



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 11, 2019 – 08:46 AM EST

PDB ID : 4V6Y  
EMDB ID: : EMD-1716  
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in classic pre-translocation state (pre1a)  
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.  
Deposited on : 2013-10-14  
Resolution : 12.00 Å(reported)  
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

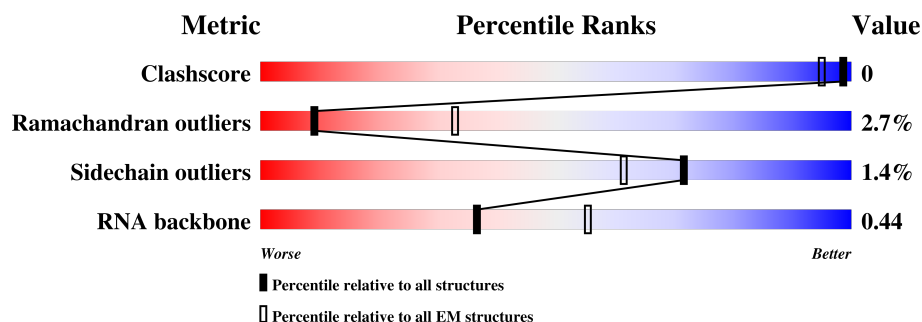
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 12.00 Å.

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



















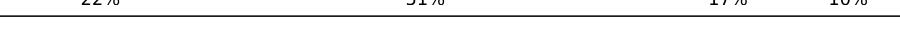





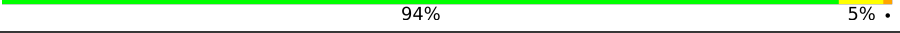
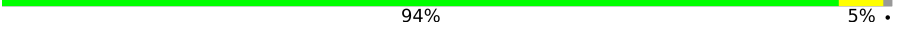

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	93% 7%
2	AC	208	92% 7%
3	AD	206	87% 12%
4	AE	152	89% 11% .
5	AF	101	87% 13%
6	AG	152	88% 13%
7	AH	130	91% 8% .
8	AI	128	81% 18% .











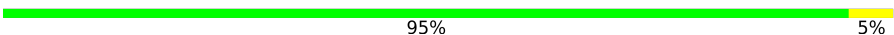












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Mol	Chain	Length	Quality of chain
9	AJ	100	 84% 16%
10	AK	118	 89% 11%
11	AL	124	 85% 15% .
12	AM	115	 85% 14% .
13	AN	101	 86% 12% ..
14	AO	89	 87% 12% .
15	AP	81	 84% 16%
16	AQ	82	 90% 9% .
17	AR	57	 93% 7%
18	AS	81	 89% 11%
19	AT	86	 90% 10%
20	AU	53	 66% 26% 8%
21	AA	1533	 15% 56% 24% 5%
22	A1	76	 20% 53% 22% 5%
23	A2	15	 20% 40% 20% 20%
24	A3	77	 22% 51% 17% 10%
25	BC	273	 91% 8%
26	BD	209	 89% 11%
27	BE	201	 89% 10%
28	BF	179	 89% 11% .
29	BG	177	 92% 7% ..
30	BH	149	 94% 5% .
31	BI	142	 94% 5% .
32	BJ	142	 91% 8% .
33	BK	123	 90% 10%

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Mol	Chain	Length	Quality of chain
34	BL	144	 85% 14% .
35	BM	136	 88% 12%
36	BN	121	 88% 12%
37	BO	117	 89% 10% .
38	BP	115	 83% 16% .
39	BQ	118	 84% 14% ..
40	BR	103	 89% 10% .
41	BS	110	 92% 8%
42	BT	94	 91% 7% .
43	BU	104	 90% 8% ..
44	BV	94	 95% 5%
45	BW	80	 88% 13%
46	BX	79	 84% 10% . .
47	BY	63	 90% 10%
48	BZ	59	 90% 7% ..
49	B0	57	 88% 11% .
50	B1	52	 88% 12%
51	B2	46	 76% 22% .
52	B3	65	 86% 12% .
53	B4	38	 89% 8% .
54	BA	2903	 16% 55% 24% .
55	BB	118	 15% 59% 19% 5% .
56	B5	234	 88% 6% . 5%

## 2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	7	ACE	-	acetylation	UNP P0A7V0
AB	226	NH2	-	amidation	UNP P0A7V0

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	acetylation	UNP P0A7W1
AE	159	NH2	-	amidation	UNP P0A7W1

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	1	ACE	-	acetylation	UNP P02359
AG	152	NH2	-	amidation	UNP P02359

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	4	ACE	-	acetylation	UNP P0A7R5
AJ	103	NH2	-	amidation	UNP P0A7R5

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	2	ACE	-	acetylation	UNP P0AG63
AQ	83	NH2	-	amidation	UNP P0AG63

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	ACE	-	acetylation	UNP P0A7U3
AS	81	NH2	-	amidation	UNP P0A7U3

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AU	2	ACE	-	acetylation	UNP P68679
AU	54	NH2	-	amidation	UNP P68679

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

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

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

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

- Molecule 23 is a RNA chain called 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*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 RNA chain called tRNA-fMet.

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

- Molecule 25 is a protein called 50S ribosomal protein L35.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 26 is a protein called 50S ribosomal protein L36.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

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

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	2	ACE	-	acetylation	UNP P0A7N9
B1	53	NH2	-	amidation	UNP P0A7N9

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

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

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

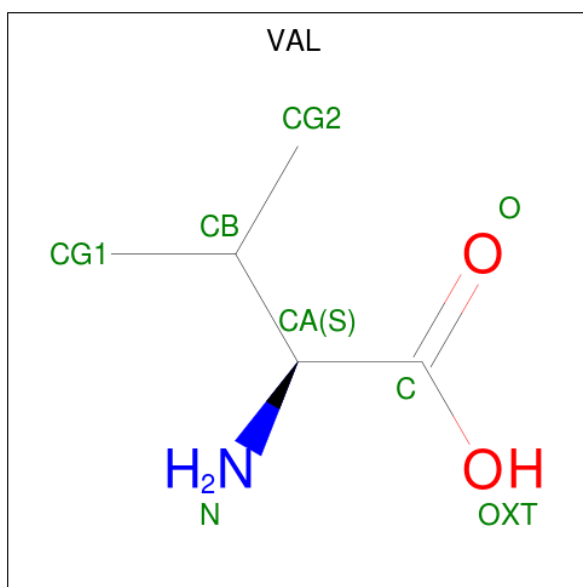
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

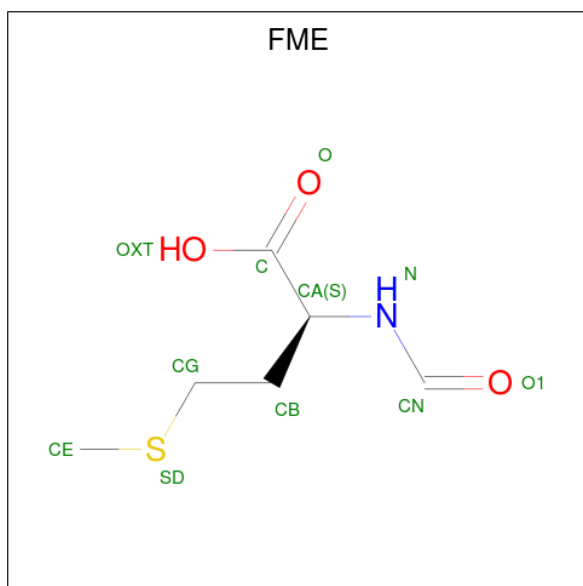
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



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

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



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

### 3 Residue-property plots [i](#)

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

- Molecule 1: 30S ribosomal protein S2

Chain AB:  93% 7%



- Molecule 2: 30S ribosomal protein S3

Chain AC:  92% 7%



- Molecule 3: 30S ribosomal protein S4

Chain AD:  87% 12%



- Molecule 4: 30S ribosomal protein S5

Chain AE:  89% 11%




- Molecule 5: 30S ribosomal protein S6

Chain AF:  87% 13%



- Molecule 6: 30S ribosomal protein S7

Chain AG:  88% 13%



- Molecule 7: 30S ribosomal protein S8

Chain AH: 91% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 81% 18%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 84% 16%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 89% 11%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 85% 15%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 85% 14%



- Molecule 13: 30S ribosomal protein S14

Chain AN: 86% 12%




- Molecule 14: 30S ribosomal protein S15

Chain AO:  87% 12%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  84% 16%



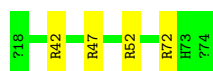
- Molecule 16: 30S ribosomal protein S17

Chain AQ:  90% 9%




- Molecule 17: 30S ribosomal protein S18

Chain AR:  93% 7%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  89% 11%



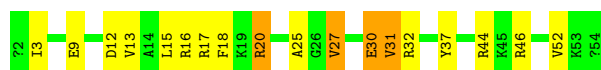
- Molecule 19: 30S ribosomal protein S20

Chain AT:  90% 10%




- Molecule 20: 30S ribosomal protein S21

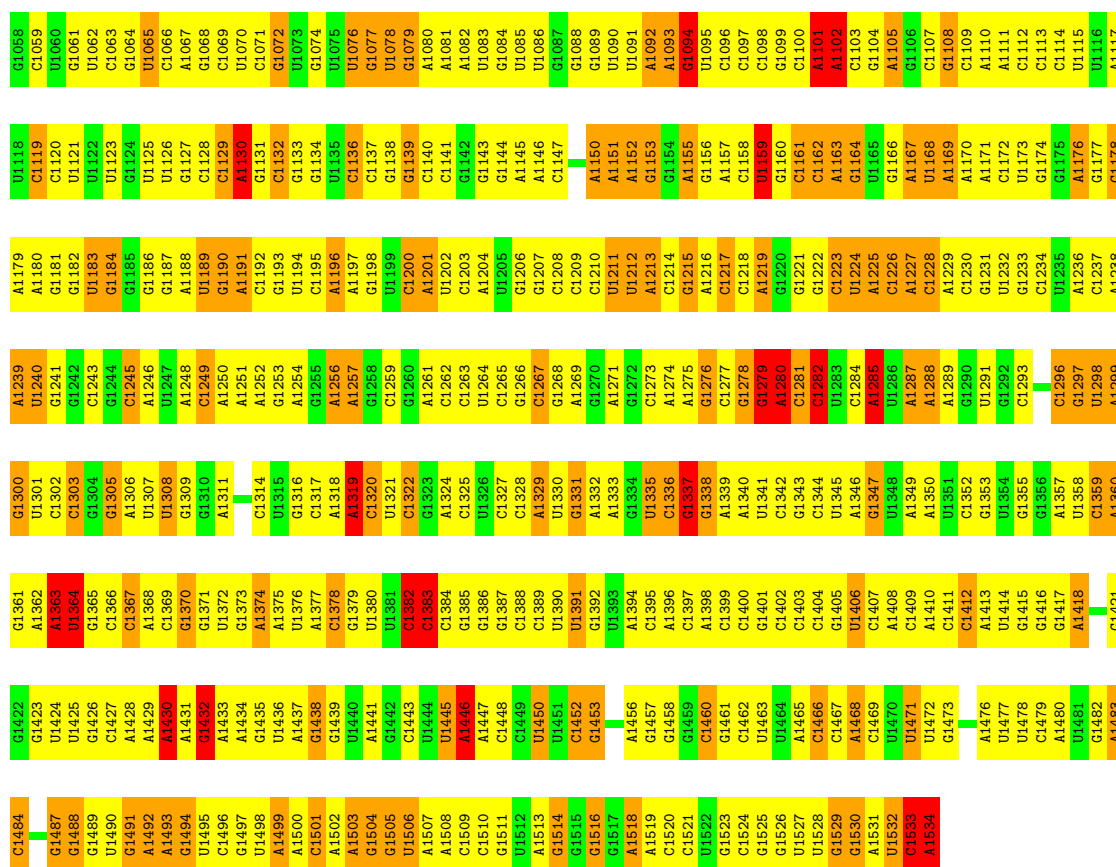
Chain AU:  66% 26% 8%



- Molecule 21: 16S ribosomal RNA

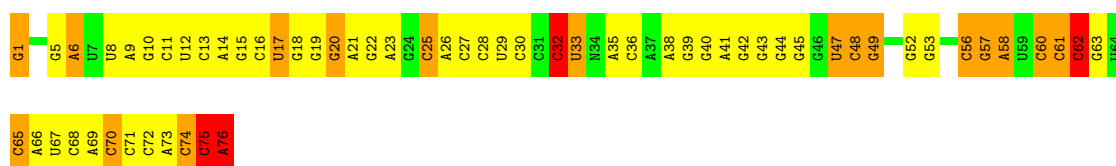
Chain AA:  15% 56% 24% 5%

A	A	A	U	U5	G6	G6	A7	A8	G9	A10	G11	G12	U13	U14	G15	A16	U17	G18	A19	U20	G21	G22	C23	U24	G25	A26	G27	A28	U29	U30	G31	A32	A33	C34	G35	C36	U37	G38	G39	C40	G41	C42	C43	A44	C47	C48	U49	A50	A51	C52	A53	C54	A55	U56	G57	A58	A59	A60	G61	U62
C63	G126	G187	U249	C311	C372	A432	A493	C556	G616	C680	U740	A802	A865	G926	U992	C63	G126	G187	U249	C311	C372	A432	A493	C556	G616	C680	U740	A802	A865	G926	U992	C63	G126	G187	U249	C311	C372	A432	A493	C556	G616	C680	U740	A802	A865	G926	U992													
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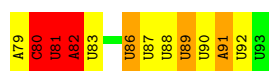
• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 20% 53% 22% 5%



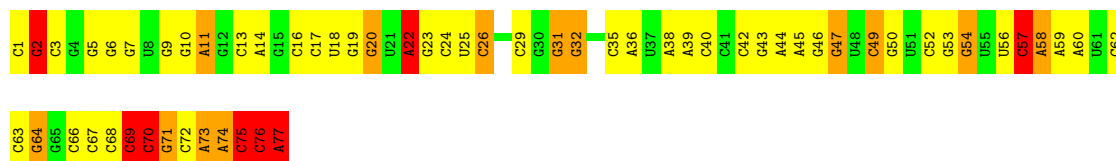
• Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'

Chain A2: 20% 40% 20% 20%

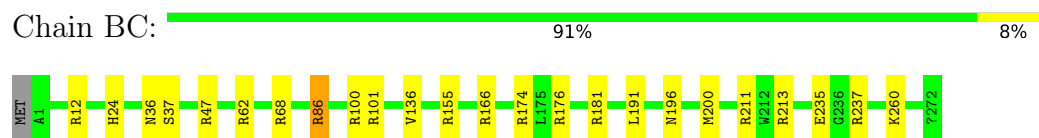


• Molecule 24: tRNA-fMet

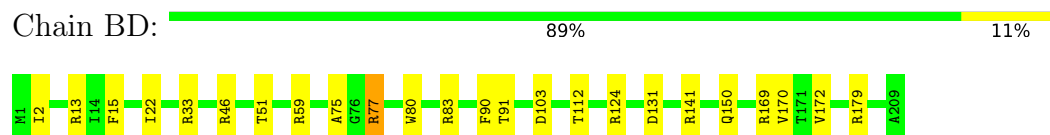
Chain A3: 22% 51% 17% 10%



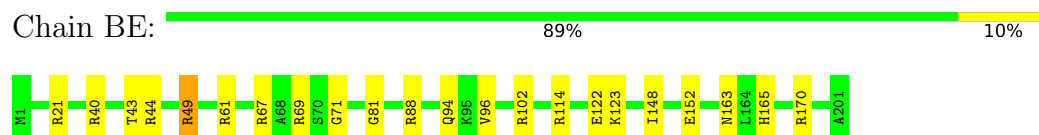
- Molecule 25: 50S ribosomal protein L35



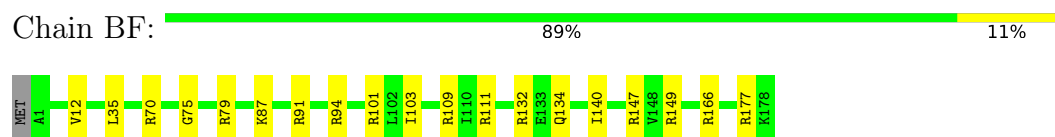
- Molecule 26: 50S ribosomal protein L36



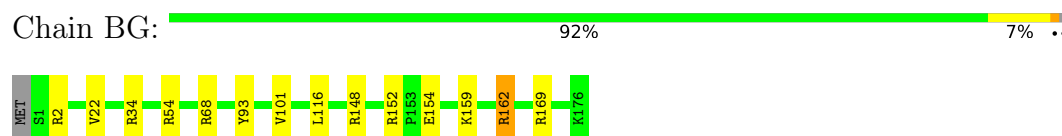
- Molecule 27: 50S ribosomal protein L2



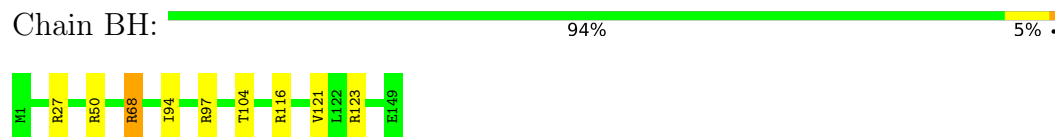
- Molecule 28: 50S ribosomal protein L3



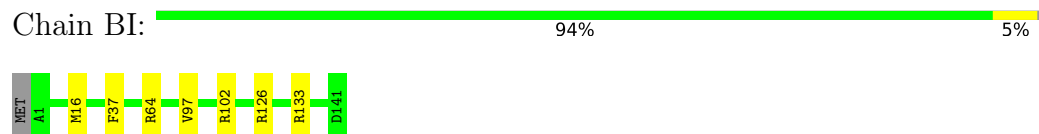
- Molecule 29: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L5



- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9

Chain BJ:  91% 8% .




- Molecule 33: 50S ribosomal protein L11

Chain BK:  90% 10%



- Molecule 34: 50S ribosomal protein L13

Chain BL:  85% 14% .




- Molecule 35: 50S ribosomal protein L14

Chain BM:  88% 12%



- Molecule 36: 50S ribosomal protein L15

Chain BN:  88% 12%



- Molecule 37: 50S ribosomal protein L16

Chain BO:  89% 10% .




- Molecule 38: 50S ribosomal protein L17

Chain BP:  83% 16% .



- Molecule 39: 50S ribosomal protein L18

Chain BQ:  84% 14% ..



- Molecule 40: 50S ribosomal protein L19

Chain BR: 89% 10% .



- Molecule 41: 50S ribosomal protein L20

Chain BS: 92% 8%



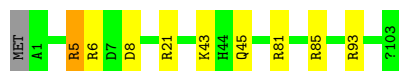
- Molecule 42: 50S ribosomal protein L21

Chain BT: 91% 7% .



- Molecule 43: 50S ribosomal protein L22

Chain BU: 90% 8% ..



- Molecule 44: 50S ribosomal protein L23

Chain BV: 95% 5%



- Molecule 45: 50S ribosomal protein L24

Chain BW: 88% 13%



- Molecule 46: 50S ribosomal protein L25

Chain BX: 84% 10% . .



- Molecule 47: 50S ribosomal protein L27

Chain BY:  90% 10%




- Molecule 48: 50S ribosomal protein L28

Chain BZ:  90% 7% ..




- Molecule 49: 50S ribosomal protein L29

Chain B0:  88% 11% .




- Molecule 50: 50S ribosomal protein L30

Chain B1:  88% 12%




- Molecule 51: 50S ribosomal protein L32

Chain B2:  76% 22% .



- Molecule 52: 50S ribosomal protein L33

Chain B3:  86% 12% .

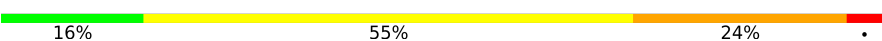


- Molecule 53: 50S ribosomal protein L34

Chain B4:  89% 8% .



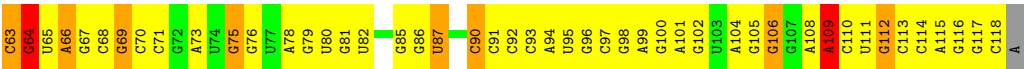
- Molecule 54: 23S ribosomal RNA

Chain BA:  16% 55% 24% .

