 (6%)	4 (2%)	9	51
27	BF	176/179 (98%)	143 (81%)	26 (15%)	7 (4%)	4	35
28	BG	174/177 (98%)	152 (87%)	18 (10%)	4 (2%)	8	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BH	147/149 (99%)	131 (89%)	15 (10%)	1 (1%)	26	71
30	BI	139/142 (98%)	128 (92%)	11 (8%)	0	100	100
31	BJ	140/142 (99%)	129 (92%)	6 (4%)	5 (4%)	4	38
32	BK	121/123 (98%)	105 (87%)	11 (9%)	5 (4%)	3	35
33	BL	141/144 (98%)	117 (83%)	14 (10%)	10 (7%)	1	22
34	BM	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	13	57
35	BN	119/121 (98%)	103 (87%)	13 (11%)	3 (2%)	7	46
36	BO	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
37	BP	112/115 (97%)	99 (88%)	10 (9%)	3 (3%)	6	45
38	BQ	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	11	55
39	BR	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	9	51
40	BS	108/110 (98%)	97 (90%)	10 (9%)	1 (1%)	21	67
41	BT	92/94 (98%)	73 (79%)	11 (12%)	8 (9%)	1	17
42	BU	101/104 (97%)	86 (85%)	10 (10%)	5 (5%)	3	31
43	BV	92/94 (98%)	82 (89%)	8 (9%)	2 (2%)	8	49
44	BW	78/80 (98%)	62 (80%)	8 (10%)	8 (10%)	1	12
45	BX	75/79 (95%)	64 (85%)	8 (11%)	3 (4%)	4	35
46	BY	61/63 (97%)	55 (90%)	4 (7%)	2 (3%)	5	40
47	BZ	56/59 (95%)	50 (89%)	5 (9%)	1 (2%)	11	53
48	B0	54/57 (95%)	50 (93%)	3 (6%)	1 (2%)	10	52
49	B1	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	9	51
50	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	8	48
51	B3	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
52	B4	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	2	28
55	B5	221/234 (94%)	211 (96%)	8 (4%)	2 (1%)	21	67
All	All	5876/6008 (98%)	5278 (90%)	447 (8%)	151 (3%)	11	45

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	105	ILE
24	BC	206	LYS
25	BD	9	VAL

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Mol	Chain	Res	Type
25	BD	150	GLN
25	BD	188	LEU
27	BF	12	VAL
33	BL	57	LEU
38	BQ	87	VAL
41	BT	81	LYS
42	BU	43	LYS
44	BW	37	VAL
46	BY	2	LYS
48	B0	24	VAL
49	B1	50	GLU
50	B2	15	SER
2	AC	4	VAL
2	AC	163	ARG
2	AC	189	HIS
3	AD	35	GLN
3	AD	84	ASN
4	AE	89	THR
6	AG	113	LYS
7	AH	105	THR
8	AI	120	ALA
10	AK	126	ARG
12	AM	85	TYR
13	AN	100	SER
16	AQ	39	ARG
18	AS	77	ARG
19	AT	84	LYS
25	BD	2	ILE
25	BD	22	ILE
25	BD	51	THR
25	BD	114	LYS
25	BD	170	VAL
27	BF	107	VAL
27	BF	135	ILE
27	BF	136	ILE
28	BG	22	VAL
28	BG	57	TYR
31	BJ	47	HIS
31	BJ	112	GLY
33	BL	4	ASN
33	BL	29	LYS
33	BL	30	THR

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Mol	Chain	Res	Type
35	BN	11	ASN
37	BP	74	GLN
39	BR	44	GLY
41	BT	63	VAL
42	BU	51	LEU
45	BX	17	ARG
46	BY	7	ARG
47	BZ	31	ILE
52	B4	4	ARG
52	B4	16	ILE
1	AB	128	LEU
6	AG	56	SER
9	AJ	75	ASP
11	AL	78	VAL
12	AM	23	GLY
12	AM	42	VAL
17	AR	20	ILE
17	AR	47	ARG
24	BC	19	VAL
24	BC	153	LEU
24	BC	228	ASP
25	BD	106	LYS
25	BD	119	ALA
26	BE	90	GLN
26	BE	165	HIS
27	BF	72	SER
31	BJ	81	ILE
32	BK	32	TYR
33	BL	55	MET
33	BL	75	ALA
35	BN	10	LEU
35	BN	103	ARG
39	BR	53	PHE
41	BT	28	ASN
41	BT	68	LYS
41	BT	88	LYS
43	BV	71	LYS
44	BW	10	ARG
44	BW	11	ASN
44	BW	14	ASP
44	BW	51	GLY
45	BX	21	LEU