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C1005	G939	G875	U810	G745	G681	A621	G559	A497	U437	U373	G313	C249	G189	A126	A64	G2
C1006	G940	C876	U811	U746	G684	G822	G560	G498	C438	A374	G314	G250	A190	A127	U66	U4
C1007	A941	A877	C812	U747	G684	G823	G561	G499	A439		G315	A251	A191	C127	C66	U3
A1008	G942	A878	U813	G748	G685	C824	U562	A501	U440	G377	G316	G252	C192	C129	U67	A5
A1009	G943	G879	C814	A749	U686	G825	A563	A502	U441	C378	G317	G253	U193	C130	G68	A6
A1010	G944	G880	C815	A750	C687	G826	C564	A503	C442		G318	G254	G194	A131	G69	G7
A1011	A945	A751	C816	A752	U688	A827	C565	A504	A443	G381	G319	A255	A195	A132	G70	C8
G1012	A946	A753	C817	A754	G689	G828	U566	A505	C444	G382	A320	A256	A196	G134	A71	C9
A1013	A947	U753	G690	U754	C691	G829	U567	A506	C445	C383	U321	C257	A197	U135	U72	A10
A1014	G948	A886	A819	U755	G692	A831	U568	G506	C446	C384	A322		C198	G136	A73	C11
U1015	G949	U756	A820	A756	C693	A832	U569	A507	U447	G385	C323	A262	A199	U139	A74	U12
G1016	G950	C757	A821	C757	A893	A833	G570	A508	U448	U387	G324	G263	U200	C140	G75	A13
	G952		G822		U694	A834	U571	C509	A449	G388	G325	A264	C201	C141	C76	A14
			G823		G695	C835	A572	C510	A450	G389	G326	A265	U202	G142	G77	G15
U1019			U824			C836	U573		U451	G390	U327	A266	A203	C143	G78	G16
A1020	G956	G891	A825	G759	C698	C837	A574	A513	A452	A391	G328	C268	G205	A144	U82	U18
A1021	C957	A892	U826	A761	A699	A838	A575	A514	A453	U392	G329	C269	G206	C145	A83	A19
G1022	U958	C893	U827	U762	G700	G839	U576	A515	A454	C393	A330	A270	U207	C146	A21	C20
U1023	U885	U885	U828	G763	G701	U839	G577	C516	C455	C394	C331	A271	A208	C147	A84	G21
G1024	A896	A829	U829	A764	U702	U840	G578	G518	A457	U395	G333	A272	C209	U148	G85	G22
G1025	C961	C765	G830	G775	G703	U841	U579	U519	C458	U396	G334	G273	C210	A149	G86	G23
A1026	C964		U832	G776	G704	U842	U580	G520	U459	U397	G335	C274	C211	U150	U87	G24
A1027	A900	G770	A833	G771	A705	A643	C581	G521	U460	C398	C336	C275	G212	C151	G88	
A1028	A901	C772	U834	C772	A706	A644	A582	U522	C461	U399	C337	U276	A213	A152	A89	
A1029	C902		G834		G707	C845	G583	A523	C462	G400	G338	U277	G214	U153	U90	A28
G1030	G966		C835		U710	U646	C584	G524	C463	A401	U339	A278	G215	U154	U91	
G1031	C967			G774	G711	G647	G585	G530	U469	G410	A340	A279	A216	U155	U92	C31
A1032	G968	G904	C838	G775	G712	G648	A586	A532	A470	G411	A341	A280	A222	A160	G97	
U1033	U970	A905	U839	G776	G713	U649	C587	U526	U466	A412	A342	C281	A223	U162	G98	
G1034	G971		C840	G777	G714	C850	U588	A527	C467	U405	A343	A282	A219	C157	A94	C33
U1035	A972				A715	G851	U589	A528	C468	G406	A344	G283	A218	U158	A95	U34
G1036	A973				A716	U852	A590	A529	U468		A345	G284	G220	G159	G96	
			A844		C717	U853	U591	G530	C469	G410	A346	U285	A221	A161	C97	
A1039	G974	A910	U845	A781	C718	A854	A592	C531	U470	G411	A347	U286	A222	U163	G98	
A1040	A975	C912	U846	A782	C719	A855	U593	A533	A471	A412	A348	G287	A223	C163	U99	A38
G1041	G976	U913	U847	A783	U720	G856	U594	G533	A472	C413	U349		U224	C164	U100	G39
G1042	G977	G885	C848	G785	A721	U857	C595		G473	C414	G350		C225	C165	U101	U40
G1043	G978		A849		U722	U858	U596	G536	C474	C415	G351	U290	A226	A166	U102	C41
A979	A979		U850	C786	A723	U859	G597	G537	C475	A416	A352	G291	A227	U167	A103	A42
A1044	A980		C851	C787	C723	G859	U598	A538	C476	U417	A353	U292	C228	U168	A104	A43
A1045	A981			A788	U724	C660	U599	G539	A477	C418	C353	U293	C229	G167	A105	A44
A1046	C982	A918	C854	A789	G725	A661	A599	G540	A478	U419	A354	A294	G230	G169	C106	
G1047	A983	U919	G855	U790	G726	G662	G600	C541	A479	U420	U355	G295	A231	U170	G107	G46
A1048	A984	A920	C856	C791	A727	G663	C601	A541	A480	C421	G356	U296	G232	U171	G108	C47
C1049	C985	C921	G857	A792	G728	G664	A602	C542	C481	A422	C357	U297	A233	A172	C109	
A1050	C986		G858	A793	G729	U665	A603	G543	A482	A423	U358	G298	U234	A173	G110	A49
G1051	C987	A794	C859	A794	A730	A666	G604	C544	A483	G424	C359	A299	U235	U174	A111	G51
C1052	A988	C795	U860	C795	C731	U667	G605	U545	A484	A425	G360	A299	U236	G175	U50	
C1053	G989		A861	C796	C732	A668	U606	U546	C484	G426	U360	A300	C236	A176	A52	
A1054	A990	A927	G862	G797	G733	G669	U607	A547	C485	C427	G361	G301	C237	G177	A53	
G1055	C991	A928	A863		A734	A870	A608	G548	C486	U428	A362	C302	C238	G178	A54	
				A800		C671	A609	G549	C487	C429	G363	G303	C239	G179	G55	
G1056	C992	U929	G864	G801	C736	C672	C610	C550	C488	A428	C364	U304	C240	C179	G56	
G993	A1057	G930	C865	A802	C737	C673	C611	G551	C489	A429	U365	C305	A241	G180	A56	
U1058	C994	U931	A866	A802	C738	C674	C612	U552	C490	A430	C366	U306	G242	A181	C57	
G1059	C995	A932	C867	G874	G739	G675	G613	U553	C491	U431	G367	G307	U243	A182	G58	
U1060	A996	A833	U868	A804	A739	A676	A613	U554	A492	A432	A368	G308	A244	C183	U59	
	C997	U934	G869	C805	C740	A876	A614	U555	A493	A433	U369	G309	G245	G121	G60	
C1064	U998	C935	U870	C806	U741	A677	U615	G556	C494	C433	U370	A310	G246	G122	G61	
U1065	C999	A936	U871	U807	A742	C678	A616	A556	C495	U434	G371	G310	C247	G123	C51	
U1066	A1000	C937	C873	G808	A743	C679		C557		C435	A371	A311	G247	G185	G124	U62

C1996	G1935	C1874	G1811	G1750	C1686	C1625	U1563	A1503	U1440	C1376	U1316	G1256	G1193	A1129	A1067
C1997	A1936	G1875	U1812	U1751	C1689	A1626	C1564	A1504	G1441	G1377	G1317	C1257	A1194	U1130	G1068
A1998	A1937	A1876	G1813	C1752	A1689	G1627	C1565	A1505	U1442	U1378	U1318	U1258	G1195	G1131	A1069
C1999	A1938	A1877	G1814	G1753	A1690	G1628	A1566	A1506	U1443	U1379	C1319	G1259	C1196	U1132	A1070
C2001	U1939	C1878	A1815	A1764	C1691	U1629	G1567	C1507	G1444	G1380	G1320	C1260	A1133	A1133	G1071
G2002	U1940	C1879	A1816	A1755	U1692	A1630	G1568	A1508	G1445	G1381	A1321	C1261	U1198	A1134	C1072
A2003	C1941	U1880	G1817	G1756	C1693	A1631	A1569	A1509	C1446	G1382	A1322	A1262	U1199	C1135	A1073
G2004	C1942	C1881	U1818	C1697	G1632	A1632	A1570	G1510	C1447	A1383	C1323	U1263	C1200	C1140	C1076
A2005	U1943	A1819	U1819	U1757	G1633	G1633	A1571	G1511	U1448	A1384	G1324	U1264	U1201	U1141	U1077
A2006	U1944	A1882	A1820	U1758	G1699	A1634	A1572	C1512	G1449	A1385	U1325	A1265	G1202	U1142	U1078
C2006	G1945	G1884	A1821	C1760	A1700	A1635	G1573	G1513	G1450	C1386	U1326	C1266	U1203	A1143	C1079
U2007	U1946	A1885	C1822	A1761	A1701	U1636	C1574	G1514	G1451	A1387	A1327	U1267	A1204	A1144	A1080
C2008	C1947	U1886	G1823	A1762	G1702	U1637	C1575	A1515	G1452	G1388	A1328	A1268	A1205	A1145	U1081
A2009	C1887	C1887	G1823	G1763	G1703	C1638	U1576	G1516	A1453	G1389	U1329	A1269	G1206	C1145	U1082
G2010	U1888	C1888	G1826	C1764	C1704	C1639	C1577	G1517	C1454	U1390	C1330	C1270	C1207	C1146	U1083
U2011	A1889	U1827	U1827	U1765	A1705	A1640	U1578	C1518	G1455	U1391	G1331	G1271	C1208	A1147	A1084
G2012	A1890	G1828	A1828	G1766	C1706	A1641	C1579	G1519	G1456	A1392	G1332	A1272	U1209	U1148	A1085
A2013	C1891	A1829	G1830	G1767	G1707	G1642	A1580	U1520	U1457	A1393	G1333	U1273	G1210	G1149	A1086
U2014	C1892	C1830	G1831	C1768	C1708	G1643	G1581	G1521	U1458	U1394	G1334	A1274	C1211	C1150	A1087
A2015	C1893	G1832	G1831	U1769	U1709	C1644	C1582	A1522	G1459	A1395	C1335	A1275	G1212	A1151	A1088
U2016	C1894	C1832	G1832	G1770	G1710	G1645	A1583	U1523	U1460	U1396	A1336	A1276	C1152	C1152	G1089
U2017	C1895	U1827	G1833	A1771	A1711	C1646	U1584	G1524	C1461	U1397	G1337	G1277	A1214	C1153	A1090
G2018	G1896	U1834	U1834	A1772	U1712	G1647	C1585	A1525	C1462	C1398	G1338	C1278	G1215	G1154	A1091
A2019	C1897	G1835	G1835	A1773	A1713	U1648	A1586	C1526	G1463	C1399	G1339	G1279	G1216	A1155	G1092
A2020	U1898	C1836	C1836	C1774	U1714	G1649	G1587	G1527	G1464	U1400	U1340	G1280	U1217	A1156	C1092
C2021	A1899	C1837	C1837	U1775	G1715	A1650	G1588	A1528	G1465	G1401	G1341	G1281	G1218	G1157	G1083
U2022	A1900	G1840	G1840	G1776	U1716	G1651	U1589	G1529	U1466	U1402	A1342	U1282	U1219	C1158	U1094
C2023	C1901	U1841	G1841	C1779	A1717	A1652	A1590	C1530	U1467	A1403	G1343	G1283	G1220	U1159	A1095
G2024	G1902	G1842	G1842	G1718	G1718	G1653	A1591	C1531	U1468	U1404	U1344	C1284	C1221	G1160	A1096
C2025	C1903	C1843	C1843	G1719	C1719	A1654	C1592	A1532	A1469	U1405	C1345	A1285	U1222	C1161	U1097
U2026	A1904	G1844	C1844	U1720	U1720	A1655	A1593	C1533	A1470	U1406	G1346	U1286	G1223	G1163	A1098
G2029	C1905	C1844	C1844	G1721	G1721	C1656	U1594	U1534	G1471	G1407	A1347	A1287	U1224	G1163	G1099
A2030	G1906	U1852	U1852	A1722	G1722	U1657	C1595	A1535	G1472	G1408	A1346	G1288	G1225	C1164	C1100
C2031	C1907	A1847	A1847	G1723	G1723	C1658	A1596	C1536	U1473	A1409	C1349	G1289	A1226	A1165	U1101
G2032	U1908	A1848	A1848	G1724	G1724	G1661	A1597	G1537	U1474	A1413	C1350	C1290	G1227	G1166	C1102
A2033	C1909	G1849	G1849	U1725	U1725	U1662	A1598	C1538	G1475	C1414	U1352	G1292	G1228	C1167	A1103
U2034	G1910	G1850	G1850	C1726	C1726	G1663	U1599	U1539	U1476	U1415	U1353	G1293	A1230	A1169	C1104
G2035	U1911	U1851	U1851	C1727	C1727	G1663	C1600	G1540	A1477	U1415	A1353	C1293	A1230	A1169	U1105
C2036	C1912	C1852	U1852	G1728	C1728	A1664	G1601	C1541	C1480	U1416	A1354	U1294	C1233	C1170	U1108
A2037	A1913	A1853	A1853	U1729	U1729	A1665	U1602	U1542	U1487	C1417	G1361	C1295	G1236	C1172	C1109
G2038	C1914	A1854	A1854	C1730	C1730	G1666	A1603	G1543	U1481	A1418	C1362	G1296	A1237	U1173	G1110
U2039	U1915	U1855	U1855	G1731	G1731	G1667	C1604	A1544	G1482	A1419	C1363	C1297	G1238	U1174	A1111
C2042	C1916	G1856	G1856	C1732	C1732	A1668	C1605	A1545	U1485	G1420	A1359	G1298	G1238	A1175	G1112
A2043	U1917	G1857	G1857	G1733	G1733	A1669	C1606	G1546	U1486	G1421	G1360	G1300	U1176	U1176	U1113
C2044	A1918	A1858	A1858	G1734	G1734	C1670	C1607	C1547	U1488	G1422	G1361	A1301	A1241	G1177	C1114
G2045	U1919	U1859	U1859	A1735	A1735	A1671	A1608	A1548	U1489	G1426	C1362	A1302	U1242	C1178	G1115
U2046	C1920	G1860	G1860	U1736	U1736	G1672	A1609	C1550	C1488	A1427	C1363	G1303	C1243	G1179	G1116
C2047	G1921	G1861	G1861	G1737	G1737	G1673	A1610	C1551	A1490	C1428	G1364	A1304	A1244	U1180	C1117
G2048	U1922	G1862	G1862	U1738	U1738	G1674	C1611	A1551	G1491	G1429	A1365	C1305	G1245	U1181	C1118
A2049	C1924	G1863	G1863	A1739	A1739	C1675	C1612	A1552	G1492	G1430	A1366	C1306	A1246	U1182	U1119
C2050	U1925	U1864	U1864	G1740	G1740	A1676	G1613	A1553	C1493	A1431	A1367	A1307	A1247	U1183	G1120
G2051	G1926	U1865	U1865	C1741	C1741	A1677	A1614	U1554	C1494	A1432	G1368	G1308	G1248	G1186	C1121
A2052	A1927	A1866	A1866	U1742	U1742	A1678	C1615	C1555	A1494	A1433	G1369	A1309	U1249	G1187	C1122
U2053	C1928	G1867	G1867	G1743	G1743	A1679	A1616	C1556	A1495	A1434	C1370	G1310	G1250	G1187	C1123
C2054	G1929	C1868	C1868	A1744	A1744	U1680	C1617	C1557	U1496	A1435	G1371	G1311	G1251	U1188	G1124
G2055	U1930	G1869	G1869	A1745	A1745	G1681	A1618	C1558	U1497	G1435	U1372	U1312	G1252	A1189	G1125
A2056	U1931	C1870	C1870	A1746	A1746	G1682	G1619	U1559	C1498	C1436	A1373	U1313	A1253	G1190	A1126
C2057	A1932	A1871	A1871	U1747	U1747	U1683	G1620	C1561	C1499	C1437	U1374	U1314	U1254	G1191	A1127
U2058	G1933	G1872	G1872	C1748	C1748	C1684	G1620	U1562	A1502	A1439	U1375	C1315	G1192	G1192	G1128





● Molecule 56: 50S ribosomal protein L1

Chain B5: 88% 6% • 5%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14235	Depositor
Resolution determination method	FSC 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	162740	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	AB	0.72	0/1736	1.11	13/2340 (0.6%)
10	AK	0.80	0/894	1.27	12/1207 (1.0%)
11	AL	0.80	0/969	1.25	13/1300 (1.0%)
12	AM	0.82	0/884	1.29	13/1181 (1.1%)
13	AN	0.82	0/817	1.25	9/1088 (0.8%)
14	AO	0.77	0/722	1.18	6/964 (0.6%)
15	AP	0.82	0/648	1.42	14/870 (1.6%)
16	AQ	0.71	0/658	1.18	8/883 (0.9%)
17	AR	0.77	0/463	1.19	5/623 (0.8%)
18	AS	0.80	0/653	1.23	7/879 (0.8%)
19	AT	0.75	0/672	1.18	7/890 (0.8%)
2	AC	0.76	0/1651	1.17	14/2225 (0.6%)
20	AU	0.87	0/431	1.59	8/572 (1.4%)
21	AA	1.88	441/36759 (1.2%)	2.29	2411/57346 (4.2%)
22	A1	1.89	18/1668 (1.1%)	2.23	102/2595 (3.9%)
23	A2	1.67	1/343 (0.3%)	2.18	19/531 (3.6%)
24	A3	1.93	26/1722 (1.5%)	2.27	102/2685 (3.8%)
25	BC	0.79	0/2121	1.28	19/2852 (0.7%)
26	BD	0.72	0/1586	1.23	12/2134 (0.6%)
27	BE	0.71	0/1571	1.17	11/2113 (0.5%)
28	BF	0.77	0/1444	1.18	13/1937 (0.7%)
29	BG	0.72	0/1343	1.16	7/1816 (0.4%)
3	AD	0.76	0/1665	1.23	21/2227 (0.9%)
30	BH	0.67	0/1122	1.14	6/1515 (0.4%)
31	BI	0.69	0/1046	1.11	7/1410 (0.5%)
32	BJ	0.74	0/1152	1.23	9/1551 (0.6%)
33	BK	0.76	0/947	1.23	11/1268 (0.9%)
34	BL	0.76	0/1054	1.28	14/1403 (1.0%)
35	BM	0.79	0/1093	1.27	11/1460 (0.8%)
36	BN	0.80	0/973	1.26	12/1301 (0.9%)
37	BO	0.80	0/902	1.28	10/1209 (0.8%)
38	BP	0.77	0/929	1.26	9/1242 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.80	0/960	1.37	17/1278 (1.3%)
4	AE	0.70	0/1119	1.12	11/1506 (0.7%)
40	BR	0.73	0/829	1.22	9/1107 (0.8%)
41	BS	0.71	0/864	1.18	7/1156 (0.6%)
42	BT	0.73	0/744	1.19	5/994 (0.5%)
43	BU	0.70	0/787	1.17	6/1051 (0.6%)
44	BV	0.72	0/766	1.12	5/1025 (0.5%)
45	BW	0.73	0/604	1.25	4/799 (0.5%)
46	BX	0.82	0/635	1.47	14/848 (1.7%)
47	BY	0.70	0/510	1.22	5/677 (0.7%)
48	BZ	0.73	0/453	1.27	4/605 (0.7%)
49	B0	0.78	0/450	1.25	4/599 (0.7%)
5	AF	0.79	0/835	1.15	7/1128 (0.6%)
50	B1	0.75	0/417	1.10	3/556 (0.5%)
51	B2	0.91	0/380	1.45	8/498 (1.6%)
52	B3	0.73	0/513	1.24	6/676 (0.9%)
53	B4	0.72	0/303	1.25	3/397 (0.8%)
54	BA	1.74	667/69796 (1.0%)	2.28	4747/108888 (4.4%)
55	BB	1.83	58/2800 (2.1%)	2.30	198/4367 (4.5%)
56	B5	0.68	0/1673	1.14	10/2255 (0.4%)
6	AG	0.77	0/1188	1.24	16/1593 (1.0%)
7	AH	0.74	0/989	1.11	7/1326 (0.5%)
8	AI	0.85	0/1035	1.33	20/1377 (1.5%)
9	AJ	0.78	0/797	1.39	16/1079 (1.5%)
All	All	1.56	1211/160085 (0.8%)	2.06	8067/239402 (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
13	AN	0	1
14	AO	0	1
21	AA	0	342
22	A1	0	13
23	A2	0	5
24	A3	0	19
3	AD	0	1
4	AE	0	1
46	BX	0	1
54	BA	0	646

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	23
56	B5	0	1
All	All	0	1054

All (1211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2048	G	C2-N2	-6.80	1.27	1.34
24	A3	75	C	N3-C4	-6.76	1.29	1.33
21	AA	1063	C	C4-N4	-6.70	1.27	1.33
23	A2	80	C	C4-N4	-6.68	1.27	1.33
55	BB	113	C	C4-N4	-6.68	1.27	1.33
54	BA	2297	A	C6-N1	-6.65	1.30	1.35
54	BA	1646	C	C4-N4	-6.64	1.27	1.33
55	BB	34	A	C6-N1	-6.62	1.30	1.35
21	AA	658	C	C4-N4	-6.60	1.28	1.33
54	BA	2091	C	C4-N4	-6.58	1.28	1.33
21	AA	341	C	C4-N4	-6.57	1.28	1.33
21	AA	1113	C	C4-N4	-6.55	1.28	1.33
54	BA	32	C	C4-N4	-6.54	1.28	1.33
55	BB	90	C	C4-N4	-6.50	1.28	1.33
24	A3	63	C	C4-N4	-6.49	1.28	1.33
21	AA	1467	C	C4-N4	-6.48	1.28	1.33
24	A3	77	A	C6-N1	-6.46	1.31	1.35
54	BA	1556	C	C4-N4	-6.45	1.28	1.33
21	AA	183	C	C4-N4	-6.44	1.28	1.33
54	BA	565	C	C4-N4	-6.43	1.28	1.33
21	AA	422	C	C4-N4	-6.43	1.28	1.33
54	BA	343	C	C4-N4	-6.42	1.28	1.33
55	BB	27	C	C4-N4	-6.41	1.28	1.33
21	AA	197	A	C6-N1	-6.40	1.31	1.35
21	AA	490	C	C4-N4	-6.39	1.28	1.33
54	BA	1768	C	C4-N4	-6.38	1.28	1.33
54	BA	671	C	C4-N4	-6.38	1.28	1.33
21	AA	1257	A	C6-N1	-6.37	1.31	1.35
54	BA	1550	C	C4-N4	-6.37	1.28	1.33
54	BA	2282	G	C2-N2	-6.34	1.28	1.34
54	BA	2863	C	C4-N4	-6.34	1.28	1.33
54	BA	774	G	C2-N2	-6.32	1.28	1.34
54	BA	1389	G	C2-N2	-6.32	1.28	1.34
54	BA	51	G	C2-N2	-6.31	1.28	1.34
54	BA	1386	C	C4-N4	-6.30	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2326	C	C4-N4	-6.29	1.28	1.33
55	BB	4	C	C4-N4	-6.29	1.28	1.33
21	AA	342	C	C4-N4	-6.28	1.28	1.33
21	AA	1457	G	C2-N2	-6.28	1.28	1.34
54	BA	577	G	C6-N1	-6.25	1.35	1.39
54	BA	2427	C	C4-N4	-6.25	1.28	1.33
54	BA	1875	G	C2-N2	-6.25	1.28	1.34
21	AA	57	G	C2-N2	-6.24	1.28	1.34
21	AA	736	C	N3-C4	-6.23	1.29	1.33
21	AA	980	C	C4-N4	-6.23	1.28	1.33
21	AA	379	C	C4-N4	-6.22	1.28	1.33
54	BA	1370	C	C4-N4	-6.22	1.28	1.33
21	AA	52	C	C4-N4	-6.22	1.28	1.33
22	A1	72	C	C4-N4	-6.21	1.28	1.33
54	BA	37	C	C4-N4	-6.20	1.28	1.33
54	BA	2359	C	C4-N4	-6.20	1.28	1.33
21	AA	732	C	C4-N4	-6.20	1.28	1.33
54	BA	2064	C	C4-N4	-6.19	1.28	1.33
54	BA	2428	G	C2-N2	-6.19	1.28	1.34
54	BA	1724	G	C2-N2	-6.18	1.28	1.34
54	BA	2285	C	C4-N4	-6.17	1.28	1.33
54	BA	1950	G	C2-N2	-6.16	1.28	1.34
21	AA	186	C	C4-N4	-6.15	1.28	1.33
54	BA	2575	C	C4-N4	-6.15	1.28	1.33
54	BA	1043	C	C4-N4	-6.15	1.28	1.33
54	BA	806	C	C4-N4	-6.15	1.28	1.33
54	BA	1595	C	C4-N4	-6.15	1.28	1.33
24	A3	68	C	C4-N4	-6.15	1.28	1.33
54	BA	1793	C	C4-N4	-6.14	1.28	1.33
54	BA	433	C	C4-N4	-6.14	1.28	1.33
54	BA	2620	C	C4-N4	-6.14	1.28	1.33
21	AA	330	C	C4-N4	-6.13	1.28	1.33
54	BA	758	C	C4-N4	-6.13	1.28	1.33
22	A1	60	C	C4-N4	-6.12	1.28	1.33
54	BA	2420	C	C4-N4	-6.12	1.28	1.33
21	AA	176	C	C4-N4	-6.12	1.28	1.33
21	AA	1054	C	C4-N4	-6.12	1.28	1.33
54	BA	1833	C	C4-N4	-6.11	1.28	1.33
21	AA	1302	C	C4-N4	-6.10	1.28	1.33
54	BA	2045	C	C4-N4	-6.10	1.28	1.33
54	BA	1426	G	C2-N2	-6.09	1.28	1.34
21	AA	1407	C	C4-N4	-6.09	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1496	C	C4-N4	-6.09	1.28	1.33
55	BB	86	G	C2-N2	-6.09	1.28	1.34
54	BA	2025	C	C4-N4	-6.08	1.28	1.33
21	AA	1347	G	C2-N2	-6.08	1.28	1.34
21	AA	1228	C	C4-N4	-6.08	1.28	1.33
54	BA	781	A	C6-N1	-6.08	1.31	1.35
55	BB	91	C	C4-N4	-6.07	1.28	1.33
21	AA	675	A	C6-N1	-6.07	1.31	1.35
54	BA	1401	G	C2-N2	-6.07	1.28	1.34
54	BA	2595	G	C2-N2	-6.06	1.28	1.34
54	BA	1667	G	C2-N2	-6.06	1.28	1.34
54	BA	564	C	C4-N4	-6.06	1.28	1.33
24	A3	71	G	C2-N2	-6.05	1.28	1.34
54	BA	411	G	C2-N2	-6.05	1.28	1.34
21	AA	494	G	C2-N2	-6.05	1.28	1.34
21	AA	1192	C	C4-N4	-6.05	1.28	1.33
54	BA	2160	C	C4-N4	-6.04	1.28	1.33
24	A3	3	C	C4-N4	-6.04	1.28	1.33
54	BA	587	C	C4-N4	-6.04	1.28	1.33
21	AA	704	A	C6-N1	-6.04	1.31	1.35
54	BA	2222	C	C4-N4	-6.03	1.28	1.33
54	BA	2794	C	C4-N4	-6.03	1.28	1.33
21	AA	359	G	C2-N2	-6.03	1.28	1.34
21	AA	1182	G	C2-N2	-6.03	1.28	1.34
21	AA	674	G	C2-N2	-6.02	1.28	1.34
21	AA	418	C	C4-N4	-6.02	1.28	1.33
21	AA	369	G	C2-N2	-6.02	1.28	1.34
21	AA	1207	G	C2-N2	-6.02	1.28	1.34
21	AA	19	A	C6-N1	-6.01	1.31	1.35
54	BA	1362	C	N3-C4	-6.01	1.29	1.33
54	BA	1832	C	C4-N4	-6.01	1.28	1.33
22	A1	75	C	C4-N4	-6.01	1.28	1.33
54	BA	986	C	C4-N4	-6.00	1.28	1.33
21	AA	233	C	C4-N4	-6.00	1.28	1.33
21	AA	308	C	C4-N4	-6.00	1.28	1.33
21	AA	976	G	C2-N2	-6.00	1.28	1.34
21	AA	1112	C	N3-C4	-6.00	1.29	1.33
21	AA	1066	C	C4-N4	-6.00	1.28	1.33
54	BA	393	C	C4-N4	-5.99	1.28	1.33
21	AA	58	C	C4-N4	-5.99	1.28	1.33
54	BA	295	G	C6-N1	-5.99	1.35	1.39
54	BA	2104	C	C4-N4	-5.99	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	145	G	C2-N2	-5.99	1.28	1.34
21	AA	372	C	C4-N4	-5.98	1.28	1.33
54	BA	11	C	C4-N4	-5.98	1.28	1.33
54	BA	784	G	C2-N2	-5.98	1.28	1.34
54	BA	1870	C	C4-N4	-5.98	1.28	1.33
24	A3	69	C	C4-N4	-5.98	1.28	1.33
54	BA	1797	G	C2-N2	-5.97	1.28	1.34
54	BA	396	G	C2-N2	-5.97	1.28	1.34
54	BA	1710	G	C2-N2	-5.97	1.28	1.34
21	AA	475	C	C4-N4	-5.97	1.28	1.33
21	AA	1171	A	C6-N1	-5.97	1.31	1.35
21	AA	1479	C	C4-N4	-5.97	1.28	1.33
54	BA	285	G	C2-N2	-5.97	1.28	1.34
54	BA	2446	G	C2-N2	-5.96	1.28	1.34
24	A3	53	G	C6-N1	-5.96	1.35	1.39
54	BA	585	G	C2-N2	-5.96	1.28	1.34
24	A3	19	G	C2-N2	-5.96	1.28	1.34
54	BA	381	G	C2-N2	-5.96	1.28	1.34
54	BA	2636	C	C4-N4	-5.95	1.28	1.33
55	BB	3	C	C4-N4	-5.95	1.28	1.33
21	AA	931	C	N3-C4	-5.95	1.29	1.33
21	AA	1509	C	C4-N4	-5.95	1.28	1.33
55	BB	19	C	C4-N4	-5.95	1.28	1.33
54	BA	33	C	C4-N4	-5.94	1.28	1.33
54	BA	143	C	N3-C4	-5.94	1.29	1.33
54	BA	914	G	N1-C2	-5.94	1.32	1.37
55	BB	31	C	C4-N4	-5.94	1.28	1.33
21	AA	990	C	C4-N4	-5.94	1.28	1.33
54	BA	386	G	C2-N2	-5.94	1.28	1.34
21	AA	1469	C	C4-N4	-5.93	1.28	1.33
21	AA	1064	G	C2-N2	-5.93	1.28	1.34
54	BA	2049	G	C2-N2	-5.93	1.28	1.34
54	BA	444	C	N3-C4	-5.93	1.29	1.33
54	BA	1533	C	C4-N4	-5.93	1.28	1.33
54	BA	1558	C	C4-N4	-5.93	1.28	1.33
21	AA	520	A	C6-N1	-5.92	1.31	1.35
54	BA	2228	G	C2-N2	-5.92	1.28	1.34
21	AA	1051	C	C4-N4	-5.92	1.28	1.33
54	BA	1357	C	N3-C4	-5.92	1.29	1.33
21	AA	1344	C	C4-N4	-5.91	1.28	1.33
54	BA	389	G	C2-N2	-5.91	1.28	1.34
54	BA	584	C	C4-N4	-5.91	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1748	C	C4-N4	-5.91	1.28	1.33
21	AA	1061	G	C2-N2	-5.91	1.28	1.34
21	AA	453	G	C2-N2	-5.90	1.28	1.34
54	BA	2824	C	N3-C4	-5.90	1.29	1.33
54	BA	1345	C	C4-N4	-5.90	1.28	1.33
21	AA	234	C	C4-N4	-5.90	1.28	1.33
54	BA	454	A	C6-N1	-5.90	1.31	1.35
54	BA	2821	A	C6-N1	-5.90	1.31	1.35
54	BA	1398	C	C4-N4	-5.90	1.28	1.33
54	BA	1430	G	C2-N2	-5.90	1.28	1.34
55	BB	24	G	C2-N2	-5.89	1.28	1.34
21	AA	618	C	C4-N4	-5.89	1.28	1.33
21	AA	634	C	C4-N4	-5.89	1.28	1.33
21	AA	730	G	C2-N2	-5.88	1.28	1.34
21	AA	775	G	C2-N2	-5.88	1.28	1.34
54	BA	748	G	C2-N2	-5.88	1.28	1.34
54	BA	442	G	C2-N2	-5.88	1.28	1.34
21	AA	929	G	C2-N2	-5.88	1.28	1.34
21	AA	776	G	C2-N2	-5.88	1.28	1.34
21	AA	783	C	N3-C4	-5.88	1.29	1.33
54	BA	1121	C	C4-N4	-5.88	1.28	1.33
21	AA	726	C	N3-C4	-5.87	1.29	1.33
54	BA	1822	C	C4-N4	-5.87	1.28	1.33
21	AA	277	C	C4-N4	-5.87	1.28	1.33
21	AA	495	A	C6-N1	-5.87	1.31	1.35
54	BA	1272	A	C6-N1	-5.87	1.31	1.35
54	BA	2619	C	C4-N4	-5.87	1.28	1.33
54	BA	1211	C	C4-N4	-5.87	1.28	1.33
54	BA	2699	C	C4-N4	-5.86	1.28	1.33
54	BA	2165	C	C4-N4	-5.86	1.28	1.33
54	BA	1990	C	N3-C4	-5.86	1.29	1.33
54	BA	24	G	C2-N2	-5.86	1.28	1.34
55	BB	64	G	C6-N1	-5.86	1.35	1.39
21	AA	779	C	C4-N4	-5.86	1.28	1.33
54	BA	2396	G	C2-N2	-5.86	1.28	1.34
55	BB	116	G	C2-N2	-5.85	1.28	1.34
21	AA	1084	G	C2-N2	-5.85	1.28	1.34
54	BA	1741	C	C4-N4	-5.85	1.28	1.33
21	AA	1143	G	C2-N2	-5.84	1.28	1.34
54	BA	889	C	N3-C4	-5.84	1.29	1.33
54	BA	1361	G	C2-N2	-5.84	1.28	1.34
54	BA	2190	G	C2-N2	-5.84	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	34	C	C4'-C3'	-5.84	1.46	1.52
21	AA	136	C	C4-N4	-5.84	1.28	1.33
21	AA	824	G	C2-N2	-5.84	1.28	1.34
54	BA	1613	G	C2-N2	-5.84	1.28	1.34
54	BA	2037	A	C6-N1	-5.83	1.31	1.35
21	AA	1103	C	N3-C4	-5.83	1.29	1.33
54	BA	1959	G	C2-N2	-5.83	1.28	1.34
54	BA	637	A	C6-N1	-5.82	1.31	1.35
24	A3	76	C	N3-C4	-5.82	1.29	1.33
54	BA	1538	G	C2-N2	-5.82	1.28	1.34
55	BB	62	C	C4-N4	-5.82	1.28	1.33
54	BA	385	C	C4-N4	-5.82	1.28	1.33
54	BA	2443	C	C4-N4	-5.82	1.28	1.33
54	BA	134	G	C2-N2	-5.82	1.28	1.34
54	BA	1947	C	C4-N4	-5.82	1.28	1.33
21	AA	314	C	C4-N4	-5.82	1.28	1.33
54	BA	2442	C	C4-N4	-5.81	1.28	1.33
21	AA	481	G	C2-N2	-5.81	1.28	1.34
21	AA	579	A	C6-N1	-5.81	1.31	1.35
21	AA	1117	A	C6-N1	-5.81	1.31	1.35
21	AA	1412	C	C4-N4	-5.81	1.28	1.33
54	BA	2073	C	N3-C4	-5.81	1.29	1.33
21	AA	914	A	C6-N1	-5.81	1.31	1.35
21	AA	919	A	C6-N1	-5.81	1.31	1.35
54	BA	473	G	C2-N2	-5.81	1.28	1.34
54	BA	2338	C	C4-N4	-5.81	1.28	1.33
54	BA	2339	C	C4-N4	-5.81	1.28	1.33
54	BA	2374	C	C4-N4	-5.81	1.28	1.33
54	BA	69	C	C4-N4	-5.81	1.28	1.33
24	A3	62	C	C4-N4	-5.80	1.28	1.33
54	BA	2770	G	C2-N2	-5.80	1.28	1.34
21	AA	918	A	C6-N1	-5.80	1.31	1.35
54	BA	2012	G	C2-N2	-5.80	1.28	1.34
21	AA	1108	G	C2-N2	-5.80	1.28	1.34
54	BA	58	G	C2-N2	-5.80	1.28	1.34
54	BA	378	C	C4-N4	-5.80	1.28	1.33
54	BA	805	G	C2-N2	-5.80	1.28	1.34
54	BA	1429	G	C2-N2	-5.80	1.28	1.34
54	BA	1470	A	C6-N1	-5.80	1.31	1.35
21	AA	1098	C	N3-C4	-5.79	1.29	1.33
21	AA	57	G	C6-N1	-5.79	1.35	1.39
21	AA	673	A	C6-N1	-5.79	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1494	G	C2-N2	-5.79	1.28	1.34
54	BA	1697	G	C2-N2	-5.79	1.28	1.34
54	BA	2365	G	C2-N2	-5.79	1.28	1.34
21	AA	878	A	C6-N1	-5.79	1.31	1.35
54	BA	318	C	C4-N4	-5.79	1.28	1.33
55	BB	51	G	C2-N2	-5.79	1.28	1.34
24	A3	53	G	C2-N2	-5.79	1.28	1.34
21	AA	1146	A	C6-N1	-5.78	1.31	1.35
54	BA	1752	C	N3-C4	-5.78	1.29	1.33
21	AA	1447	A	C6-N1	-5.78	1.31	1.35
21	AA	1482	G	C2-N2	-5.78	1.28	1.34
21	AA	124	C	C4-N4	-5.78	1.28	1.33
21	AA	501	C	C4-N4	-5.78	1.28	1.33
21	AA	127	G	C2-N2	-5.78	1.28	1.34
54	BA	1961	C	C4-N4	-5.78	1.28	1.33
54	BA	2364	C	C4-N4	-5.78	1.28	1.33
21	AA	1231	G	C2-N2	-5.78	1.28	1.34
54	BA	2752	C	C4-N4	-5.78	1.28	1.33
54	BA	982	C	N3-C4	-5.77	1.29	1.33
54	BA	2795	C	C4-N4	-5.77	1.28	1.33
54	BA	2050	C	C4-N4	-5.77	1.28	1.33
54	BA	1541	C	C4-N4	-5.77	1.28	1.33
54	BA	2801	G	C2-N2	-5.77	1.28	1.34
21	AA	1226	C	N3-C4	-5.77	1.29	1.33
21	AA	1369	C	C4-N4	-5.76	1.28	1.33
21	AA	1502	A	C6-N1	-5.76	1.31	1.35
21	AA	1139	G	C2-N2	-5.76	1.28	1.34
54	BA	267	C	C4-N4	-5.76	1.28	1.33
54	BA	2353	G	C2-N2	-5.76	1.28	1.34
54	BA	729	G	C2-N2	-5.76	1.28	1.34
21	AA	235	C	C4-N4	-5.75	1.28	1.33
54	BA	1441	G	C2-N2	-5.75	1.28	1.34
21	AA	1209	C	C4-N4	-5.75	1.28	1.33
21	AA	1462	C	N3-C4	-5.75	1.29	1.33
54	BA	1382	G	C2-N2	-5.75	1.28	1.34
54	BA	1404	C	C4-N4	-5.75	1.28	1.33
54	BA	1985	C	N3-C4	-5.74	1.29	1.33
21	AA	676	A	C6-N1	-5.74	1.31	1.35
21	AA	1461	G	C2-N2	-5.74	1.28	1.34
21	AA	1433	A	C6-N1	-5.74	1.31	1.35
22	A1	61	C	C4-N4	-5.74	1.28	1.33
54	BA	1557	C	C4-N4	-5.74	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2850	A	C6-N1	-5.74	1.31	1.35
21	AA	848	C	C4-N4	-5.73	1.28	1.33
54	BA	1266	G	N1-C2	-5.73	1.33	1.37
54	BA	1093	G	C2-N2	-5.73	1.28	1.34
21	AA	880	C	C4-N4	-5.73	1.28	1.33
21	AA	1223	C	C4-N4	-5.73	1.28	1.33
54	BA	116	C	C4-N4	-5.73	1.28	1.33
54	BA	823	C	C4-N4	-5.73	1.28	1.33
55	BB	75	G	C2-N2	-5.73	1.28	1.34
21	AA	926	G	C6-N1	-5.72	1.35	1.39
54	BA	2717	C	C4-N4	-5.72	1.28	1.33
21	AA	1193	G	C2-N2	-5.72	1.28	1.34
54	BA	2067	G	C2-N2	-5.72	1.28	1.34