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Mol	Chain	Res	Type
2	AC	180	ASP
2	AC	195	ILE
6	AG	129	ASN
8	AI	55	ASP
9	AJ	33	GLY
11	AL	33	CYS
11	AL	117	GLY
18	AS	6	LYS
19	AT	43	LYS
24	BC	47	ARG
24	BC	196	ASN
24	BC	197	ALA
24	BC	204	LEU
25	BD	27	ILE
29	BH	10	ALA
37	BP	31	VAL
40	BS	41	LYS
41	BT	15	HIS
41	BT	36	LYS
42	BU	5	ARG
44	BW	23	LYS
44	BW	41	GLY
44	BW	78	PHE
45	BX	27	ARG
2	AC	167	TYR
4	AE	121	ASN
6	AG	114	SER
9	AJ	41	PRO
18	AS	79	TYR
26	BE	94	GLN
27	BF	148	VAL
28	BG	9	VAL
31	BJ	79	GLY
32	BK	47	ILE
33	BL	3	LEU
33	BL	7	SER
34	BM	134	THR
37	BP	85	VAL
42	BU	12	VAL
42	BU	45	GLN
43	BV	54	ALA
55	B5	207	VAL

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Mol	Chain	Res	Type
2	AC	144	GLY
4	AE	43	GLY
5	AF	6	ILE
13	AN	63	ARG
31	BJ	78	THR
32	BK	46	ALA
38	BQ	90	ASP
41	BT	11	LEU
10	AK	73	VAL
11	AL	43	LYS
25	BD	73	VAL
33	BL	101	ILE
55	B5	91	GLY
26	BE	59	PRO
27	BF	103	ILE
33	BL	88	GLY
19	AT	3	ILE
28	BG	116	LEU
32	BK	93	GLN
2	AC	13	ILE
32	BK	26	GLY
34	BM	36	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%)	169 (99%)	1 (1%)	90	95
3	AD	172/173 (99%)	171 (99%)	1 (1%)	90	95
4	AE	113/113 (100%)	112 (99%)	1 (1%)	84	93
5	AF	87/87 (100%)	85 (98%)	2 (2%)	58	83
6	AG	123/123 (100%)	122 (99%)	1 (1%)	86	94
7	AH	104/105 (99%)	103 (99%)	1 (1%)	82	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AI	105/105 (100%)	102 (97%)	3 (3%)	50	78
9	AJ	86/86 (100%)	84 (98%)	2 (2%)	58	83
10	AK	90/90 (100%)	88 (98%)	2 (2%)	60	83
11	AL	103/104 (99%)	101 (98%)	2 (2%)	65	86
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	80 (96%)	3 (4%)	42	74
14	AO	76/77 (99%)	74 (97%)	2 (3%)	54	80
15	AP	65/65 (100%)	64 (98%)	1 (2%)	72	88
16	AQ	74/74 (100%)	73 (99%)	1 (1%)	74	89
17	AR	48/48 (100%)	47 (98%)	1 (2%)	61	84
18	AS	70/70 (100%)	67 (96%)	3 (4%)	35	70
19	AT	65/65 (100%)	64 (98%)	1 (2%)	72	88
20	AU	44/44 (100%)	43 (98%)	1 (2%)	58	83
24	BC	216/217 (100%)	214 (99%)	2 (1%)	84	93
25	BD	164/164 (100%)	162 (99%)	2 (1%)	78	90
26	BE	165/165 (100%)	161 (98%)	4 (2%)	57	82
27	BF	149/150 (99%)	144 (97%)	5 (3%)	44	75
28	BG	137/138 (99%)	134 (98%)	3 (2%)	60	83
29	BH	114/114 (100%)	113 (99%)	1 (1%)	84	93
30	BI	109/110 (99%)	108 (99%)	1 (1%)	84	93
31	BJ	116/116 (100%)	115 (99%)	1 (1%)	84	93
32	BK	103/103 (100%)	98 (95%)	5 (5%)	31	67
33	BL	102/103 (99%)	100 (98%)	2 (2%)	63	85
34	BM	109/109 (100%)	106 (97%)	3 (3%)	51	78
35	BN	100/100 (100%)	98 (98%)	2 (2%)	63	85
36	BO	86/87 (99%)	85 (99%)	1 (1%)	78	90
37	BP	99/100 (99%)	98 (99%)	1 (1%)	82	92
38	BQ	89/90 (99%)	89 (100%)	0	100	100
39	BR	84/84 (100%)	82 (98%)	2 (2%)	57	82
40	BS	93/93 (100%)	91 (98%)	2 (2%)	60	83
41	BT	80/80 (100%)	78 (98%)	2 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BU	83/84 (99%)	83 (100%)	0	100	100
43	BV	78/78 (100%)	76 (97%)	2 (3%)	54	80
44	BW	59/59 (100%)	55 (93%)	4 (7%)	20	57
45	BX	67/68 (98%)	65 (97%)	2 (3%)	48	77
46	BY	55/55 (100%)	55 (100%)	0	100	100
47	BZ	48/49 (98%)	45 (94%)	3 (6%)	22	59
48	B0	47/48 (98%)	46 (98%)	1 (2%)	61	84
49	B1	45/45 (100%)	44 (98%)	1 (2%)	60	83
50	B2	38/38 (100%)	37 (97%)	1 (3%)	54	80
51	B3	51/52 (98%)	48 (94%)	3 (6%)	24	61
52	B4	34/34 (100%)	34 (100%)	0	100	100
55	B5	173/181 (96%)	167 (96%)	6 (4%)	43	74
All	All	4842/4870 (99%)	4748 (98%)	94 (2%)	67	86