21	AA	868	C	C4-N4	-5.72	1.28	1.33
54	BA	2	G	C2-N2	-5.72	1.28	1.34
54	BA	2238	G	C2-N2	-5.72	1.28	1.34
55	BB	7	G	C2-N2	-5.72	1.28	1.34
54	BA	776	G	C2-N2	-5.72	1.28	1.34
54	BA	2033	A	C6-N1	-5.72	1.31	1.35
54	BA	1435	G	C2-N2	-5.71	1.28	1.34
54	BA	2228	G	C6-N1	-5.71	1.35	1.39
54	BA	2289	G	C2-N2	-5.71	1.28	1.34
54	BA	1701	A	C6-N1	-5.71	1.31	1.35
55	BB	75	G	C6-N1	-5.71	1.35	1.39
54	BA	2854	G	C2-N2	-5.71	1.28	1.34
54	BA	2083	G	C2-N2	-5.71	1.28	1.34
54	BA	2426	A	C6-N1	-5.70	1.31	1.35
54	BA	2521	C	C4-N4	-5.70	1.28	1.33
54	BA	1407	G	C2-N2	-5.70	1.28	1.34
54	BA	2361	G	C2-N2	-5.70	1.28	1.34
55	BB	105	G	C2-N2	-5.70	1.28	1.34
21	AA	370	C	C4-N4	-5.70	1.28	1.33
21	AA	128	G	C2-N2	-5.70	1.28	1.34
21	AA	1267	C	N3-C4	-5.69	1.29	1.33
54	BA	549	G	N1-C2	-5.69	1.33	1.37
55	BB	100	G	C2-N2	-5.69	1.28	1.34
21	AA	741	G	C2-N2	-5.69	1.28	1.34
21	AA	1482	G	C6-N1	-5.69	1.35	1.39
54	BA	719	C	N3-C4	-5.69	1.29	1.33
54	BA	1711	A	C5-C4	-5.69	1.34	1.38
21	AA	1516	G	C2-N2	-5.68	1.28	1.34
54	BA	845	A	C6-N1	-5.68	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	215	C	N3-C4	-5.68	1.29	1.33
54	BA	1080	A	C6-N1	-5.68	1.31	1.35
54	BA	1413	A	C6-N1	-5.68	1.31	1.35
55	BB	118	C	C4-N4	-5.68	1.28	1.33
54	BA	1472	C	C4-N4	-5.67	1.28	1.33
54	BA	2831	G	C2-N2	-5.67	1.28	1.34
54	BA	1984	G	C2-N2	-5.67	1.28	1.34
54	BA	1112	G	C2-N2	-5.67	1.28	1.34
54	BA	1114	C	C4-N4	-5.67	1.28	1.33
54	BA	176	A	C6-N1	-5.67	1.31	1.35
54	BA	1836	C	C4-N4	-5.67	1.28	1.33
54	BA	2200	C	N3-C4	-5.67	1.29	1.33
54	BA	2128	G	C2-N2	-5.66	1.28	1.34
21	AA	1195	C	C4-N4	-5.66	1.28	1.33
54	BA	164	C	C4-N4	-5.65	1.28	1.33
54	BA	295	G	C2-N2	-5.65	1.28	1.34
21	AA	385	C	N3-C4	-5.65	1.29	1.33
21	AA	1226	C	C4-N4	-5.65	1.28	1.33
54	BA	2607	G	C2-N2	-5.64	1.28	1.34
54	BA	2601	C	N3-C4	-5.64	1.30	1.33
21	AA	915	A	C6-N6	-5.64	1.29	1.33
21	AA	1438	G	C2-N2	-5.64	1.28	1.34
22	A1	30	C	C4-N4	-5.64	1.28	1.33
54	BA	145	C	C4-N4	-5.64	1.28	1.33
54	BA	445	C	C4-N4	-5.64	1.28	1.33
55	BB	60	C	C4-N4	-5.64	1.28	1.33
54	BA	1436	G	C2-N2	-5.64	1.28	1.34
54	BA	1710	G	C6-N1	-5.64	1.35	1.39
22	A1	52	G	C6-N1	-5.64	1.35	1.39
54	BA	531	C	N3-C4	-5.64	1.30	1.33
54	BA	1804	C	C4-N4	-5.64	1.28	1.33
21	AA	348	G	C2-N2	-5.63	1.28	1.34
54	BA	1314	C	C4-N4	-5.63	1.28	1.33
54	BA	2802	G	C6-N1	-5.63	1.35	1.39
21	AA	164	G	C2-N2	-5.63	1.28	1.34
21	AA	456	A	C6-N1	-5.63	1.31	1.35
21	AA	1215	G	C2-N2	-5.63	1.28	1.34
21	AA	1280	A	C6-N1	-5.63	1.31	1.35
54	BA	1601	G	C2-N2	-5.63	1.28	1.34
21	AA	144	G	C2-N2	-5.62	1.28	1.34
55	BB	98	G	C2-N2	-5.62	1.28	1.34
21	AA	271	C	C4-N4	-5.62	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2721	A	C6-N1	-5.62	1.31	1.35
21	AA	1234	C	C4-N4	-5.62	1.28	1.33
21	AA	1511	G	C2-N2	-5.62	1.28	1.34
21	AA	222	C	C4-N4	-5.62	1.28	1.33
21	AA	519	C	C4-N4	-5.61	1.28	1.33
21	AA	582	C	C4-N4	-5.61	1.28	1.33
54	BA	1679	A	C6-N1	-5.61	1.31	1.35
21	AA	1349	A	C6-N1	-5.61	1.31	1.35
21	AA	243	A	C6-N1	-5.61	1.31	1.35
21	AA	719	C	C4-N4	-5.61	1.28	1.33
21	AA	755	G	C2-N2	-5.61	1.28	1.34
21	AA	932	C	C4-N4	-5.61	1.28	1.33
54	BA	2805	C	C4-N4	-5.61	1.28	1.33
21	AA	191	G	C2-N2	-5.61	1.28	1.34
54	BA	1826	G	C2-N2	-5.61	1.28	1.34
54	BA	2383	G	C2-N2	-5.61	1.28	1.34
54	BA	2655	G	C2-N2	-5.61	1.28	1.34
55	BB	116	G	C6-N1	-5.61	1.35	1.39
54	BA	620	G	C2-N2	-5.61	1.28	1.34
55	BB	71	C	C4-N4	-5.61	1.28	1.33
21	AA	985	C	C4-N4	-5.60	1.28	1.33
54	BA	717	C	C4-N4	-5.60	1.28	1.33
54	BA	1045	C	C4-N4	-5.60	1.28	1.33
54	BA	1447	C	C4-N4	-5.60	1.28	1.33
21	AA	207	C	N3-C4	-5.60	1.30	1.33
21	AA	1210	C	C4-N4	-5.60	1.28	1.33
54	BA	54	G	C6-N1	-5.60	1.35	1.39
21	AA	192	A	C5-C4	-5.59	1.34	1.38
54	BA	2038	G	C6-N1	-5.59	1.35	1.39
21	AA	876	C	C4-N4	-5.59	1.28	1.33
21	AA	1361	G	C2-N2	-5.59	1.28	1.34
54	BA	1593	A	C6-N1	-5.59	1.31	1.35
54	BA	2263	C	N3-C4	-5.59	1.30	1.33
54	BA	2328	A	C6-N1	-5.59	1.31	1.35
21	AA	408	A	C6-N1	-5.58	1.31	1.35
54	BA	674	G	C2-N2	-5.58	1.28	1.34
21	AA	284	C	C4-N4	-5.58	1.28	1.33
54	BA	2520	C	C4-N4	-5.58	1.28	1.33
55	BB	64	G	C2-N2	-5.58	1.28	1.34
24	A3	1	C	N3-C4	-5.58	1.30	1.33
54	BA	2813	A	C6-N1	-5.58	1.31	1.35
54	BA	937	C	N3-C4	-5.58	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1356	G	C2-N2	-5.58	1.28	1.34
54	BA	1395	A	C6-N1	-5.58	1.31	1.35
54	BA	1802	A	C6-N1	-5.58	1.31	1.35
54	BA	1974	C	C4-N4	-5.58	1.28	1.33
21	AA	355	C	C4-N4	-5.58	1.28	1.33
54	BA	2815	C	C4-N4	-5.58	1.28	1.33
54	BA	2323	G	C2-N2	-5.57	1.28	1.34
54	BA	2499	C	C4-N4	-5.57	1.28	1.33
21	AA	1166	G	C2-N2	-5.57	1.28	1.34
54	BA	151	C	C4-N4	-5.57	1.28	1.33
54	BA	1376	C	C4-N4	-5.57	1.28	1.33
54	BA	2823	A	C6-N1	-5.57	1.31	1.35
54	BA	60	G	C2-N2	-5.57	1.28	1.34
54	BA	1538	G	C6-N1	-5.57	1.35	1.39
54	BA	2710	C	C4-N4	-5.57	1.28	1.33
54	BA	585	G	C6-N1	-5.56	1.35	1.39
21	AA	498	A	C5-C4	-5.56	1.34	1.38
54	BA	1954	G	C2-N2	-5.56	1.28	1.34
21	AA	1128	C	C4-N4	-5.56	1.28	1.33
54	BA	757	G	N1-C2	-5.56	1.33	1.37
54	BA	2175	C	C4-N4	-5.56	1.28	1.33
21	AA	1421	G	C2-N2	-5.56	1.28	1.34
21	AA	879	C	N3-C4	-5.55	1.30	1.33
54	BA	383	C	C4-N4	-5.55	1.28	1.33
21	AA	953	G	C2-N2	-5.55	1.28	1.34
54	BA	985	C	C4-N4	-5.55	1.28	1.33
54	BA	1772	A	C5-C4	-5.55	1.34	1.38
55	BB	29	A	C6-N1	-5.55	1.31	1.35
54	BA	2365	G	C6-N1	-5.55	1.35	1.39
54	BA	2452	C	C4-N4	-5.55	1.28	1.33
21	AA	347	G	C2-N2	-5.54	1.29	1.34
21	AA	376	G	C2-N2	-5.54	1.29	1.34
21	AA	568	G	C2-N2	-5.54	1.29	1.34
21	AA	1144	G	C2-N2	-5.54	1.29	1.34
54	BA	2723	C	C4-N4	-5.54	1.28	1.33
21	AA	725	G	C2-N2	-5.54	1.29	1.34
54	BA	128	C	N3-C4	-5.54	1.30	1.33
54	BA	2201	G	C2-N2	-5.54	1.29	1.34
21	AA	34	C	C4-N4	-5.54	1.28	1.33
54	BA	1290	C	C4-N4	-5.54	1.28	1.33
54	BA	1972	G	C2-N2	-5.54	1.29	1.34
54	BA	2626	C	C4-N4	-5.54	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	601	C	C4-N4	-5.54	1.28	1.33
54	BA	1490	A	C6-N1	-5.54	1.31	1.35
54	BA	1555	G	N1-C2	-5.54	1.33	1.37
54	BA	2591	C	N3-C4	-5.54	1.30	1.33
55	BB	8	C	N3-C4	-5.53	1.30	1.33
21	AA	384	G	C2-N2	-5.53	1.29	1.34
54	BA	809	G	C2-N2	-5.53	1.29	1.34
54	BA	2394	C	C4-N4	-5.53	1.28	1.33
21	AA	734	G	C2-N2	-5.53	1.29	1.34
54	BA	1092	C	C4-N4	-5.53	1.28	1.33
21	AA	217	C	C4-N4	-5.53	1.28	1.33
21	AA	354	G	C2-N2	-5.53	1.29	1.34
54	BA	1570	A	C6-N1	-5.53	1.31	1.35
21	AA	528	C	C4-N4	-5.53	1.28	1.33
21	AA	869	G	C6-N1	-5.53	1.35	1.39
21	AA	1418	A	C5-C4	-5.52	1.34	1.38
24	A3	5	G	C2-N2	-5.52	1.29	1.34
55	BB	94	A	C6-N1	-5.52	1.31	1.35
21	AA	727	G	N1-C2	-5.52	1.33	1.37
21	AA	1151	A	C6-N1	-5.52	1.31	1.35
54	BA	333	G	C2-N2	-5.52	1.29	1.34
24	A3	6	G	C2-N2	-5.51	1.29	1.34
21	AA	496	A	C6-N1	-5.51	1.31	1.35
21	AA	1388	C	C4-N4	-5.51	1.28	1.33
54	BA	936	A	C6-N1	-5.51	1.31	1.35
54	BA	2747	G	C2-N2	-5.51	1.29	1.34
54	BA	2162	G	C2-N2	-5.51	1.29	1.34
54	BA	2722	G	N1-C2	-5.51	1.33	1.37
21	AA	806	C	N3-C4	-5.50	1.30	1.33
55	BB	26	C	C4-N4	-5.50	1.28	1.33
21	AA	1421	G	C6-N1	-5.50	1.35	1.39
54	BA	1608	A	C6-N1	-5.50	1.31	1.35
21	AA	462	G	C2-N2	-5.50	1.29	1.34
21	AA	1342	C	C4-N4	-5.50	1.29	1.33
54	BA	2422	C	C4-N4	-5.50	1.29	1.33
54	BA	2901	C	C4-N4	-5.50	1.29	1.33
21	AA	1483	A	C6-N1	-5.49	1.31	1.35
54	BA	2301	C	C4-N4	-5.49	1.29	1.33
54	BA	2870	C	C4-N4	-5.49	1.29	1.33
21	AA	48	C	C4-N4	-5.49	1.29	1.33
54	BA	291	G	C2-N2	-5.49	1.29	1.34
21	AA	1217	C	C4-N4	-5.49	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1410	A	C6-N1	-5.49	1.31	1.35
54	BA	1044	C	C4-N4	-5.49	1.29	1.33
54	BA	1787	A	C6-N1	-5.49	1.31	1.35
54	BA	2747	G	C6-N1	-5.49	1.35	1.39
21	AA	77	A	C6-N1	-5.48	1.31	1.35
21	AA	444	G	C6-N1	-5.48	1.35	1.39
21	AA	525	C	C4-N4	-5.48	1.29	1.33
54	BA	130	C	C4-N4	-5.48	1.29	1.33
54	BA	291	G	C6-N1	-5.48	1.35	1.39
54	BA	2623	G	C2-N2	-5.48	1.29	1.34
54	BA	2712	C	C4-N4	-5.48	1.29	1.33
21	AA	392	C	C4-N4	-5.48	1.29	1.33
21	AA	419	C	C4-N4	-5.48	1.29	1.33
54	BA	1428	C	C4-N4	-5.48	1.29	1.33
21	AA	685	G	C6-N1	-5.47	1.35	1.39
21	AA	356	A	C5-C4	-5.47	1.34	1.38
54	BA	2875	C	C4-N4	-5.47	1.29	1.33
55	BB	52	A	C6-N1	-5.47	1.31	1.35
21	AA	178	C	C4-N4	-5.47	1.29	1.33
21	AA	266	G	C4'-O4'	-5.47	1.38	1.45
54	BA	2152	G	C2-N2	-5.47	1.29	1.34
54	BA	752	A	C6-N1	-5.47	1.31	1.35
55	BB	33	G	C2-N2	-5.47	1.29	1.34
21	AA	498	A	C6-N6	-5.47	1.29	1.33
54	BA	736	C	C4-N4	-5.46	1.29	1.33
54	BA	1401	G	C6-N1	-5.46	1.35	1.39
21	AA	1404	C	N3-C4	-5.46	1.30	1.33
54	BA	2024	G	C2-N2	-5.46	1.29	1.34
21	AA	685	G	C2-N2	-5.46	1.29	1.34
54	BA	1343	G	C2-N2	-5.46	1.29	1.34
54	BA	1464	G	C2-N2	-5.46	1.29	1.34
21	AA	206	C	N3-C4	-5.46	1.30	1.33
21	AA	1208	C	N3-C4	-5.46	1.30	1.33
54	BA	2258	C	N3-C4	-5.46	1.30	1.33
21	AA	1231	G	C6-N1	-5.46	1.35	1.39
22	A1	22	G	C2-N2	-5.46	1.29	1.34
54	BA	1077	A	C6-N1	-5.46	1.31	1.35
54	BA	1792	G	C2-N2	-5.46	1.29	1.34
54	BA	1879	C	C4-N4	-5.46	1.29	1.33
55	BB	6	G	C2-N2	-5.46	1.29	1.34
55	BB	49	C	C4-N4	-5.46	1.29	1.33
21	AA	164	G	C6-N1	-5.45	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2846	G	C2-N2	-5.45	1.29	1.34
21	AA	67	C	N3-C4	-5.45	1.30	1.33
21	AA	141	G	C2-N2	-5.45	1.29	1.34
54	BA	1986	C	C4-N4	-5.45	1.29	1.33
21	AA	425	G	C2-N2	-5.45	1.29	1.34
54	BA	910	A	C6-N1	-5.45	1.31	1.35
54	BA	2888	C	C4-N4	-5.45	1.29	1.33
54	BA	265	A	C6-N1	-5.44	1.31	1.35
21	AA	1109	C	C4-N4	-5.44	1.29	1.33
55	BB	2	G	C2-N2	-5.44	1.29	1.34
21	AA	281	G	C2-N2	-5.44	1.29	1.34
54	BA	334	C	N3-C4	-5.44	1.30	1.33
21	AA	21	G	N1-C2	-5.44	1.33	1.37
54	BA	2827	C	N3-C4	-5.44	1.30	1.33
21	AA	413	G	C2-N2	-5.44	1.29	1.34
21	AA	744	C	C4-N4	-5.44	1.29	1.33
54	BA	1339	G	C2-N2	-5.43	1.29	1.34
55	BB	117	G	C2-N2	-5.43	1.29	1.34
54	BA	942	G	C2-N2	-5.43	1.29	1.34
21	AA	227	G	C6-N1	-5.43	1.35	1.39
54	BA	1759	A	C6-N1	-5.43	1.31	1.35
54	BA	1034	G	C2-N2	-5.43	1.29	1.34
21	AA	708	C	N3-C4	-5.43	1.30	1.33
21	AA	1164	G	N1-C2	-5.43	1.33	1.37
54	BA	45	G	C2-N2	-5.43	1.29	1.34
54	BA	2038	G	C2-N2	-5.43	1.29	1.34
21	AA	382	A	C5-C4	-5.42	1.34	1.38
54	BA	384	A	C6-N1	-5.42	1.31	1.35
54	BA	1857	G	C2-N2	-5.42	1.29	1.34
21	AA	1405	G	C2-N2	-5.42	1.29	1.34
54	BA	396	G	C6-N1	-5.42	1.35	1.39
54	BA	2346	A	O3'-P	-5.42	1.54	1.61
21	AA	1193	G	C6-N1	-5.42	1.35	1.39
54	BA	1446	C	N3-C4	-5.42	1.30	1.33
21	AA	1225	A	C6-N1	-5.42	1.31	1.35
54	BA	2295	C	C4-N4	-5.42	1.29	1.33
54	BA	2802	G	C2-N2	-5.42	1.29	1.34
21	AA	586	C	C4-N4	-5.41	1.29	1.33
21	AA	803	G	C2-N2	-5.41	1.29	1.34
54	BA	7	G	C2-N2	-5.41	1.29	1.34
54	BA	885	C	C4-N4	-5.41	1.29	1.33
54	BA	2862	G	N1-C2	-5.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1047	G	C2-N2	-5.41	1.29	1.34
54	BA	1353	A	C6-N1	-5.41	1.31	1.35
54	BA	398	C	C4-N4	-5.41	1.29	1.33
54	BA	1718	G	C2-N2	-5.41	1.29	1.34
54	BA	1954	G	C6-N1	-5.41	1.35	1.39
54	BA	2396	G	C6-N1	-5.41	1.35	1.39
21	AA	1188	A	C6-N1	-5.41	1.31	1.35
54	BA	425	G	C2-N2	-5.41	1.29	1.34
55	BB	110	C	N3-C4	-5.41	1.30	1.33
54	BA	121	G	C2-N2	-5.40	1.29	1.34
21	AA	1426	G	C2-N2	-5.40	1.29	1.34
54	BA	54	G	C2-N2	-5.40	1.29	1.34
54	BA	1726	C	C4-N4	-5.40	1.29	1.33
54	BA	1564	C	C4-N4	-5.40	1.29	1.33
54	BA	2755	C	N3-C4	-5.40	1.30	1.33
21	AA	356	A	C6-N6	-5.39	1.29	1.33
21	AA	220	G	C2-N2	-5.39	1.29	1.34
54	BA	134	G	C6-N1	-5.39	1.35	1.39
54	BA	426	C	N3-C4	-5.39	1.30	1.33
54	BA	2304	G	C2-N2	-5.39	1.29	1.34
54	BA	1984	G	C6-N1	-5.39	1.35	1.39
54	BA	2043	C	N3-C4	-5.39	1.30	1.33
21	AA	750	C	C4-N4	-5.39	1.29	1.33
24	A3	43	G	C2-N2	-5.39	1.29	1.34
54	BA	516	C	C4-N4	-5.39	1.29	1.33
21	AA	95	C	N3-C4	-5.38	1.30	1.33
21	AA	394	G	C2-N2	-5.38	1.29	1.34
21	AA	455	G	C2-N2	-5.38	1.29	1.34
21	AA	403	C	C4-N4	-5.38	1.29	1.33
22	A1	13	C	C4-N4	-5.38	1.29	1.33
54	BA	651	G	C2-N2	-5.38	1.29	1.34
54	BA	1450	G	C2-N2	-5.38	1.29	1.34
54	BA	1960	A	C6-N1	-5.38	1.31	1.35
54	BA	2102	G	C2-N2	-5.37	1.29	1.34
24	A3	54	G	C2-N2	-5.37	1.29	1.34
54	BA	2140	G	C2-N2	-5.37	1.29	1.34
54	BA	175	G	C2-N2	-5.37	1.29	1.34
54	BA	1575	C	N3-C4	-5.37	1.30	1.33
24	A3	58	A	C5-C4	-5.37	1.34	1.38
54	BA	1526	C	N3-C4	-5.37	1.30	1.33
54	BA	2644	G	C2-N2	-5.37	1.29	1.34
54	BA	706	A	C6-N1	-5.36	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1353	G	C2-N2	-5.36	1.29	1.34
21	AA	1048	G	C2-N2	-5.36	1.29	1.34
54	BA	1368	G	C2-N2	-5.36	1.29	1.34
21	AA	939	G	C2-N2	-5.36	1.29	1.34
21	AA	1418	A	C6-N6	-5.36	1.29	1.33
54	BA	2856	A	C5-C4	-5.35	1.35	1.38
54	BA	160	A	C6-N1	-5.35	1.31	1.35
54	BA	1084	A	C6-N6	-5.35	1.29	1.33
54	BA	1872	A	C6-N1	-5.35	1.31	1.35
54	BA	2371	G	C2-N2	-5.35	1.29	1.34
21	AA	338	A	C6-N1	-5.35	1.31	1.35
21	AA	970	C	C4-N4	-5.35	1.29	1.33
21	AA	1524	C	C4-N4	-5.35	1.29	1.33
54	BA	1750	G	C2-N2	-5.35	1.29	1.34
54	BA	2127	G	C2-N2	-5.35	1.29	1.34
54	BA	2260	C	C4-N4	-5.35	1.29	1.33
54	BA	2603	G	N1-C2	-5.35	1.33	1.37
54	BA	217	A	C6-N1	-5.35	1.31	1.35
54	BA	1270	C	N3-C4	-5.35	1.30	1.33
54	BA	711	G	C2-N2	-5.35	1.29	1.34
21	AA	522	C	C4-N4	-5.34	1.29	1.33
21	AA	1147	C	C4-N4	-5.34	1.29	1.33
24	A3	40	C	C4-N4	-5.34	1.29	1.33
54	BA	9	G	C2-N2	-5.34	1.29	1.34
54	BA	624	C	C4-N4	-5.34	1.29	1.33
54	BA	668	A	C6-N1	-5.34	1.31	1.35
54	BA	2389	G	C2-N2	-5.34	1.29	1.34
21	AA	146	G	C2-N2	-5.34	1.29	1.34
54	BA	456	C	C4-N4	-5.34	1.29	1.33
54	BA	979	A	C6-N6	-5.34	1.29	1.33
54	BA	1256	G	C2-N2	-5.34	1.29	1.34
54	BA	2150	C	C4-N4	-5.34	1.29	1.33
21	AA	1416	G	C2-N2	-5.34	1.29	1.34
54	BA	2391	G	N1-C2	-5.34	1.33	1.37
54	BA	2686	G	C2-N2	-5.34	1.29	1.34
55	BB	51	G	C6-N1	-5.34	1.35	1.39
54	BA	391	A	C6-N1	-5.33	1.31	1.35
54	BA	672	C	C4-N4	-5.33	1.29	1.33
54	BA	1719	G	C2-N2	-5.33	1.29	1.34
21	AA	382	A	C6-N6	-5.33	1.29	1.33
21	AA	527	G	C2-N2	-5.33	1.29	1.34
21	AA	1468	A	C5-C4	-5.33	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1388	G	C2-N2	-5.33	1.29	1.34
54	BA	1681	G	C2-N2	-5.33	1.29	1.34
54	BA	1760	C	N3-C4	-5.33	1.30	1.33
54	BA	2842	G	C2-N2	-5.33	1.29	1.34
54	BA	287	G	N1-C2	-5.33	1.33	1.37
54	BA	627	A	C6-N1	-5.33	1.31	1.35
54	BA	1585	C	C4-N4	-5.33	1.29	1.33
54	BA	2899	A	C6-N1	-5.33	1.31	1.35
21	AA	359	G	C6-N1	-5.33	1.35	1.39
21	AA	468	A	C6-N1	-5.33	1.31	1.35
21	AA	511	C	N3-C4	-5.33	1.30	1.33
21	AA	877	G	C2-N2	-5.33	1.29	1.34
54	BA	536	G	C2-N2	-5.33	1.29	1.34
21	AA	205	A	C6-N1	-5.33	1.31	1.35
24	A3	19	G	C6-N1	-5.33	1.35	1.39
54	BA	49	A	C6-N6	-5.33	1.29	1.33
54	BA	669	G	N1-C2	-5.33	1.33	1.37
54	BA	1295	C	C4-N4	-5.33	1.29	1.33
54	BA	825	A	C6-N1	-5.32	1.31	1.35
21	AA	153	C	C4-N4	-5.32	1.29	1.33
54	BA	1615	C	C4-N4	-5.32	1.29	1.33
54	BA	2332	C	C4-N4	-5.32	1.29	1.33
21	AA	349	A	C5-C4	-5.32	1.35	1.38
21	AA	1366	C	N3-C4	-5.32	1.30	1.33
21	AA	1501	C	N3-C4	-5.32	1.30	1.33
54	BA	978	G	C2-N2	-5.32	1.29	1.34
54	BA	1980	G	N1-C2	-5.32	1.33	1.37
54	BA	2067	G	C6-N1	-5.32	1.35	1.39
54	BA	2896	C	C4-N4	-5.32	1.29	1.33
55	BB	114	C	C4-N4	-5.32	1.29	1.33
21	AA	930	C	N3-C4	-5.32	1.30	1.33
21	AA	15	G	C2-N2	-5.32	1.29	1.34
21	AA	1402	C	C4-N4	-5.32	1.29	1.33
54	BA	2624	G	N1-C2	-5.32	1.33	1.37
54	BA	1567	G	N1-C2	-5.31	1.33	1.37
21	AA	248	C	C4-N4	-5.31	1.29	1.33
21	AA	489	C	C4-N4	-5.31	1.29	1.33
21	AA	915	A	C5-C4	-5.31	1.35	1.38
21	AA	1305	G	C2-N2	-5.31	1.29	1.34
54	BA	518	G	C2-N2	-5.31	1.29	1.34
54	BA	2102	G	C6-N1	-5.31	1.35	1.39
54	BA	2762	C	N3-C4	-5.31	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	326	G	C2-N2	-5.31	1.29	1.34
54	BA	31	C	C4-N4	-5.31	1.29	1.33
54	BA	1436	G	C6-N1	-5.31	1.35	1.39
21	AA	844	G	C2-N2	-5.31	1.29	1.34
21	AA	236	A	C6-N1	-5.31	1.31	1.35
21	AA	191	G	C6-N1	-5.30	1.35	1.39
54	BA	1569	A	C6-N1	-5.30	1.31	1.35
21	AA	557	G	C2-N2	-5.30	1.29	1.34
21	AA	845	A	C6-N1	-5.30	1.31	1.35
21	AA	1172	C	N3-C4	-5.30	1.30	1.33
21	AA	497	G	N1-C2	-5.30	1.33	1.37
21	AA	941	G	C2-N2	-5.30	1.29	1.34
21	AA	1038	C	C4-N4	-5.30	1.29	1.33
54	BA	1036	G	C2-N2	-5.30	1.29	1.34
54	BA	2692	G	C6-N1	-5.30	1.35	1.39
55	BB	81	G	C2-N2	-5.30	1.29	1.34
22	A1	62	C	C4-C5	-5.30	1.38	1.43
21	AA	260	G	C2-N2	-5.30	1.29	1.34
21	AA	156	C	C4-N4	-5.29	1.29	1.33
21	AA	1503	A	C6-N1	-5.29	1.31	1.35
54	BA	1831	G	C2-N2	-5.29	1.29	1.34
21	AA	147	G	N1-C2	-5.29	1.33	1.37
21	AA	1497	G	N1-C2	-5.29	1.33	1.37
21	AA	31	G	N1-C2	-5.29	1.33	1.37
21	AA	1398	A	C6-N6	-5.29	1.29	1.33
24	A3	67	C	C4-N4	-5.29	1.29	1.33
54	BA	2405	G	C2-N2	-5.29	1.29	1.34
21	AA	1473	G	N1-C2	-5.29	1.33	1.37
54	BA	41	C	N3-C4	-5.29	1.30	1.33
54	BA	2123	G	C2-N2	-5.29	1.29	1.34
54	BA	2824	C	C4-N4	-5.29	1.29	1.33
54	BA	2080	A	C5-C4	-5.28	1.35	1.38
54	BA	700	G	C2-N2	-5.28	1.29	1.34
55	BB	23	G	C2-N2	-5.28	1.29	1.34
54	BA	1962	C	C4-N4	-5.28	1.29	1.33
54	BA	2084	C	N3-C4	-5.28	1.30	1.33
54	BA	1738	G	C2-N2	-5.28	1.29	1.34
21	AA	380	G	C2-N2	-5.28	1.29	1.34
54	BA	1708	C	C4-N4	-5.28	1.29	1.33
21	AA	459	A	C6-N1	-5.27	1.31	1.35
54	BA	1403	A	C5-C4	-5.27	1.35	1.38
21	AA	604	G	C2-N2	-5.27	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	315	G	C2-N2	-5.27	1.29	1.34
54	BA	418	C	C4-N4	-5.27	1.29	1.33
54	BA	1251	C	N3-C4	-5.27	1.30	1.33
54	BA	1704	C	C4-N4	-5.27	1.29	1.33
21	AA	728	A	C5-C4	-5.27	1.35	1.38
54	BA	352	A	C6-N1	-5.27	1.31	1.35
21	AA	737	C	C4-N4	-5.27	1.29	1.33
54	BA	2103	C	N3-C4	-5.27	1.30	1.33
21	AA	776	G	C6-N1	-5.26	1.35	1.39
54	BA	738	G	C2-N2	-5.26	1.29	1.34
54	BA	1703	G	N1-C2	-5.26	1.33	1.37
54	BA	1289	C	N3-C4	-5.26	1.30	1.33
54	BA	2337	G	C2-N2	-5.26	1.29	1.34
21	AA	188	C	C4-N4	-5.26	1.29	1.33
54	BA	2708	G	C2-N2	-5.26	1.29	1.34
21	AA	444	G	C2-N2	-5.26	1.29	1.34
54	BA	1102	C	C4-N4	-5.26	1.29	1.33
54	BA	2682	A	C6-N1	-5.26	1.31	1.35
54	BA	2777	G	C2-N2	-5.26	1.29	1.34
54	BA	281	C	C4-N4	-5.26	1.29	1.33
54	BA	342	A	C5-C4	-5.26	1.35	1.38
54	BA	979	A	C5-C4	-5.26	1.35	1.38
55	BB	37	C	N3-C4	-5.26	1.30	1.33
21	AA	363	A	C6-N1	-5.26	1.31	1.35
54	BA	1334	G	C2-N2	-5.26	1.29	1.34
21	AA	781	A	C5-C4	-5.25	1.35	1.38
54	BA	297	G	N1-C2	-5.25	1.33	1.37
54	BA	1934	C	C4-N4	-5.25	1.29	1.33
54	BA	2234	G	C2-N2	-5.25	1.29	1.34
54	BA	2350	C	C4-N4	-5.25	1.29	1.33
54	BA	2683	C	C4-N4	-5.25	1.29	1.33
55	BB	15	A	C6-N6	-5.25	1.29	1.33
21	AA	469	C	N3-C4	-5.25	1.30	1.33
54	BA	2177	C	C4-N4	-5.25	1.29	1.33
54	BA	2281	A	C6-N1	-5.25	1.31	1.35
54	BA	577	G	C2-N2	-5.25	1.29	1.34
54	BA	1069	A	C6-N1	-5.25	1.31	1.35
54	BA	1363	C	C4-N4	-5.25	1.29	1.33
21	AA	187	G	N1-C2	-5.25	1.33	1.37
21	AA	242	G	C2-N2	-5.25	1.29	1.34
21	AA	838	G	C2-N2	-5.25	1.29	1.34
54	BA	719	C	C4-N4	-5.25	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2600	A	C6-N1	-5.25	1.31	1.35
54	BA	1072	C	C4-N4	-5.25	1.29	1.33
54	BA	2692	G	C2-N2	-5.25	1.29	1.34
54	BA	1382	G	C6-N1	-5.25	1.35	1.39
55	BB	9	G	C2-N2	-5.25	1.29	1.34
24	A3	1	C	C4-N4	-5.24	1.29	1.33
54	BA	60	G	C6-N1	-5.24	1.35	1.39
21	AA	874	G	N1-C2	-5.24	1.33	1.37
54	BA	879	G	C2-N2	-5.24	1.29	1.34
54	BA	2314	A	C6-N1	-5.24	1.31	1.35
21	AA	680	C	N3-C4	-5.24	1.30	1.33
54	BA	167	A	C6-N1	-5.24	1.31	1.35
54	BA	1973	G	C2-N2	-5.24	1.29	1.34
54	BA	2029	G	C2-N2	-5.24	1.29	1.34
54	BA	2330	G	C2-N2	-5.24	1.29	1.34
21	AA	192	A	C6-N6	-5.24	1.29	1.33
21	AA	175	C	N3-C4	-5.24	1.30	1.33
54	BA	2611	C	N3-C4	-5.24	1.30	1.33
54	BA	2750	A	C6-N1	-5.24	1.31	1.35
21	AA	63	C	C4-N4	-5.23	1.29	1.33
21	AA	1322	C	C4-N4	-5.23	1.29	1.33
54	BA	2349	G	C2-N2	-5.23	1.29	1.34
54	BA	2683	C	N3-C4	-5.23	1.30	1.33
21	AA	357	G	C2-N2	-5.23	1.29	1.34
21	AA	1371	G	C2-N2	-5.23	1.29	1.34
54	BA	2042	A	C6-N1	-5.23	1.31	1.35
21	AA	1132	C	N3-C4	-5.23	1.30	1.33
54	BA	684	G	C2-N2	-5.23	1.29	1.34
21	AA	386	C	N3-C4	-5.23	1.30	1.33
21	AA	106	C	N3-C4	-5.22	1.30	1.33
21	AA	735	C	N3-C4	-5.22	1.30	1.33
54	BA	1355	G	C2-N2	-5.22	1.29	1.34
54	BA	2174	C	N3-C4	-5.22	1.30	1.33
21	AA	184	G	C2-N2	-5.22	1.29	1.34
21	AA	1159	U	C4'-O4'	-5.22	1.38	1.45
21	AA	1526	G	C2-N2	-5.22	1.29	1.34
54	BA	1514	G	C2-N2	-5.22	1.29	1.34
54	BA	1989	G	C2-N2	-5.22	1.29	1.34
21	AA	310	G	C2-N2	-5.22	1.29	1.34
54	BA	438	G	N1-C2	-5.22	1.33	1.37
54	BA	844	A	C6-N1	-5.22	1.31	1.35
54	BA	2196	C	N3-C4	-5.22	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2224	G	C2-N2	-5.22	1.29	1.34
54	BA	2294	G	C2-N2	-5.22	1.29	1.34
54	BA	2385	C	C4-N4	-5.22	1.29	1.33
21	AA	1156	G	C2-N2	-5.22	1.29	1.34
54	BA	68	G	N1-C2	-5.22	1.33	1.37
54	BA	347	A	C6-N1	-5.22	1.31	1.35
54	BA	1417	C	N3-C4	-5.22	1.30	1.33
54	BA	1753	G	C2-N2	-5.22	1.29	1.34
54	BA	1788	C	N3-C4	-5.22	1.30	1.33
22	A1	32	C	N3-C4	-5.21	1.30	1.33
54	BA	2078	C	N3-C4	-5.21	1.30	1.33
54	BA	1373	A	C6-N1	-5.21	1.31	1.35
54	BA	473	G	C6-N1	-5.21	1.35	1.39
54	BA	520	G	C2-N2	-5.21	1.29	1.34
54	BA	1543	G	C2-N2	-5.21	1.29	1.34
54	BA	1620	G	C2-N2	-5.21	1.29	1.34
54	BA	1800	C	C4-N4	-5.21	1.29	1.33
21	AA	457	G	C2-N2	-5.21	1.29	1.34
54	BA	35	G	C2-N2	-5.21	1.29	1.34
21	AA	364	A	C5-C4	-5.21	1.35	1.38
54	BA	2005	A	C6-N1	-5.21	1.31	1.35
54	BA	2093	G	N1-C2	-5.21	1.33	1.37
54	BA	2748	A	C6-N1	-5.21	1.31	1.35
55	BB	7	G	C6-N1	-5.21	1.35	1.39
24	A3	2	G	N1-C2	-5.21	1.33	1.37
54	BA	2616	C	C4-N4	-5.21	1.29	1.33
54	BA	544	C	C4-N4	-5.20	1.29	1.33
54	BA	2745	C	C4-N4	-5.20	1.29	1.33
21	AA	852	G	C2-N2	-5.20	1.29	1.34
21	AA	171	A	C6-N1	-5.20	1.31	1.35
21	AA	226	G	C2-N2	-5.20	1.29	1.34
21	AA	802	A	C6-N1	-5.20	1.31	1.35
21	AA	862	C	N3-C4	-5.20	1.30	1.33
21	AA	1428	A	C5-C4	-5.20	1.35	1.38
21	AA	1466	C	C4-N4	-5.20	1.29	1.33
54	BA	49	A	C5-C4	-5.20	1.35	1.38
54	BA	760	G	C2-N2	-5.20	1.29	1.34
21	AA	39	G	C2-N2	-5.20	1.29	1.34
21	AA	1249	C	C4-N4	-5.20	1.29	1.33
21	AA	1378	C	N3-C4	-5.20	1.30	1.33
54	BA	129	C	C4-N4	-5.20	1.29	1.33
54	BA	1544	A	C6-N1	-5.20	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1428	A	C6-N6	-5.19	1.29	1.33
21	AA	129	A	C5-C4	-5.19	1.35	1.38
54	BA	983	A	C6-N1	-5.19	1.31	1.35
54	BA	1740	G	C2-N2	-5.19	1.29	1.34
54	BA	2239	G	C2-N2	-5.19	1.29	1.34
54	BA	2893	A	C6-N1	-5.19	1.31	1.35
54	BA	1945	G	C2-N2	-5.19	1.29	1.34
21	AA	726	C	C4-N4	-5.19	1.29	1.33
54	BA	680	C	N3-C4	-5.18	1.30	1.33
54	BA	2221	G	C2-N2	-5.18	1.29	1.34
54	BA	1686	C	N3-C4	-5.18	1.30	1.33
54	BA	1788	C	C4-N4	-5.18	1.29	1.33
54	BA	2498	C	C4-N4	-5.18	1.29	1.33
21	AA	1102	A	C6-N1	-5.18	1.31	1.35
54	BA	449	A	C6-N1	-5.18	1.31	1.35
54	BA	2719	G	C2-N2	-5.18	1.29	1.34
21	AA	247	G	C2-N2	-5.18	1.29	1.34
21	AA	825	A	C6-N1	-5.18	1.31	1.35
54	BA	1766	G	C2-N2	-5.18	1.29	1.34
21	AA	35	G	C2-N2	-5.18	1.29	1.34
54	BA	2208	C	C4-N4	-5.18	1.29	1.33
54	BA	2789	C	C4-N4	-5.18	1.29	1.33
54	BA	447	A	C5-C4	-5.17	1.35	1.38
54	BA	2063	C	C4-N4	-5.17	1.29	1.33
54	BA	2230	G	N1-C2	-5.17	1.33	1.37
21	AA	16	A	C5-C4	-5.17	1.35	1.38
22	A1	1	G	C2-N2	-5.17	1.29	1.34
21	AA	97	G	N1-C2	-5.17	1.33	1.37
21	AA	470	C	C4-N4	-5.17	1.29	1.33
54	BA	2065	C	C4-N4	-5.17	1.29	1.33
55	BB	105	G	C6-N1	-5.17	1.35	1.39
21	AA	1100	C	C4-N4	-5.17	1.29	1.33