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	187	ASP
1	AB	204	ASP
1	AB	209	VAL
2	AC	35	ASP
3	AD	55	ARG
4	AE	105	ILE
5	AF	36	ILE
5	AF	41	ASP
6	AG	51	GLN
7	AH	105	THR
8	AI	3	ASN
8	AI	66	VAL
8	AI	98	ARG
9	AJ	48	ARG
9	AJ	50	THR
10	AK	55	ARG
10	AK	84	MET
11	AL	19	ASN
11	AL	34	THR
13	AN	6	MET
13	AN	40	ASP

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Mol	Chain	Res	Type
13	AN	41	ARG
14	AO	5	GLU
14	AO	45	HIS
15	AP	1	MET
16	AQ	41	THR
17	AR	69	TYR
18	AS	11	ASP
18	AS	30	LEU
18	AS	54	ARG
19	AT	27	MET
20	AU	20	ARG
24	BC	89	ASN
24	BC	263	ASP
25	BD	148	GLN
25	BD	164	GLN
26	BE	3	LEU
26	BE	60	TRP
26	BE	69	ARG
26	BE	120	VAL
27	BF	41	GLU
27	BF	46	LYS
27	BF	113	PHE
27	BF	122	ASP
27	BF	129	MET
28	BG	154	GLU
28	BG	162	ARG
28	BG	163	TYR
29	BH	104	THR
30	BI	16	MET
31	BJ	1	MET
32	BK	4	GLU
32	BK	29	HIS
32	BK	32	TYR
32	BK	80	ASP
32	BK	105	ARG
33	BL	21	ARG
33	BL	39	LYS
34	BM	81	ARG
34	BM	97	GLN
34	BM	126	ILE
35	BN	1	MET
35	BN	3	HIS

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Mol	Chain	Res	Type
36	BO	36	TYR
37	BP	74	GLN
39	BR	2	TYR
39	BR	82	HIS
40	BS	15	GLN
40	BS	77	ASP
41	BT	60	THR
41	BT	86	THR
43	BV	12	GLN
43	BV	51	GLN
44	BW	31	LEU
44	BW	38	ARG
44	BW	39	GLN
44	BW	55	ASP
45	BX	26	ARG
45	BX	31	ASN
47	BZ	28	LEU
47	BZ	31	ILE
47	BZ	33	HIS
48	B0	41	HIS
49	B1	24	LYS
50	B2	1	MET
51	B3	23	HIS
51	B3	27	ASN
51	B3	48	MET
55	B5	40	GLU
55	B5	51	ASP
55	B5	97	MET
55	B5	109	MET
55	B5	126	GLN
55	B5	148	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
52	B4	37	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	195 (12%)	46 (3%)
22	A1	73/76 (96%)	7 (9%)	2 (2%)
23	A2	14/15 (93%)	4 (28%)	2 (14%)
53	BA	2902/2903 (99%)	455 (15%)	123 (4%)
54	BB	116/118 (98%)	19 (16%)	2 (1%)
All	All	4635/4645 (99%)	680 (14%)	175 (3%)

All (680) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	8	A
21	AA	9	G
21	AA	16	A
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	50	A
21	AA	51	A
21	AA	66	A
21	AA	80	A
21	AA	81	A
21	AA	83	C
21	AA	85	U
21	AA	86	G
21	AA	87	C
21	AA	109	A
21	AA	110	C
21	AA	112	G
21	AA	121	U
21	AA	144	G
21	AA	148	G
21	AA	188	C
21	AA	194	C
21	AA	198	G
21	AA	209	U
21	AA	225	C
21	AA	240	G
21	AA	245	U
21	AA	247	G
21	AA	251	G
21	AA	266	G