21	AA	349	A	C6-N6	-5.17	1.29	1.33
21	AA	518	C	N3-C4	-5.17	1.30	1.33
54	BA	1674	G	N1-C2	-5.17	1.33	1.37
21	AA	544	G	C2-N2	-5.17	1.29	1.34
21	AA	1409	C	N3-C4	-5.17	1.30	1.33
21	AA	1488	G	C2-N2	-5.17	1.29	1.34
54	BA	359	G	C2-N2	-5.17	1.29	1.34
54	BA	761	A	C6-N1	-5.17	1.31	1.35
21	AA	453	G	C6-N1	-5.16	1.35	1.39
24	A3	66	C	N3-C4	-5.16	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1127	A	C6-N1	-5.16	1.31	1.35
54	BA	2054	A	C6-N1	-5.16	1.31	1.35
21	AA	1493	A	C6-N6	-5.16	1.29	1.33
22	A1	18	G	C2-N2	-5.16	1.29	1.34
54	BA	1434	A	C5-C4	-5.16	1.35	1.38
54	BA	1512	C	C4-N4	-5.16	1.29	1.33
54	BA	2226	C	C4-N4	-5.16	1.29	1.33
54	BA	2428	G	C6-N1	-5.16	1.35	1.39
54	BA	1826	G	C6-N1	-5.16	1.35	1.39
21	AA	383	A	C6-N6	-5.16	1.29	1.33
54	BA	55	G	N1-C2	-5.16	1.33	1.37
54	BA	943	A	C6-N1	-5.16	1.31	1.35
21	AA	728	A	C6-N6	-5.16	1.29	1.33
54	BA	48	G	C2-N2	-5.16	1.29	1.34
54	BA	320	A	C6-N1	-5.16	1.31	1.35
54	BA	1972	G	C6-N1	-5.16	1.35	1.39
21	AA	959	A	C6-N1	-5.15	1.31	1.35
54	BA	496	G	C2-N2	-5.15	1.29	1.34
54	BA	192	C	C4-N4	-5.15	1.29	1.33
54	BA	1090	A	C5-C4	-5.15	1.35	1.38
54	BA	1319	C	C4-N4	-5.15	1.29	1.33
55	BB	79	G	C2-N2	-5.15	1.29	1.34
55	BB	86	G	C6-N1	-5.15	1.35	1.39
21	AA	730	G	C6-N1	-5.15	1.35	1.39
21	AA	770	C	C4'-C3'	-5.15	1.47	1.52
21	AA	1129	C	C4-N4	-5.15	1.29	1.33
54	BA	733	G	C2-N2	-5.15	1.29	1.34
55	BB	85	G	C2-N2	-5.15	1.29	1.34
54	BA	2446	G	C6-N1	-5.15	1.35	1.39
54	BA	42	A	C5-C4	-5.14	1.35	1.38
54	BA	597	G	C2-N2	-5.14	1.29	1.34
54	BA	1371	G	C2-N2	-5.14	1.29	1.34
21	AA	156	C	N3-C4	-5.14	1.30	1.33
21	AA	840	C	C4-N4	-5.14	1.29	1.33
21	AA	1141	C	C4-N4	-5.14	1.29	1.33
22	A1	15	G	C2-N2	-5.14	1.29	1.34
22	A1	53	G	C2-N2	-5.14	1.29	1.34
54	BA	411	G	C6-N1	-5.14	1.35	1.39
21	AA	604	G	C6-N1	-5.14	1.35	1.39
54	BA	2885	G	C2-N2	-5.14	1.29	1.34
21	AA	395	C	N3-C4	-5.14	1.30	1.33
21	AA	1071	C	N3-C4	-5.14	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	731	C	C4-N4	-5.14	1.29	1.33
54	BA	1530	G	C2-N2	-5.14	1.29	1.34
54	BA	2306	C	C4-N4	-5.14	1.29	1.33
21	AA	113	G	C2-N2	-5.14	1.29	1.34
54	BA	1536	C	C4-N4	-5.14	1.29	1.33
54	BA	1929	G	C2-N2	-5.14	1.29	1.34
54	BA	2362	C	C4-N4	-5.14	1.29	1.33
21	AA	1415	G	C2-N2	-5.14	1.29	1.34
54	BA	484	C	C4-N4	-5.14	1.29	1.33
54	BA	1821	A	C5-C4	-5.14	1.35	1.38
54	BA	1874	C	C4-N4	-5.14	1.29	1.33
54	BA	142	A	C6-N1	-5.13	1.31	1.35
54	BA	718	A	C5-C4	-5.13	1.35	1.38
54	BA	1451	C	N3-C4	-5.13	1.30	1.33
54	BA	1461	C	C4-N4	-5.13	1.29	1.33
54	BA	2545	G	C2-N2	-5.13	1.29	1.34
54	BA	2761	A	C6-N1	-5.13	1.31	1.35
54	BA	2062	A	C6-N1	-5.13	1.31	1.35
21	AA	386	C	C4-N4	-5.13	1.29	1.33
21	AA	1519	A	C5-C4	-5.13	1.35	1.38
54	BA	424	G	C2-N2	-5.13	1.29	1.34
21	AA	272	C	C4-N4	-5.13	1.29	1.33
21	AA	988	G	C2-N2	-5.13	1.29	1.34
54	BA	675	A	C6-N1	-5.13	1.31	1.35
54	BA	1746	A	C6-N1	-5.13	1.31	1.35
21	AA	292	G	C2-N2	-5.12	1.29	1.34
54	BA	2625	G	N1-C2	-5.12	1.33	1.37
21	AA	105	G	C2-N2	-5.12	1.29	1.34
22	A1	9	A	C6-N1	-5.12	1.31	1.35
54	BA	1434	A	C6-N6	-5.12	1.29	1.33
21	AA	370	C	N3-C4	-5.12	1.30	1.33
21	AA	228	A	C6-N6	-5.12	1.29	1.33
21	AA	853	C	C4-N4	-5.12	1.29	1.33
21	AA	1320	C	C4-N4	-5.12	1.29	1.33
54	BA	1	G	C2-N2	-5.12	1.29	1.34
54	BA	1112	G	C6-N1	-5.12	1.35	1.39
54	BA	2379	G	C2-N2	-5.12	1.29	1.34
21	AA	348	G	C6-N1	-5.12	1.35	1.39
21	AA	655	A	C6-N1	-5.12	1.31	1.35
21	AA	823	C	C4-N4	-5.12	1.29	1.33
21	AA	1178	G	N1-C2	-5.12	1.33	1.37
24	A3	58	A	C6-N6	-5.12	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	275	C	C4-N4	-5.12	1.29	1.33
21	AA	424	G	C2-N2	-5.11	1.29	1.34
54	BA	1973	G	C6-N1	-5.11	1.35	1.39
21	AA	312	C	C4-N4	-5.11	1.29	1.33
54	BA	39	G	C2-N2	-5.11	1.29	1.34
54	BA	1975	G	N1-C2	-5.11	1.33	1.37
54	BA	23	G	C2-N2	-5.11	1.29	1.34
54	BA	1514	G	C6-N1	-5.11	1.35	1.39
54	BA	2308	G	N1-C2	-5.11	1.33	1.37
21	AA	440	C	C4-N4	-5.11	1.29	1.33
21	AA	1187	G	C2-N2	-5.11	1.29	1.34
21	AA	1336	C	N3-C4	-5.11	1.30	1.33
21	AA	1396	A	C6-N1	-5.11	1.31	1.35
54	BA	797	G	N1-C2	-5.11	1.33	1.37
55	BB	97	C	C4-N4	-5.11	1.29	1.33
21	AA	570	G	N1-C2	-5.11	1.33	1.37
21	AA	575	G	C2-N2	-5.11	1.29	1.34
21	AA	1432	G	C2-N2	-5.11	1.29	1.34
54	BA	381	G	C6-N1	-5.11	1.35	1.39
54	BA	2767	C	C4-N4	-5.11	1.29	1.33
21	AA	611	C	C4-N4	-5.10	1.29	1.33
54	BA	1957	C	C4-N4	-5.10	1.29	1.33
21	AA	334	C	N3-C4	-5.10	1.30	1.33
54	BA	679	C	N3-C4	-5.10	1.30	1.33
21	AA	145	G	C6-N1	-5.10	1.35	1.39
21	AA	803	G	C6-N1	-5.10	1.35	1.39
54	BA	1743	G	C2-N2	-5.10	1.29	1.34
21	AA	443	C	N3-C4	-5.10	1.30	1.33
54	BA	1377	G	C2-N2	-5.10	1.29	1.34
54	BA	2015	A	C6-N1	-5.10	1.31	1.35
54	BA	2142	A	C6-N1	-5.10	1.31	1.35
21	AA	1107	C	C4-N4	-5.10	1.29	1.33
54	BA	1430	G	C6-N1	-5.10	1.35	1.39
55	BB	39	A	C6-N1	-5.10	1.31	1.35
21	AA	1484	C	C4-N4	-5.10	1.29	1.33
55	BB	69	G	C2-N2	-5.10	1.29	1.34
21	AA	494	G	C6-N1	-5.09	1.35	1.39
54	BA	1711	A	C6-N6	-5.09	1.29	1.33
54	BA	2174	C	C4-N4	-5.09	1.29	1.33
21	AA	1269	A	C6-N1	-5.09	1.31	1.35
21	AA	1346	A	C6-N6	-5.09	1.29	1.33
54	BA	2890	G	C2-N2	-5.09	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1084	G	C6-N1	-5.09	1.35	1.39
54	BA	563	A	C6-N1	-5.09	1.31	1.35
54	BA	2293	G	C2-N2	-5.09	1.29	1.34
21	AA	255	G	C2-N2	-5.09	1.29	1.34
21	AA	869	G	C2-N2	-5.09	1.29	1.34
22	A1	28	C	C4-N4	-5.09	1.29	1.33
54	BA	1084	A	C5-C4	-5.09	1.35	1.38
54	BA	1987	A	C6-N6	-5.09	1.29	1.33
21	AA	506	G	C2-N2	-5.08	1.29	1.34
54	BA	394	C	C4-N4	-5.08	1.29	1.33
54	BA	595	C	C4-N4	-5.08	1.29	1.33
54	BA	808	G	C2-N2	-5.08	1.29	1.34
54	BA	2606	C	N3-C4	-5.08	1.30	1.33
54	BA	972	A	O3'-P	-5.08	1.55	1.61
54	BA	1588	G	C2-N2	-5.08	1.29	1.34
54	BA	2791	G	C2-N2	-5.08	1.29	1.34
54	BA	795	C	N3-C4	-5.08	1.30	1.33
54	BA	1645	G	C2-N2	-5.08	1.29	1.34
55	BB	12	C	C4-N4	-5.08	1.29	1.33
21	AA	381	C	N3-C4	-5.08	1.30	1.33
21	AA	1267	C	C4-N4	-5.08	1.29	1.33
24	A3	69	C	C4'-C3'	-5.08	1.47	1.52
21	AA	179	A	C6-N1	-5.08	1.31	1.35
54	BA	1920	C	C4-N4	-5.08	1.29	1.33
54	BA	2237	G	C2-N2	-5.08	1.29	1.34
54	BA	1407	G	C6-N1	-5.08	1.35	1.39
21	AA	681	A	C6-N6	-5.08	1.29	1.33
21	AA	794	A	C6-N1	-5.08	1.31	1.35
21	AA	1385	G	C2-N2	-5.08	1.29	1.34
54	BA	74	A	C5-C4	-5.08	1.35	1.38
54	BA	74	A	C6-N6	-5.08	1.29	1.33
54	BA	423	A	C6-N1	-5.08	1.31	1.35
54	BA	1767	G	N1-C2	-5.08	1.33	1.37
54	BA	1813	G	C2-N2	-5.08	1.29	1.34
54	BA	1291	C	C4-N4	-5.07	1.29	1.33
54	BA	2215	C	N3-C4	-5.07	1.30	1.33
55	BB	30	C	N3-C4	-5.07	1.30	1.33
21	AA	16	A	C6-N6	-5.07	1.29	1.33
21	AA	1133	G	C2-N2	-5.07	1.29	1.34
54	BA	1374	G	N1-C2	-5.07	1.33	1.37
54	BA	89	A	C6-N1	-5.07	1.32	1.35
54	BA	876	C	C4-N4	-5.07	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1359	A	C5-C4	-5.07	1.35	1.38
54	BA	2736	A	C6-N1	-5.07	1.32	1.35
54	BA	2759	G	C2-N2	-5.07	1.29	1.34
55	BB	53	A	C6-N1	-5.07	1.32	1.35
21	AA	748	G	C2-N2	-5.07	1.29	1.34
54	BA	45	G	C6-N1	-5.07	1.36	1.39
54	BA	1809	A	C6-N1	-5.07	1.32	1.35
54	BA	2090	A	C5-C4	-5.07	1.35	1.38
54	BA	2169	A	C6-N1	-5.07	1.32	1.35
54	BA	2644	G	C6-N1	-5.07	1.36	1.39
22	A1	5	G	C2-N2	-5.06	1.29	1.34
54	BA	2280	G	C2-N2	-5.06	1.29	1.34
54	BA	2505	G	C6-N1	-5.06	1.36	1.39
54	BA	2549	G	C2-N2	-5.06	1.29	1.34
54	BA	2830	C	C4-N4	-5.06	1.29	1.33
54	BA	1361	G	C6-N1	-5.06	1.36	1.39
54	BA	1895	C	C4-N4	-5.06	1.29	1.33
54	BA	2354	C	N3-C4	-5.06	1.30	1.33
55	BB	37	C	C4-N4	-5.06	1.29	1.33
54	BA	2803	G	N1-C2	-5.06	1.33	1.37
54	BA	353	C	N3-C4	-5.06	1.30	1.33
54	BA	354	A	C5-C4	-5.06	1.35	1.38
54	BA	475	C	C4-N4	-5.06	1.29	1.33
54	BA	1803	A	C6-N1	-5.06	1.32	1.35
54	BA	2191	A	C5-C4	-5.06	1.35	1.38
54	BA	2729	G	C2-N2	-5.06	1.29	1.34
55	BB	2	G	C6-N1	-5.06	1.36	1.39
54	BA	1437	C	N3-C4	-5.06	1.30	1.33
54	BA	1970	A	C6-N1	-5.06	1.32	1.35
54	BA	1431	A	C5-C4	-5.06	1.35	1.38
54	BA	2060	A	C5-C4	-5.06	1.35	1.38
54	BA	977	G	C2-N2	-5.05	1.29	1.34
54	BA	1867	G	C2-N2	-5.05	1.29	1.34
54	BA	2544	G	C2-N2	-5.05	1.29	1.34
54	BA	2735	G	C2-N2	-5.05	1.29	1.34
54	BA	2757	A	C6-N6	-5.05	1.29	1.33
21	AA	738	C	C4-N4	-5.05	1.29	1.33
21	AA	846	G	C6-N1	-5.05	1.36	1.39
21	AA	440	C	N3-C4	-5.05	1.30	1.33
21	AA	1108	G	C6-N1	-5.05	1.36	1.39
54	BA	1351	C	N3-C4	-5.05	1.30	1.33
54	BA	1831	G	C6-N1	-5.05	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	139	A	C6-N1	-5.05	1.32	1.35
21	AA	339	C	N3-C4	-5.05	1.30	1.33
21	AA	457	G	C6-N1	-5.05	1.36	1.39
21	AA	650	G	C2-N2	-5.05	1.29	1.34
21	AA	784	A	C5-C4	-5.05	1.35	1.38
21	AA	1099	G	C2-N2	-5.05	1.29	1.34
21	AA	1111	A	C6-N1	-5.05	1.32	1.35
21	AA	1177	G	C2-N2	-5.05	1.29	1.34
54	BA	47	C	C4-N4	-5.05	1.29	1.33
54	BA	2590	A	C6-N1	-5.05	1.32	1.35
21	AA	211	G	N1-C2	-5.05	1.33	1.37
21	AA	729	A	C6-N6	-5.05	1.29	1.33
21	AA	1331	G	C2-N2	-5.05	1.29	1.34
21	AA	1411	C	C4-N4	-5.05	1.29	1.33
54	BA	1463	C	N3-C4	-5.05	1.30	1.33
21	AA	954	G	C2-N2	-5.04	1.29	1.34
54	BA	2315	G	C2-N2	-5.04	1.29	1.34
54	BA	351	C	C4-N4	-5.04	1.29	1.33
21	AA	578	C	N3-C4	-5.04	1.30	1.33
21	AA	1200	C	N3-C4	-5.04	1.30	1.33
54	BA	1441	G	C6-N1	-5.04	1.36	1.39
54	BA	2141	G	C2-N2	-5.04	1.29	1.34
54	BA	2153	C	N3-C4	-5.04	1.30	1.33
54	BA	2209	G	N1-C2	-5.04	1.33	1.37
54	BA	2367	G	C2-N2	-5.04	1.29	1.34
54	BA	2856	A	C6-N6	-5.04	1.29	1.33
55	BB	21	G	C2-N2	-5.04	1.29	1.34
21	AA	462	G	C6-N1	-5.04	1.36	1.39
21	AA	545	C	C4-N4	-5.04	1.29	1.33
21	AA	681	A	C5-C4	-5.04	1.35	1.38
21	AA	940	C	N3-C4	-5.04	1.30	1.33
21	AA	1150	A	C6-N1	-5.04	1.32	1.35
54	BA	2097	A	C6-N1	-5.04	1.32	1.35
54	BA	2633	G	C2-N2	-5.04	1.29	1.34
21	AA	882	C	C4-N4	-5.03	1.29	1.33
21	AA	1218	C	C4-N4	-5.03	1.29	1.33
54	BA	159	G	C2-N2	-5.03	1.29	1.34
54	BA	804	A	C6-N1	-5.03	1.32	1.35
54	BA	1587	G	C2-N2	-5.03	1.29	1.34
21	AA	376	G	C6-N1	-5.03	1.36	1.39
21	AA	39	G	C6-N1	-5.03	1.36	1.39
21	AA	177	G	N1-C2	-5.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	762	U	C4'-O4'	-5.03	1.39	1.45
21	AA	1207	G	C6-N1	-5.03	1.36	1.39
22	A1	52	G	C2-N2	-5.03	1.29	1.34
54	BA	432	A	C5-C4	-5.03	1.35	1.38
54	BA	2124	G	N1-C2	-5.03	1.33	1.37
54	BA	2890	G	C6-N1	-5.03	1.36	1.39
21	AA	237	G	C2-N2	-5.03	1.29	1.34
54	BA	447	A	C6-N6	-5.03	1.29	1.33
54	BA	510	C	C4-N4	-5.03	1.29	1.33
54	BA	2069	G	N1-C2	-5.03	1.33	1.37
54	BA	704	G	C2-N2	-5.02	1.29	1.34
54	BA	172	A	C5-C4	-5.02	1.35	1.38
54	BA	988	A	C6-N1	-5.02	1.32	1.35
54	BA	1582	C	C4-N4	-5.02	1.29	1.33
54	BA	2501	C	C4-N4	-5.02	1.29	1.33
54	BA	2587	A	C6-N1	-5.02	1.32	1.35
54	BA	1762	A	C6-N1	-5.02	1.32	1.35
21	AA	450	G	C2-N2	-5.02	1.29	1.34
21	AA	703	G	C2-N2	-5.02	1.29	1.34
21	AA	1521	C	N3-C4	-5.02	1.30	1.33
54	BA	210	C	C4-N4	-5.02	1.29	1.33
54	BA	1902	C	C4-N4	-5.02	1.29	1.33
54	BA	2792	A	C6-N1	-5.02	1.32	1.35
21	AA	553	A	C6-N6	-5.02	1.29	1.33
21	AA	647	C	C4-N4	-5.02	1.29	1.33
54	BA	201	C	C4-N4	-5.02	1.29	1.33
21	AA	1456	A	C6-N1	-5.01	1.32	1.35
54	BA	1936	A	C5-C4	-5.01	1.35	1.38
21	AA	1096	C	C4-N4	-5.01	1.29	1.33
54	BA	1869	G	C2-N2	-5.01	1.29	1.34
21	AA	993	G	C2-N2	-5.01	1.29	1.34
54	BA	2241	A	C5-C4	-5.01	1.35	1.38
21	AA	503	C	C4-N4	-5.00	1.29	1.33
54	BA	1925	C	C4-N4	-5.00	1.29	1.33
21	AA	428	G	C2-N2	-5.00	1.29	1.34
21	AA	560	A	C5-C4	-5.00	1.35	1.38
21	AA	1452	C	C4-N4	-5.00	1.29	1.33
54	BA	2760	C	N3-C4	-5.00	1.30	1.33
21	AA	1281	C	C4-N4	-5.00	1.29	1.33
54	BA	1900	A	C5-C4	-5.00	1.35	1.38
54	BA	1967	C	C4-N4	-5.00	1.29	1.33
54	BA	2255	G	N1-C2	-5.00	1.33	1.37

All (8067) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	34	A	N1-C6-N6	-13.76	110.34	118.60
54	BA	323	C	O4'-C1'-N1	13.51	119.01	108.20
54	BA	547	A	O4'-C1'-N9	12.98	118.58	108.20
54	BA	1943	U	O4'-C1'-N1	12.88	118.50	108.20
54	BA	1340	U	O4'-C1'-N1	12.80	118.44	108.20
54	BA	2284	A	N1-C6-N6	-12.62	111.03	118.60
54	BA	2176	A	N1-C6-N6	-12.59	111.05	118.60
21	AA	1188	A	N1-C6-N6	-12.29	111.23	118.60
54	BA	1566	A	N1-C6-N6	-12.28	111.23	118.60
21	AA	78	A	N1-C6-N6	-12.21	111.27	118.60
21	AA	914	A	N1-C6-N6	-12.18	111.29	118.60
54	BA	2439	A	N1-C6-N6	-12.10	111.34	118.60
54	BA	943	A	N1-C6-N6	-12.09	111.34	118.60
21	AA	397	A	N1-C6-N6	-12.07	111.36	118.60
54	BA	1815	A	N1-C6-N6	-12.07	111.36	118.60
54	BA	1427	A	N1-C6-N6	-12.06	111.36	118.60
54	BA	348	A	N1-C6-N6	-11.99	111.41	118.60
54	BA	280	U	O4'-C1'-N1	11.89	117.71	108.20
21	AA	749	A	N1-C6-N6	-11.87	111.48	118.60
54	BA	1021	A	N1-C6-N6	-11.86	111.48	118.60
21	AA	1398	A	N1-C6-N6	-11.84	111.50	118.60
24	A3	77	A	N1-C6-N6	-11.84	111.50	118.60
54	BA	346	A	N1-C6-N6	-11.82	111.50	118.60
54	BA	716	A	N1-C6-N6	-11.79	111.52	118.60
54	BA	2666	C	O4'-C1'-N1	11.78	117.62	108.20
54	BA	1088	A	N1-C6-N6	-11.73	111.56	118.60
54	BA	910	A	N1-C6-N6	-11.70	111.58	118.60
21	AA	408	A	N1-C6-N6	-11.69	111.58	118.60
21	AA	1005	A	N1-C6-N6	-11.67	111.60	118.60
54	BA	2297	A	N1-C6-N6	-11.65	111.61	118.60
54	BA	1783	A	N1-C6-N6	-11.63	111.62	118.60
54	BA	382	A	N1-C6-N6	-11.63	111.62	118.60
54	BA	1871	A	N1-C6-N6	-11.58	111.65	118.60
21	AA	129	A	N1-C6-N6	-11.54	111.67	118.60
54	BA	1505	A	N1-C6-N6	-11.48	111.71	118.60
54	BA	1285	A	N1-C6-N6	-11.47	111.72	118.60
21	AA	1502	A	N1-C6-N6	-11.47	111.72	118.60
54	BA	1272	A	N1-C6-N6	-11.46	111.73	118.60
54	BA	2513	A	N1-C6-N6	-11.44	111.74	118.60
54	BA	2241	A	N1-C6-N6	-11.43	111.74	118.60
55	BB	15	A	O4'-C1'-N9	11.42	117.33	108.20
21	AA	1246	A	N1-C6-N6	-11.41	111.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1257	A	N1-C6-N6	-11.41	111.75	118.60
54	BA	1679	A	N1-C6-N6	-11.40	111.76	118.60
21	AA	344	A	N1-C6-N6	-11.34	111.79	118.60
54	BA	925	A	N1-C6-N6	-11.32	111.81	118.60
54	BA	2733	A	N1-C6-N6	-11.32	111.81	118.60
54	BA	1960	A	N1-C6-N6	-11.31	111.82	118.60
21	AA	373	A	N1-C6-N6	-11.24	111.86	118.60
54	BA	945	A	N1-C6-N6	-11.23	111.86	118.60
54	BA	104	A	N1-C6-N6	-11.22	111.87	118.60
54	BA	2191	A	N1-C6-N6	-11.22	111.87	118.60
21	AA	546	A	N1-C6-N6	-11.19	111.89	118.60
21	AA	364	A	N1-C6-N6	-11.18	111.89	118.60
21	AA	728	A	N1-C6-N6	-11.17	111.90	118.60
39	BQ	12	ARG	NE-CZ-NH2	11.16	125.88	120.30
46	BX	71	ARG	NE-CZ-NH1	11.15	125.87	120.30
54	BA	1821	A	N1-C6-N6	-11.14	111.92	118.60
21	AA	1171	A	N1-C6-N6	-11.13	111.92	118.60
54	BA	2381	A	N1-C6-N6	-11.12	111.93	118.60
21	AA	1441	A	N1-C6-N6	-11.09	111.94	118.60
21	AA	1081	A	N1-C6-N6	-11.06	111.96	118.60
21	AA	363	A	N1-C6-N6	-11.03	111.98	118.60
54	BA	2109	U	O4'-C1'-N1	11.01	117.01	108.20
21	AA	452	A	N1-C6-N6	-11.00	112.00	118.60
54	BA	1204	A	N1-C6-N6	-10.99	112.00	118.60
54	BA	2590	A	N1-C6-N6	-10.97	112.02	118.60
21	AA	873	A	N1-C6-N6	-10.96	112.03	118.60
21	AA	1467	C	N3-C2-O2	-10.94	114.25	121.90
21	AA	807	A	N1-C6-N6	-10.91	112.06	118.60
54	BA	213	A	N1-C6-N6	-10.89	112.07	118.60
54	BA	1762	A	N1-C6-N6	-10.88	112.07	118.60
21	AA	466	A	N1-C6-N6	-10.88	112.07	118.60
46	BX	73	ARG	NE-CZ-NH1	10.87	125.74	120.30
21	AA	1346	A	N1-C6-N6	-10.87	112.08	118.60
54	BA	2311	A	N1-C6-N6	-10.86	112.08	118.60
54	BA	2031	A	N1-C6-N6	-10.86	112.09	118.60
54	BA	1509	A	N1-C6-N6	-10.84	112.09	118.60
54	BA	219	A	N1-C6-N6	-10.84	112.10	118.60
54	BA	83	A	N1-C6-N6	-10.83	112.10	118.60
21	AA	918	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	270	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	222	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	2358	A	N1-C6-N6	-10.79	112.13	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	481	G	O4'-C1'-N9	10.77	116.82	108.20
54	BA	1803	A	N1-C6-N6	-10.76	112.14	118.60
54	BA	1490	A	N1-C6-N6	-10.76	112.14	118.60
54	BA	1545	A	N1-C6-N6	-10.76	112.14	118.60
54	BA	233	A	N1-C6-N6	-10.75	112.15	118.60
2	AC	171	ARG	NE-CZ-NH1	10.74	125.67	120.30
54	BA	569	U	O4'-C1'-N1	10.73	116.78	108.20
54	BA	514	A	N1-C6-N6	-10.73	112.16	118.60
54	BA	1773	A	N1-C6-N6	-10.72	112.17	118.60
21	AA	130	A	N1-C6-N6	-10.69	112.19	118.60
11	AL	53	ARG	NE-CZ-NH1	10.68	125.64	120.30
25	BC	235	GLU	OE1-CD-OE2	-10.68	110.48	123.30
54	BA	847	U	O4'-C1'-N1	10.68	116.75	108.20
22	A1	41	A	N1-C6-N6	-10.67	112.20	118.60
54	BA	423	A	N1-C6-N6	-10.67	112.20	118.60
21	AA	499	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	1496	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	1635	A	N1-C6-N6	-10.65	112.21	118.60
21	AA	969	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	1701	A	N1-C6-N6	-10.64	112.22	118.60
54	BA	2835	A	N1-C6-N6	-10.64	112.22	118.60
54	BA	1353	A	N1-C6-N6	-10.63	112.22	118.60
21	AA	1152	A	N1-C6-N6	-10.63	112.22	118.60
54	BA	1810	A	N1-C6-N6	-10.62	112.23	118.60
54	BA	980	A	N1-C6-N6	-10.61	112.23	118.60
21	AA	768	A	N1-C6-N6	-10.60	112.24	118.60
54	BA	1616	A	N1-C6-N6	-10.59	112.24	118.60
54	BA	1569	A	N1-C6-N6	-10.59	112.25	118.60
21	AA	26	A	N1-C6-N6	-10.58	112.25	118.60
54	BA	10	A	N1-C6-N6	-10.58	112.25	118.60
54	BA	2899	A	N1-C6-N6	-10.57	112.26	118.60
54	BA	2646	C	O4'-C1'-N1	10.57	116.65	108.20
21	AA	675	A	N1-C6-N6	-10.56	112.27	118.60
10	AK	92	ARG	NE-CZ-NH1	10.54	125.57	120.30
21	AA	236	A	N1-C6-N6	-10.54	112.28	118.60
54	BA	1352	U	O4'-C1'-N1	10.53	116.63	108.20
54	BA	2158	A	N1-C6-N6	-10.53	112.28	118.60
2	AC	10	ARG	NE-CZ-NH1	10.52	125.56	120.30
35	BM	40	ARG	NE-CZ-NH1	10.51	125.56	120.30
21	AA	509	A	N1-C6-N6	-10.51	112.29	118.60
21	AA	547	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	1784	A	N1-C6-N6	-10.49	112.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1396	A	N1-C6-N6	-10.49	112.31	118.60
54	BA	172	A	N1-C6-N6	-10.48	112.31	118.60
21	AA	288	A	N1-C6-N6	-10.45	112.33	118.60
54	BA	1713	A	N1-C6-N6	-10.45	112.33	118.60
21	AA	1467	C	N1-C2-O2	10.44	125.17	118.90
21	AA	1117	A	N1-C6-N6	-10.44	112.33	118.60
54	BA	602	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	2776	A	N1-C6-N6	-10.44	112.34	118.60
37	BO	9	ARG	NE-CZ-NH1	10.44	125.52	120.30
21	AA	205	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	1969	A	N1-C6-N6	-10.43	112.34	118.60
37	BO	16	ARG	NE-CZ-NH1	10.42	125.51	120.30
21	AA	872	A	C1'-O4'-C4'	-10.40	101.58	109.90
21	AA	539	A	N1-C6-N6	-10.38	112.37	118.60
21	AA	968	A	N1-C6-N6	-10.38	112.37	118.60
2	AC	130	ARG	NE-CZ-NH1	10.37	125.48	120.30
21	AA	1519	A	N1-C6-N6	-10.37	112.38	118.60
54	BA	821	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	1084	A	N1-C6-N6	-10.34	112.39	118.60
21	AA	1150	A	N1-C6-N6	-10.32	112.41	118.60
32	BJ	37	ARG	NE-CZ-NH1	10.32	125.46	120.30
54	BA	1901	A	N1-C6-N6	-10.32	112.41	118.60
21	AA	468	A	N1-C6-N6	-10.31	112.41	118.60
54	BA	161	A	N1-C6-N6	-10.31	112.41	118.60
54	BA	1690	A	N1-C6-N6	-10.30	112.42	118.60
54	BA	2270	A	N1-C6-N6	-10.29	112.43	118.60
7	AH	83	ARG	NE-CZ-NH1	10.29	125.44	120.30
54	BA	372	G	O4'-C1'-N9	10.28	116.43	108.20
38	BP	61	ARG	NE-CZ-NH1	10.26	125.43	120.30
54	BA	1226	A	N1-C6-N6	-10.26	112.44	118.60
54	BA	1932	A	N1-C6-N6	-10.26	112.44	118.60
54	BA	1434	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	1819	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	1789	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	2665	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	715	A	N1-C6-N6	-10.24	112.45	118.60
21	AA	845	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	673	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	1021	A	N1-C6-N6	-10.23	112.46	118.60
14	AO	53	ARG	NE-CZ-NH1	10.23	125.41	120.30
54	BA	513	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	1533	C	N3-C2-O2	-10.22	114.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2425	A	N1-C6-N6	-10.21	112.47	118.60
21	AA	1269	A	N1-C6-N6	-10.21	112.48	118.60
54	BA	920	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	13	A	N1-C6-N6	-10.20	112.48	118.60
21	AA	704	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	1847	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	2598	A	N1-C6-N6	-10.18	112.49	118.60
21	AA	33	A	N1-C6-N6	-10.16	112.50	118.60
39	BQ	91	ARG	NE-CZ-NH1	10.15	125.37	120.30
21	AA	715	A	N1-C6-N6	-10.14	112.51	118.60
54	BA	1532	A	N1-C6-N6	-10.14	112.52	118.60
54	BA	2900	A	N1-C6-N6	-10.14	112.52	118.60
12	AM	97	ARG	NE-CZ-NH2	10.12	125.36	120.30
21	AA	1105	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	1801	A	O4'-C1'-N9	10.11	116.29	108.20
54	BA	1626	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	676	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	609	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	1036	A	N1-C6-N6	-10.09	112.55	118.60
21	AA	356	A	N1-C6-N6	-10.09	112.55	118.60
21	AA	872	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	2163	A	N1-C6-N6	-10.09	112.55	118.60
21	AA	687	A	N1-C6-N6	-10.08	112.55	118.60
21	AA	1349	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	627	A	N1-C6-N6	-10.08	112.55	118.60
21	AA	1146	A	N1-C6-N6	-10.07	112.56	118.60
21	AA	161	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	825	A	N1-C6-N6	-10.07	112.56	118.60
21	AA	120	A	N1-C6-N6	-10.06	112.56	118.60
21	AA	915	A	C5-C6-N1	10.05	122.73	117.70
21	AA	1299	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	761	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	1084	A	C5-C6-N1	10.05	122.73	117.70
21	AA	414	A	N1-C6-N6	-10.05	112.57	118.60
21	AA	183	C	N3-C2-O2	-10.05	114.86	121.90
21	AA	344	A	C5-C6-N1	10.04	122.72	117.70
54	BA	2766	A	N1-C6-N6	-10.04	112.58	118.60
54	BA	443	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	2813	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	197	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	1431	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	80	A	N1-C6-N6	-10.01	112.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	22	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	1637	A	N1-C6-N6	-10.00	112.60	118.60
55	BB	52	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	155	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	152	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	2635	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	681	A	N1-C6-N6	-9.99	112.60	118.60
54	BA	1746	A	N1-C6-N6	-9.99	112.61	118.60
54	BA	2721	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	412	A	N1-C6-N6	-9.97	112.61	118.60
54	BA	2080	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	2761	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	959	A	N1-C6-N6	-9.96	112.62	118.60
54	BA	1610	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	1216	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	1213	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	721	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	1528	A	N1-C6-N6	-9.93	112.64	118.60
27	BE	114	ARG	NE-CZ-NH1	9.93	125.26	120.30
54	BA	346	A	C5-C6-N1	9.92	122.66	117.70
54	BA	972	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	675	A	N1-C6-N6	-9.91	112.65	118.60
22	A1	38	A	N1-C6-N6	-9.91	112.66	118.60
54	BA	1089	A	N1-C6-N6	-9.91	112.65	118.60
21	AA	553	A	N1-C6-N6	-9.90	112.66	118.60
21	AA	815	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	1785	A	N1-C6-N6	-9.89	112.66	118.60
54	BA	2126	A	N1-C6-N6	-9.89	112.66	118.60
54	BA	272	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	1889	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	1614	A	N1-C6-N6	-9.87	112.68	118.60
21	AA	1468	A	N1-C6-N6	-9.87	112.68	118.60
9	AJ	9	ARG	NE-CZ-NH1	9.86	125.23	120.30
55	BB	109	A	O4'-C1'-N9	9.85	116.08	108.20
10	AK	97	ARG	NE-CZ-NH1	9.85	125.22	120.30
21	AA	919	A	N1-C6-N6	-9.85	112.69	118.60
21	AA	1082	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	95	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	1205	A	N1-C6-N6	-9.85	112.69	118.60
21	AA	975	A	N1-C6-N6	-9.84	112.70	118.60
21	AA	1169	A	N1-C6-N6	-9.82	112.70	118.60
54	BA	1665	A	N1-C6-N6	-9.82	112.70	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1403	A	N1-C6-N6	-9.82	112.71	118.60
21	AA	1533	C	O4'-C1'-N1	9.82	116.05	108.20
56	B5	74	ARG	NE-CZ-NH1	9.81	125.21	120.30
9	AJ	68	ARG	NE-CZ-NH1	9.81	125.20	120.30
37	BO	10	ARG	NE-CZ-NH1	9.81	125.20	120.30
54	BA	429	A	N1-C6-N6	-9.81	112.72	118.60
24	A3	58	A	N1-C6-N6	-9.80	112.72	118.60
21	AA	19	A	N1-C6-N6	-9.79	112.72	118.60
54	BA	2750	A	N1-C6-N6	-9.79	112.72	118.60
55	BB	94	A	N1-C6-N6	-9.79	112.72	118.60
54	BA	482	A	N1-C6-N6	-9.79	112.73	118.60
54	BA	1928	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	1548	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	1456	A	N1-C6-N6	-9.76	112.74	118.60
54	BA	1630	A	N1-C6-N6	-9.76	112.75	118.60
15	AP	35	ARG	NE-CZ-NH1	9.75	125.18	120.30
21	AA	665	A	N1-C6-N6	-9.75	112.75	118.60
9	AJ	48	ARG	NE-CZ-NH1	9.74	125.17	120.30
34	BL	2	ARG	NE-CZ-NH1	9.74	125.17	120.30
21	AA	60	A	N1-C6-N6	-9.74	112.76	118.60
54	BA	2450	A	N1-C6-N6	-9.74	112.76	118.60
21	AA	192	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	2602	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1077	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	979	A	C5-C6-N1	9.72	122.56	117.70
54	BA	149	A	N1-C6-N6	-9.71	112.77	118.60
21	AA	579	A	N1-C6-N6	-9.71	112.78	118.60
54	BA	730	A	N1-C6-N6	-9.71	112.78	118.60
54	BA	354	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	877	A	N1-C6-N6	-9.70	112.78	118.60
21	AA	1196	A	N1-C6-N6	-9.70	112.78	118.60
21	AA	1428	A	N1-C6-N6	-9.69	112.79	118.60
18	AS	36	ARG	NE-CZ-NH1	9.69	125.14	120.30
54	BA	2833	U	O4'-C1'-N1	9.69	115.95	108.20
55	BB	29	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	592	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	2058	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	204	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	223	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	2287	A	N1-C6-N6	-9.67	112.80	118.60
10	AK	121	ARG	NE-CZ-NH2	9.66	125.13	120.30
21	AA	10	A	N1-C6-N6	-9.66	112.80	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1938	A	N1-C6-N6	-9.66	112.81	118.60
54	BA	2170	A	N1-C6-N6	-9.66	112.81	118.60
54	BA	1772	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	520	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	131	A	N1-C6-N6	-9.65	112.81	118.60
41	BS	84	ARG	NE-CZ-NH1	9.64	125.12	120.30
21	AA	116	A	N1-C6-N6	-9.64	112.82	118.60
21	AA	320	A	N1-C6-N6	-9.64	112.82	118.60
54	BA	91	A	O4'-C1'-N9	9.63	115.91	108.20
54	BA	1900	A	N1-C6-N6	-9.64	112.82	118.60
55	BB	59	A	N1-C6-N6	-9.63	112.82	118.60
8	AI	17	ARG	NE-CZ-NH1	9.62	125.11	120.30
54	BA	1359	A	N1-C6-N6	-9.62	112.83	118.60
55	BB	101	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	479	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	2307	G	O4'-C1'-N9	9.62	115.90	108.20
54	BA	2851	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	909	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	2169	A	N1-C6-N6	-9.61	112.83	118.60
21	AA	356	A	C5-C6-N1	9.61	122.50	117.70
54	BA	1204	A	C5-C6-N1	9.60	122.50	117.70
54	BA	1970	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	2317	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	2411	A	C5-C6-N1	9.59	122.50	117.70
54	BA	699	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	1088	A	C5-C6-N1	9.59	122.50	117.70
21	AA	746	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	125	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	900	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	372	C	N3-C2-O2	-9.58	115.19	121.90
15	AP	51	ARG	NE-CZ-NH1	9.58	125.09	120.30
54	BA	866	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	1046	A	O4'-C1'-N9	9.58	115.86	108.20
54	BA	670	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	1365	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	2385	C	O4'-C1'-N1	9.55	115.84	108.20
13	AN	63	ARG	NE-CZ-NH1	9.55	125.07	120.30
54	BA	2015	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	2176	A	C5-C6-N1	9.55	122.47	117.70
21	AA	559	A	N1-C6-N6	-9.54	112.87	118.60
21	AA	336	A	N1-C6-N6	-9.54	112.88	118.60
22	A1	69	A	N1-C6-N6	-9.54	112.88	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	608	A	N1-C6-N6	-9.54	112.88	118.60
21	AA	243	A	N1-C6-N6	-9.54	112.88	118.60
21	AA	451	A	N1-C6-N6	-9.54	112.88	118.60
21	AA	949	A	N1-C6-N6	-9.53	112.88	118.60
55	BB	78	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	637	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	2736	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	71	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	1549	A	C5-C6-N1	9.51	122.46	117.70
21	AA	366	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	983	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	2873	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	1129	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	1251	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	1069	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	1780	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	973	A	N1-C6-N6	-9.49	112.90	118.60
54	BA	2814	A	N1-C6-N6	-9.49	112.90	118.60
21	AA	382	A	C5-C6-N1	9.49	122.44	117.70
21	AA	622	A	N1-C6-N6	-9.49	112.91	118.60
21	AA	1503	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	42	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	629	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	1057	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	1654	A	N1-C6-N6	-9.47	112.92	118.60
55	BB	109	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1147	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1953	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	466	A	C5-C6-N1	9.46	122.43	117.70
21	AA	415	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1169	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	101	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	504	A	O4'-C1'-N9	9.45	115.76	108.20
54	BA	1010	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1783	A	C5-C6-N1	9.44	122.42	117.70
24	A3	60	A	N1-C6-N6	-9.44	112.93	118.60