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Mol	Chain	Res	Type
21	AA	275	G
21	AA	280	C
21	AA	289	G
21	AA	324	G
21	AA	329	A
21	AA	331	G
21	AA	332	G
21	AA	347	G
21	AA	352	C
21	AA	354	G
21	AA	367	U
21	AA	372	C
21	AA	373	A
21	AA	381	C
21	AA	389	A
21	AA	397	A
21	AA	398	U
21	AA	411	A
21	AA	412	A
21	AA	413	G
21	AA	414	A
21	AA	421	U
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	451	A
21	AA	463	U
21	AA	464	U
21	AA	465	A
21	AA	466	A
21	AA	468	A
21	AA	479	U
21	AA	481	G
21	AA	484	G
21	AA	511	C
21	AA	512	U
21	AA	518	C
21	AA	527	G
21	AA	530	G
21	AA	531	U
21	AA	532	A
21	AA	533	A

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Mol	Chain	Res	Type
21	AA	534	U
21	AA	535	A
21	AA	547	A
21	AA	557	G
21	AA	559	A
21	AA	560	A
21	AA	563	A
21	AA	564	C
21	AA	567	G
21	AA	572	A
21	AA	574	A
21	AA	576	C
21	AA	633	G
21	AA	665	A
21	AA	673	A
21	AA	674	G
21	AA	687	A
21	AA	695	A
21	AA	700	G
21	AA	702	A
21	AA	704	A
21	AA	723	U
21	AA	733	G
21	AA	734	G
21	AA	755	G
21	AA	794	A
21	AA	812	G
21	AA	816	A
21	AA	817	C
21	AA	819	A
21	AA	821	G
21	AA	841	C
21	AA	843	U
21	AA	845	A
21	AA	864	A
21	AA	872	A
21	AA	873	A
21	AA	877	G
21	AA	890	G
21	AA	918	A
21	AA	927	G
21	AA	934	C

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Mol	Chain	Res	Type
21	AA	935	A
21	AA	945	G
21	AA	960	U
21	AA	969	A
21	AA	971	G
21	AA	974	A
21	AA	975	A
21	AA	977	A
21	AA	978	A
21	AA	991	U
21	AA	993	G
21	AA	995	C
21	AA	1004	A
21	AA	1008	U
21	AA	1017	U
21	AA	1020	G
21	AA	1030	U
21	AA	1031	C
21	AA	1033	G
21	AA	1037	C
21	AA	1054	C
21	AA	1065	U
21	AA	1066	C
21	AA	1094	G
21	AA	1101	A
21	AA	1136	C
21	AA	1137	C
21	AA	1138	G
21	AA	1139	G
21	AA	1145	A
21	AA	1159	U
21	AA	1190	G
21	AA	1191	A
21	AA	1197	A
21	AA	1200	C
21	AA	1201	A
21	AA	1202	U
21	AA	1212	U
21	AA	1217	C
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A

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Mol	Chain	Res	Type
21	AA	1238	A
21	AA	1256	A
21	AA	1257	A
21	AA	1267	C
21	AA	1279	G
21	AA	1280	A
21	AA	1281	C
21	AA	1285	A
21	AA	1286	U
21	AA	1287	A
21	AA	1290	G
21	AA	1300	G
21	AA	1301	U
21	AA	1302	C
21	AA	1303	C
21	AA	1305	G
21	AA	1320	C
21	AA	1323	G
21	AA	1330	U
21	AA	1338	G
21	AA	1340	A
21	AA	1346	A
21	AA	1349	A
21	AA	1379	G
21	AA	1397	C
21	AA	1398	A
21	AA	1399	C
21	AA	1401	G
21	AA	1411	C
21	AA	1418	A
21	AA	1419	G
21	AA	1432	G
21	AA	1447	A
21	AA	1459	G
21	AA	1460	C
21	AA	1499	A
22	A1	10	G
22	A1	16	C
22	A1	17	U
22	A1	45	G
22	A1	49	G
22	A1	74	C

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Mol	Chain	Res	Type
22	A1	75	C
23	A2	81	U
23	A2	82	A
23	A2	85	G
23	A2	92	U
53	BA	9	G
53	BA	10	A
53	BA	15	G
53	BA	20	C
53	BA	34	U
53	BA	46	G
53	BA	50	U
53	BA	62	U
53	BA	71	A
53	BA	74	A
53	BA	75	G
53	BA	77	G
53	BA	91	A
53	BA	101	A
53	BA	119	A
53	BA	120	U
53	BA	122	G
53	BA	126	A
53	BA	127	A
53	BA	142	A
53	BA	149	A
53	BA	181	A
53	BA	196	A
53	BA	197	A
53	BA	199	A
53	BA	200	U
53	BA	205	G
53	BA	216	A
53	BA	222	A
53	BA	224	U
53	BA	233	A
53	BA	242	G
53	BA	243	U
53	BA	248	G
53	BA	250	G
53	BA	265	A
53	BA	272	A

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Mol	Chain	Res	Type
53	BA	273	G
53	BA	277	G
53	BA	278	A
53	BA	299	A
53	BA	330	A
53	BA	331	C
53	BA	332	A
53	BA	345	A
53	BA	370	G
53	BA	373	U
53	BA	374	A
53	BA	386	G
53	BA	387	U
53	BA	388	G
53	BA	390	U
53	BA	391	A
53	BA	411	G
53	BA	430	A
53	BA	435	C
53	BA	447	A
53	BA	451	U
53	BA	452	G
53	BA	454	A
53	BA	455	C
53	BA	457	A
53	BA	472	A
53	BA	473	G
53	BA	474	G
53	BA	480	A
53	BA	481	G
53	BA	482	A
53	BA	505	A
53	BA	506	G
53	BA	508	A
53	BA	510	C
53	BA	511	U
53	BA	512	G
53	BA	526	A
53	BA	527	C
53	BA	528	A
53	BA	529	A
53	BA	530	G

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Mol	Chain	Res	Type
53	BA	531	C
53	BA	532	A
53	BA	533	G
53	BA	546	U
53	BA	547	A
53	BA	572	A
53	BA	574	A
53	BA	581	C
53	BA	587	C
53	BA	588	U
53	BA	590	A
53	BA	603	A
53	BA	607	U
53	BA	613	A
53	BA	614	A
53	BA	615	U
53	BA	616	A
53	BA	617	G
53	BA	627	A
53	BA	631	A
53	BA	637	A
53	BA	644	A
53	BA	645	C
53	BA	653	U
53	BA	655	A
53	BA	671	C
53	BA	672	C
53	BA	686	U
53	BA	717	C
53	BA	719	C
53	BA	730	A
53	BA	747	U
53	BA	752	A
53	BA	753	A
53	BA	763	G
53	BA	764	A
53	BA	765	C
53	BA	776	G
53	BA	782	A
53	BA	783	A
53	BA	784	G
53	BA	785	G

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Mol	Chain	Res	Type
53	BA	792	A
53	BA	793	A
53	BA	805	G
53	BA	811	U
53	BA	812	C
53	BA	827	U
53	BA	829	A
53	BA	830	G
53	BA	831	G
53	BA	846	U
53	BA	858	G
53	BA	888	C
53	BA	889	C
53	BA	896	A
53	BA	897	C
53	BA	910	A
53	BA	914	G
53	BA	915	C
53	BA	931	U
53	BA	932	U
53	BA	941	A
53	BA	946	C
53	BA	960	A
53	BA	961	C
53	BA	962	G
53	BA	974	G
53	BA	975	A
53	BA	976	G
53	BA	977	G
53	BA	982	C
53	BA	983	A
53	BA	984	A
53	BA	996	A
53	BA	1012	U
53	BA	1013	C
53	BA	1021	A
53	BA	1022	G
53	BA	1026	G
53	BA	1034	G
53	BA	1038	G
53	BA	1046	A
53	BA	1057	A

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Mol	Chain	Res	Type
53	BA	1060	U
53	BA	1063	G
53	BA	1070	A
53	BA	1071	G
53	BA	1073	A
53	BA	1076	C
53	BA	1078	U
53	BA	1079	C
53	BA	1088	A
53	BA	1089	A
53	BA	1091	G
53	BA	1112	G
53	BA	1124	G
53	BA	1127	A
53	BA	1128	G
53	BA	1129	A
53	BA	1132	U
53	BA	1133	A
53	BA	1134	A
53	BA	1135	C
53	BA	1141	U
53	BA	1142	A
53	BA	1143	A
53	BA	1149	G
53	BA	1150	C
53	BA	1156	A
53	BA	1176	U
53	BA	1186	G
53	BA	1204	A
53	BA	1213	A
53	BA	1230	A
53	BA	1231	U
53	BA	1236	G
53	BA	1237	A
53	BA	1241	A
53	BA	1244	A
53	BA	1247	A
53	BA	1250	G
53	BA	1253	A
53	BA	1256	G
53	BA	1261	C
53	BA	1266	G

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Mol	Chain	Res	Type
53	BA	1267	U
53	BA	1272	A
53	BA	1274	A
53	BA	1275	A
53	BA	1276	A
53	BA	1291	C
53	BA	1300	G
53	BA	1301	A
53	BA	1309	G
53	BA	1314	C
53	BA	1315	C
53	BA	1320	C
53	BA	1325	U
53	BA	1333	G
53	BA	1341	G
53	BA	1345	C
53	BA	1350	C
53	BA	1365	A
53	BA	1366	A
53	BA	1374	G
53	BA	1379	U
53	BA	1383	A
53	BA	1390	U
53	BA	1396	U
53	BA	1416	G
53	BA	1420	A
53	BA	1427	A
53	BA	1428	C
53	BA	1452	G
53	BA	1453	A
53	BA	1455	G
53	BA	1458	U
53	BA	1459	G
53	BA	1461	C
53	BA	1475	G
53	BA	1482	G
53	BA	1490	A
53	BA	1494	A
53	BA	1508	A
53	BA	1509	A
53	BA	1535	A
53	BA	1537	G

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Mol	Chain	Res	Type
53	BA	1538	G
53	BA	1539	U
53	BA	1554	U
53	BA	1555	G
53	BA	1560	G
53	BA	1566	A
53	BA	1569	A
53	BA	1584	U
53	BA	1585	C
53	BA	1597	A
53	BA	1600	C
53	BA	1607	C
53	BA	1608	A
53	BA	1609	A
53	BA	1610	A
53	BA	1615	C
53	BA	1626	A
53	BA	1636	U
53	BA	1646	C
53	BA	1647	U
53	BA	1648	U
53	BA	1654	A
53	BA	1655	A
53	BA	1670	C
53	BA	1674	G
53	BA	1683	U
53	BA	1684	G
53	BA	1728	C
53	BA	1731	G
53	BA	1739	A
53	BA	1758	U
53	BA	1764	C
53	BA	1773	A
53	BA	1780	A
53	BA	1782	U
53	BA	1800	C
53	BA	1808	A
53	BA	1810	A
53	BA	1816	C
53	BA	1821	A
53	BA	1847	A
53	BA	1876	A

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Mol	Chain	Res	Type
53	BA	1877	A
53	BA	1884	G
53	BA	1906	G
53	BA	1913	A
53	BA	1914	C
53	BA	1929	G
53	BA	1937	A
53	BA	1939	U
53	BA	1943	U
53	BA	1953	A
53	BA	1954	G
53	BA	1963	U
53	BA	1964	G
53	BA	1965	C
53	BA	1966	A
53	BA	1967	C
53	BA	1970	A
53	BA	1972	G
53	BA	1992	G
53	BA	1993	U
53	BA	1996	C
53	BA	1997	C
53	BA	2022	U
53	BA	2023	C
53	BA	2030	A
53	BA	2031	A
53	BA	2032	G
53	BA	2033	A
53	BA	2034	U
53	BA	2043	C
53	BA	2053	G
53	BA	2055	C
53	BA	2056	G
53	BA	2059	A
53	BA	2060	A
53	BA	2061	G
53	BA	2069	G
53	BA	2073	C
53	BA	2093	G
53	BA	2094	A
53	BA	2102	G
53	BA	2104	C

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Mol	Chain	Res	Type
53	BA	2112	G
53	BA	2113	U
53	BA	2115	G
53	BA	2116	G
53	BA	2130	U
53	BA	2131	U
53	BA	2133	G
53	BA	2134	A
53	BA	2136	G
53	BA	2137	U
53	BA	2155	U
53	BA	2159	G
53	BA	2169	A
53	BA	2172	U
53	BA	2173	A
53	BA	2174	C
53	BA	2204	G
53	BA	2207	C
53	BA	2212	A
53	BA	2213	U
53	BA	2225	A
53	BA	2238	G
53	BA	2239	G
53	BA	2262	U
53	BA	2266	A
53	BA	2267	A
53	BA	2269	G
53	BA	2283	C
53	BA	2297	A
53	BA	2304	G
53	BA	2305	U
53	BA	2308	G
53	BA	2313	C
53	BA	2320	U
53	BA	2321	U
53	BA	2322	A
53	BA	2325	G
53	BA	2333	A
53	BA	2334	U
53	BA	2335	A
53	BA	2339	C
53	BA	2347	C

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Mol	Chain	Res	Type
53	BA	2350	C
53	BA	2352	A
53	BA	2353	G
53	BA	2383	G
53	BA	2385	C
53	BA	2390	U
53	BA	2391	G
53	BA	2403	C
53	BA	2407	A
53	BA	2420	C
53	BA	2424	C
53	BA	2427	C
53	BA	2429	G
53	BA	2430	A
53	BA	2432	A
53	BA	2438	U
53	BA	2439	A
53	BA	2441	U
53	BA	2448	A
53	BA	2452	C
53	BA	2468	A
53	BA	2469	A
53	BA	2476	A
53	BA	2488	G
53	BA	2491	U
53	BA	2498	C
53	BA	2500	U
53	BA	2501	C
53	BA	2502	G
53	BA	2503	A
53	BA	2504	U
53	BA	2505	G
53	BA	2518	A
53	BA	2529	G
53	BA	2530	A
53	BA	2531	A
53	BA	2534	A
53	BA	2543	G
53	BA	2566	A
53	BA	2567	G
53	BA	2573	C
53	BA	2578	G

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Mol	Chain	Res	Type
53	BA	2582	G
53	BA	2584	U
53	BA	2588	G
53	BA	2599	G
53	BA	2613	U
53	BA	2614	A
53	BA	2615	U
53	BA	2616	C
53	BA	2629	U
53	BA	2639	A
53	BA	2640	G
53	BA	2646	C
53	BA	2660	A
53	BA	2669	G
53	BA	2689	U
53	BA	2690	U
53	BA	2712	C
53	BA	2755	C
53	BA	2757	A
53	BA	2765	A
53	BA	2777	G
53	BA	2778	A
53	BA	2780	G
53	BA	2790	U
53	BA	2791	G
53	BA	2797	U
53	BA	2798	U
53	BA	2799	A
53	BA	2800	A
53	BA	2809	A
53	BA	2817	U
53	BA	2820	A
53	BA	2823	A
53	BA	2835	A
53	BA	2836	U
53	BA	2868	A
53	BA	2880	C
53	BA	2886	A
53	BA	2894	G
53	BA	2895	G
54	BB	13	G
54	BB	14	U

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Mol	Chain	Res	Type
54	BB	15	A
54	BB	16	G
54	BB	25	U
54	BB	35	C
54	BB	36	C
54	BB	42	C
54	BB	44	G
54	BB	45	A
54	BB	56	G
54	BB	57	A
54	BB	74	U
54	BB	81	G
54	BB	87	U
54	BB	90	C
54	BB	91	C
54	BB	109	A
54	BB	118	C

All (175) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	32	A
21	AA	80	A
21	AA	109	A
21	AA	173	U
21	AA	239	U
21	AA	279	A
21	AA	329	A
21	AA	372	C
21	AA	451	A
21	AA	461	A
21	AA	530	G
21	AA	532	A
21	AA	533	A
21	AA	559	A
21	AA	575	G
21	AA	618	C
21	AA	700	G
21	AA	723	U
21	AA	812	G
21	AA	841	C

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Mol	Chain	Res	Type
21	AA	872	A
21	AA	934	C
21	AA	944	G
21	AA	958	A
21	AA	974	A
21	AA	978	A
21	AA	992	U
21	AA	1053	G
21	AA	1065	U
21	AA	1137	C
21	AA	1139	G
21	AA	1159	U
21	AA	1190	G
21	AA	1200	C
21	AA	1201	A
21	AA	1225	A
21	AA	1296	C
21	AA	1358	U
21	AA	1398	A
21	AA	1399	C
21	AA	1432	G
21	AA	1447	A
21	AA	1455	G
21	AA	1459	G
21	AA	1529	G
22	A1	10	G
22	A1	16	C
23	A2	81	U
23	A2	84	G
53	BA	9	G
53	BA	48	G
53	BA	49	A
53	BA	60	G
53	BA	142	A
53	BA	196	A
53	BA	215	G
53	BA	242	G
53	BA	249	C
53	BA	276	U
53	BA	278	A
53	BA	323	C
53	BA	386	G

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Mol	Chain	Res	Type
53	BA	387	U
53	BA	424	G
53	BA	446	G
53	BA	473	G
53	BA	479	A
53	BA	482	A
53	BA	505	A
53	BA	510	C
53	BA	511	U
53	BA	520	G
53	BA	571	U
53	BA	573	U
53	BA	587	C
53	BA	613	A
53	BA	627	A
53	BA	629	G
53	BA	643	A
53	BA	670	A
53	BA	686	U
53	BA	728	G
53	BA	752	A
53	BA	762	U
53	BA	764	A
53	BA	776	G
53	BA	792	A
53	BA	811	U
53	BA	816	C
53	BA	829	A
53	BA	888	C
53	BA	914	G
53	BA	941	A
53	BA	944	C
53	BA	957	C
53	BA	961	C
53	BA	962	G
53	BA	963	U
53	BA	975	A
53	BA	976	G
53	BA	1021	A
53	BA	1056	G
53	BA	1062	G
53	BA	1070	A

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Mol	Chain	Res	Type
53	BA	1072	C
53	BA	1078	U
53	BA	1087	G
53	BA	1088	A
53	BA	1126	A
53	BA	1128	G
53	BA	1134	A
53	BA	1204	A
53	BA	1236	G
53	BA	1252	G
53	BA	1266	G
53	BA	1272	A
53	BA	1275	A
53	BA	1288	G
53	BA	1289	C
53	BA	1300	G
53	BA	1325	U
53	BA	1365	A
53	BA	1451	C
53	BA	1458	U
53	BA	1508	A
53	BA	1539	U
53	BA	1554	U
53	BA	1608	A
53	BA	1610	A
53	BA	1625	C
53	BA	1637	A
53	BA	1655	A
53	BA	1668	A
53	BA	1780	A
53	BA	1929	G
53	BA	1936	A
53	BA	1952	A
53	BA	1953	A
53	BA	1966	A
53	BA	1972	G
53	BA	2033	A
53	BA	2060	A
53	BA	2062	A
53	BA	2115	G
53	BA	2130	U
53	BA	2225	A

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Mol	Chain	Res	Type
53	BA	2261	C
53	BA	2266	A
53	BA	2275	C
53	BA	2288	A
53	BA	2321	U
53	BA	2335	A
53	BA	2438	U
53	BA	2451	A
53	BA	2468	A
53	BA	2487	G
53	BA	2503	A
53	BA	2518	A
53	BA	2531	A
53	BA	2566	A
53	BA	2581	G
53	BA	2602	A
53	BA	2665	A
53	BA	2666	C
53	BA	2712	C
53	BA	2756	U
53	BA	2777	G
53	BA	2778	A
53	BA	2790	U
53	BA	2799	A
53	BA	2832	U
53	BA	2884	U
54	BB	12	C
54	BB	56	G

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

6 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	1.84	2 (13%)	18,37,40	3.22	2 (11%)
22	6MZ	A1	37	22	17,25,26	1.01	2 (11%)	15,36,39	1.30	1 (6%)
22	7MG	A1	46	22	20,26,27	2.40	3 (15%)	23,39,42	2.01	2 (8%)
22	5MU	A1	54	22	13,22,23	1.11	1 (7%)	16,32,35	4.62	3 (18%)
22	PSU	A1	55	22	15,21,22	1.19	2 (13%)	16,30,33	3.26	3 (18%)
22	4SU	A1	7	22	12,21,22	1.07	1 (8%)	15,30,33	1.96	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 Torsions 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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-9.61	1.31	1.45
22	A1	34	CM0	O5-C5	-5.80	1.25	1.37
22	A1	46	7MG	C8-N7	-2.76	1.30	1.43
22	A1	37	6MZ	C8-N7	-2.30	1.30	1.34
22	A1	55	PSU	C2'-C1'	-2.21	1.51	1.53
22	A1	37	6MZ	C5-C4	-2.09	1.35	1.40
22	A1	46	7MG	C2-N2	-2.07	1.29	1.34
22	A1	7	4SU	C6-N1	2.05	1.38	1.35
22	A1	34	CM0	C4-N3	2.46	1.37	1.33
22	A1	55	PSU	C4-N3	2.61	1.37	1.33
22	A1	54	5MU	C4-N3	2.69	1.37	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C5-C4-N3	-12.80	114.61	125.35
22	A1	7	4SU	C5-C4-N3	-7.17	115.95	123.56
22	A1	46	7MG	C5-C6-N1	-6.63	113.52	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	55	PSU	C5-C6-N1	-2.85	120.41	124.38
22	A1	34	CM0	O5-C7-C8	2.10	112.36	108.01
22	A1	54	5MU	O4'-C1'-N1	2.31	112.50	108.10
22	A1	55	PSU	O4'-C1'-C2'	2.67	107.58	104.69
22	A1	37	6MZ	C2-N1-C6	3.63	119.08	116.47
22	A1	46	7MG	C6-N1-C2	6.09	123.02	115.88
22	A1	55	PSU	C4-N3-C2	12.08	125.24	115.16
22	A1	54	5MU	C4-N3-C2	12.70	125.75	115.16
22	A1	34	CM0	C4-N3-C2	12.70	125.75	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	$\# Z  > 2$
56	VAL	A1	101	57,22	5,6,7	0.49	0	5,7,9	1.81	1 (20%)
57	FME	BA	3001	56	8,9,10	0.61	0	5,9,11	1.27	1 (20%)

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
56	VAL	A1	101	57,22	-	0/4/6/8	0/0/0/0
57	FME	BA	3001	56	-	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( $^{\circ}$ )
56	A1	101	VAL	O-C-CA	-3.71	115.55	125.69
57	BA	3001	FME	O-C-CA	-2.11	119.92	125.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	BA	3001	FME	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.