54	BA	1494	A	N1-C6-N6	-9.44	112.93	118.60
21	AA	728	A	C5-C6-N1	9.44	122.42	117.70
4	AE	67	ARG	NE-CZ-NH1	9.44	125.02	120.30
54	BA	2458	G	O4'-C1'-N9	9.44	115.75	108.20
54	BA	1535	A	O4'-C1'-N9	9.43	115.74	108.20
54	BA	1936	A	N1-C6-N6	-9.43	112.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	228	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	270	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	825	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	1111	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	2542	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	508	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1156	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	1327	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	527	C	N1-C2-O2	9.41	124.54	118.90
54	BA	141	G	O4'-C1'-N9	9.40	115.72	108.20
54	BA	735	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	845	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	977	A	N1-C6-N6	-9.39	112.96	118.60
21	AA	50	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	990	A	N1-C6-N6	-9.38	112.97	118.60
21	AA	1493	A	C5-C6-N1	9.37	122.39	117.70
54	BA	2333	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	156	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	2765	A	N1-C6-N6	-9.36	112.99	118.60
54	BA	2566	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	2726	A	N1-C6-N6	-9.35	112.99	118.60
21	AA	1318	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	127	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	1544	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	2497	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	2097	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	2212	A	O4'-C1'-N9	9.34	115.67	108.20
54	BA	368	A	N1-C6-N6	-9.33	113.00	118.60
21	AA	608	A	N1-C6-N6	-9.33	113.00	118.60
21	AA	1346	A	C5-C6-N1	9.33	122.36	117.70
54	BA	1246	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	466	A	N1-C6-N6	-9.32	113.00	118.60
54	BA	1858	A	N1-C6-N6	-9.32	113.00	118.60
54	BA	756	A	N1-C6-N6	-9.32	113.01	118.60
55	BB	15	A	C5-C6-N1	9.32	122.36	117.70
21	AA	1046	A	C5-C6-N1	9.32	122.36	117.70
54	BA	1805	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	1418	A	C5-C6-N1	9.31	122.36	117.70
54	BA	541	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	759	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	1239	A	N1-C6-N6	-9.31	113.01	118.60
40	BR	90	ARG	NE-CZ-NH1	9.31	124.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	782	A	N1-C6-N6	-9.31	113.01	118.60
54	BA	527	C	N3-C2-O2	-9.31	115.39	121.90
21	AA	143	A	N1-C6-N6	-9.30	113.02	118.60
21	AA	264	C	N3-C2-O2	-9.29	115.40	121.90
21	AA	300	A	N1-C6-N6	-9.29	113.03	118.60
42	BT	69	ARG	NE-CZ-NH1	9.28	124.94	120.30
21	AA	595	A	N1-C6-N6	-9.28	113.03	118.60
25	BC	211	ARG	NE-CZ-NH1	9.28	124.94	120.30
54	BA	988	A	N1-C6-N6	-9.27	113.04	118.60
26	BD	83	ARG	NE-CZ-NH1	9.27	124.94	120.30
54	BA	1872	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	1098	A	N1-C6-N6	-9.26	113.04	118.60
21	AA	665	A	C5-C6-N1	9.26	122.33	117.70
54	BA	21	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	155	A	N1-C6-N6	-9.25	113.05	118.60
22	A1	66	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	144	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	947	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	896	A	N1-C6-N6	-9.25	113.05	118.60
55	BB	26	C	N3-C2-O2	-9.25	115.42	121.90
54	BA	2606	C	N3-C2-O2	-9.24	115.43	121.90
25	BC	181	ARG	NE-CZ-NH1	9.24	124.92	120.30
54	BA	2287	A	C5-C6-N1	9.24	122.32	117.70
54	BA	2589	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	574	A	N1-C6-N6	-9.23	113.06	118.60
22	A1	38	A	C5-C6-N1	9.22	122.31	117.70
54	BA	1284	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	2468	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	384	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	1322	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	1144	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	221	A	N1-C6-N6	-9.21	113.08	118.60
54	BA	241	A	N1-C6-N6	-9.21	113.08	118.60
56	B5	9	ARG	NE-CZ-NH1	9.21	124.90	120.30
54	BA	2451	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	313	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	1009	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	2274	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	2577	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	911	A	N1-C6-N6	-9.19	113.08	118.60
21	AA	251	G	O4'-C1'-N9	9.19	115.55	108.20
54	BA	207	A	N1-C6-N6	-9.18	113.09	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2346	A	N1-C6-N6	-9.18	113.09	118.60
21	AA	784	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	101	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	1451	C	N3-C2-O2	-9.17	115.48	121.90
54	BA	1853	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	1591	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	228	A	C5-C6-N1	9.16	122.28	117.70
21	AA	129	A	C5-C6-N1	9.16	122.28	117.70
55	BB	50	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	2090	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	2872	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	2614	A	C5-C6-N1	9.16	122.28	117.70
54	BA	1320	C	N3-C2-O2	-9.16	115.49	121.90
54	BA	2748	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	441	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	1420	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	1937	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	71	A	C5-C6-N1	9.13	122.27	117.70
55	BB	73	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	1393	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	938	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	160	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	1252	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	1885	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	1434	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	2154	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	364	A	C5-C6-N1	9.10	122.25	117.70
21	AA	1311	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	718	A	C5-C6-N1	9.09	122.24	117.70
21	AA	246	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	668	A	N1-C6-N6	-9.09	113.15	118.60
21	AA	349	A	C5-C6-N1	9.08	122.24	117.70
54	BA	2872	A	C5-C6-N1	9.08	122.24	117.70
21	AA	978	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	2850	A	N1-C6-N6	-9.08	113.16	118.60
54	BA	599	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	412	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	1374	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	1016	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	322	A	C5-C6-N1	9.07	122.23	117.70
54	BA	1791	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	781	A	N1-C6-N6	-9.06	113.16	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	6	A	N1-C6-N6	-9.06	113.16	118.60
54	BA	1302	A	N1-C6-N6	-9.06	113.16	118.60
54	BA	1434	A	C5-C6-N1	9.06	122.23	117.70
21	AA	270	A	C5-C6-N1	9.05	122.23	117.70
54	BA	1711	A	C5-C6-N1	9.06	122.23	117.70
39	BQ	50	ARG	NE-CZ-NH2	9.05	124.83	120.30
54	BA	975	A	N1-C6-N6	-9.05	113.17	118.60
21	AA	563	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	983	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1384	A	N1-C6-N6	-9.05	113.17	118.60
21	AA	72	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	1287	A	N1-C6-N6	-9.04	113.17	118.60
21	AA	383	A	N1-C6-N6	-9.04	113.18	118.60
21	AA	1428	A	C5-C6-N1	9.04	122.22	117.70
54	BA	1403	A	C5-C6-N1	9.04	122.22	117.70
54	BA	2170	A	C5-C6-N1	9.04	122.22	117.70
22	A1	76	A	C4-C5-C6	-9.04	112.48	117.00
54	BA	1755	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2448	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2531	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2108	A	N1-C6-N6	-9.03	113.18	118.60
21	AA	1368	A	N1-C6-N6	-9.03	113.18	118.60
21	AA	183	C	N1-C2-O2	9.02	124.31	118.90
21	AA	873	A	C5-C6-N1	9.02	122.21	117.70
22	A1	23	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	614	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	1549	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	1392	A	N1-C6-N6	-9.01	113.19	118.60
1	AB	212	TYR	CB-CG-CD2	-9.01	115.59	121.00
54	BA	980	A	C5-C6-N1	9.01	122.20	117.70
54	BA	2171	A	C5-C6-N1	9.01	122.20	117.70
21	AA	430	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	518	C	N3-C2-O2	-9.00	115.60	121.90
21	AA	1398	A	C4-C5-C6	-9.00	112.50	117.00
23	A2	79	A	C5-C6-N1	9.00	122.20	117.70
21	AA	1534	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	2453	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	263	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	2450	A	C5-C6-N1	9.00	122.20	117.70
54	BA	751	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	250	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	1262	A	N1-C6-N6	-8.98	113.21	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1854	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2499	C	N3-C2-O2	-8.98	115.61	121.90
21	AA	1513	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	706	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2054	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	515	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	1459	G	O4'-C1'-N9	8.97	115.37	108.20
54	BA	294	A	C5-C6-N1	8.96	122.18	117.70
54	BA	1286	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1610	A	O4'-C1'-N9	8.96	115.37	108.20
54	BA	1089	A	C5-C6-N1	8.96	122.18	117.70
54	BA	74	A	C5-C6-N1	8.96	122.18	117.70
21	AA	1019	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	1260	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	432	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	1027	A	N1-C6-N6	-8.95	113.23	118.60
32	BJ	34	ARG	NE-CZ-NH1	8.95	124.77	120.30
54	BA	1668	A	N1-C6-N6	-8.94	113.23	118.60
21	AA	695	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	1570	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	2062	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	1802	A	N1-C6-N6	-8.94	113.24	118.60
10	AK	127	ARG	NE-CZ-NH1	8.93	124.77	120.30
21	AA	1082	A	C4-C5-C6	-8.93	112.53	117.00
54	BA	1711	A	N1-C6-N6	-8.93	113.24	118.60
21	AA	468	A	C5-C6-N1	8.93	122.16	117.70
54	BA	203	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	1495	A	N1-C6-N6	-8.93	113.24	118.60
20	AU	32	ARG	NE-CZ-NH1	8.93	124.76	120.30
54	BA	531	C	O4'-C1'-N1	8.93	115.34	108.20
21	AA	1429	A	N1-C6-N6	-8.93	113.25	118.60
54	BA	547	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	2882	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	933	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	1046	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	1301	A	N1-C6-N6	-8.91	113.25	118.60
3	AD	110	ARG	NE-CZ-NH1	8.91	124.75	120.30
21	AA	502	A	C4-C5-C6	-8.91	112.55	117.00
21	AA	913	A	N1-C6-N6	-8.91	113.26	118.60
54	BA	2818	U	O4'-C1'-N1	8.91	115.33	108.20
21	AA	329	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	2628	C	O4'-C1'-N1	8.90	115.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	26	A	C5-C6-N1	8.89	122.15	117.70
21	AA	498	A	C5-C6-N1	8.89	122.15	117.70
21	AA	546	A	C4-C5-C6	-8.89	112.55	117.00
54	BA	1772	A	C5-C6-N1	8.89	122.15	117.70
21	AA	1287	A	N1-C6-N6	-8.89	113.27	118.60
54	BA	1998	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	687	A	C5-C6-N1	8.89	122.14	117.70
54	BA	1420	A	C5-C6-N1	8.89	122.14	117.70
17	AR	72	ARG	NE-CZ-NH1	8.88	124.74	120.30
21	AA	1468	A	C5-C6-N1	8.88	122.14	117.70
54	BA	2003	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	1809	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	2734	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	1329	A	N1-C6-N6	-8.88	113.27	118.60
24	A3	73	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	2675	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	1142	A	C5-C6-N1	8.87	122.14	117.70
54	BA	2733	A	C5-C6-N1	8.87	122.14	117.70
54	BA	1641	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1086	A	C5-C6-N1	8.87	122.14	117.70
21	AA	288	A	C5-C6-N1	8.87	122.13	117.70
54	BA	176	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	861	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	764	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	2391	G	O4'-C1'-N9	8.86	115.29	108.20
24	A3	74	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	63	A	C5-C6-N1	8.85	122.13	117.70
54	BA	2824	C	N3-C2-O2	-8.85	115.70	121.90
21	AA	1163	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	793	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	172	A	N1-C6-N6	-8.84	113.29	118.60
29	BG	68	ARG	NE-CZ-NH1	8.84	124.72	120.30
21	AA	1441	A	C5-C6-N1	8.83	122.12	117.70
54	BA	282	A	C5-C6-N1	8.83	122.12	117.70
54	BA	750	A	N1-C6-N6	-8.83	113.30	118.60
21	AA	371	A	C5-C6-N1	8.83	122.11	117.70
24	A3	1	C	N3-C2-O2	-8.83	115.72	121.90
54	BA	362	A	N1-C6-N6	-8.83	113.30	118.60
35	BM	6	ARG	NE-CZ-NH1	8.83	124.71	120.30
54	BA	1194	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	167	A	N1-C6-N6	-8.82	113.31	118.60
22	A1	21	A	N1-C6-N6	-8.82	113.31	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1785	A	C5-C6-N1	8.82	122.11	117.70
21	AA	44	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	1556	C	N3-C2-O2	-8.81	115.73	121.90
21	AA	1151	A	N1-C6-N6	-8.81	113.31	118.60
18	AS	31	ARG	NE-CZ-NH1	8.81	124.71	120.30
21	AA	969	A	C5-C6-N1	8.81	122.11	117.70
54	BA	1758	U	O4'-C1'-N1	8.81	115.25	108.20
54	BA	2386	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	1276	A	N1-C6-N6	-8.81	113.32	118.60
54	BA	2060	A	N1-C6-N6	-8.81	113.32	118.60
21	AA	262	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	313	A	C4-C5-C6	-8.80	112.60	117.00
21	AA	336	A	C4-C5-C6	-8.80	112.60	117.00
54	BA	1385	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	560	A	C5-C6-N1	8.80	122.10	117.70
21	AA	1519	A	C5-C6-N1	8.80	122.10	117.70
21	AA	553	A	C5-C6-N1	8.80	122.10	117.70
54	BA	2241	A	C5-C6-N1	8.80	122.10	117.70
54	BA	2080	A	C5-C6-N1	8.80	122.10	117.70
21	AA	1350	A	C5-C6-N1	8.80	122.10	117.70
54	BA	2059	A	C5-C6-N1	8.80	122.10	117.70
54	BA	693	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	1101	A	N1-C6-N6	-8.79	113.32	118.60
12	AM	89	ARG	NE-CZ-NH1	8.79	124.70	120.30
21	AA	1109	C	N3-C2-O2	-8.79	115.75	121.90
11	AL	49	ARG	NE-CZ-NH1	8.79	124.69	120.30
21	AA	996	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	573	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	909	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	2435	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	2820	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	1515	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	792	A	C5-C6-N1	8.78	122.09	117.70
21	AA	1214	C	N3-C2-O2	-8.78	115.76	121.90
54	BA	472	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	1350	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2376	A	C5-C6-N1	8.78	122.09	117.70
54	BA	2711	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2657	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	1248	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	1271	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	546	A	C5-C6-N1	8.77	122.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	373	A	C5-C6-N1	8.77	122.08	117.70
54	BA	1593	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	2154	A	C5-C6-N1	8.77	122.08	117.70
54	BA	19	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	1320	C	N3-C2-O2	-8.76	115.77	121.90
54	BA	1404	C	N3-C2-O2	-8.76	115.77	121.90
54	BA	2033	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	1067	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	1905	C	O4'-C1'-N1	8.76	115.20	108.20
54	BA	76	C	O4'-C1'-N1	8.76	115.20	108.20
54	BA	2266	A	N1-C6-N6	-8.76	113.35	118.60
26	BD	141	ARG	NE-CZ-NH1	8.75	124.68	120.30
54	BA	2823	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	958	A	C5-C6-N1	8.75	122.08	117.70
54	BA	1029	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	1987	A	C4-C5-C6	-8.75	112.62	117.00
54	BA	249	C	O4'-C1'-N1	8.75	115.20	108.20
54	BA	1936	A	C5-C6-N1	8.75	122.07	117.70
21	AA	937	A	C5-C6-N1	8.74	122.07	117.70
54	BA	2090	A	C5-C6-N1	8.74	122.07	117.70
21	AA	441	A	C5-C6-N1	8.74	122.07	117.70
54	BA	1665	A	C4-C5-C6	-8.74	112.63	117.00
21	AA	1431	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	344	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	1829	A	C5-C6-N1	8.74	122.07	117.70
54	BA	199	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	1339	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1698	A	C5-C6-N1	8.73	122.06	117.70
21	AA	792	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1308	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	975	A	C5-C6-N1	8.72	122.06	117.70
21	AA	1533	C	N1-C2-O2	8.72	124.14	118.90
54	BA	347	A	N1-C6-N6	-8.72	113.36	118.60
54	BA	2469	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	1280	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	1654	A	C5-C6-N1	8.72	122.06	117.70
21	AA	1014	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	1336	C	N3-C2-O2	-8.72	115.80	121.90
24	A3	45	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	789	A	C5-C6-N1	8.72	122.06	117.70
54	BA	982	C	N3-C2-O2	-8.72	115.80	121.90
54	BA	1111	A	C5-C6-N1	8.72	122.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	729	A	C5-C6-N1	8.71	122.06	117.70
54	BA	510	C	N3-C2-O2	-8.71	115.80	121.90
21	AA	1518	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	892	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	575	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	1899	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	2025	C	N3-C2-O2	-8.70	115.81	121.90
21	AA	328	C	N3-C2-O2	-8.70	115.81	121.90
54	BA	152	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	503	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	1759	A	N1-C6-N6	-8.69	113.39	118.60
21	AA	10	A	C4-C5-C6	-8.68	112.66	117.00
54	BA	2284	A	C5-C6-N1	8.68	122.04	117.70
54	BA	1735	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	1509	A	C5-C6-N1	8.67	122.03	117.70
26	BD	33	ARG	NE-CZ-NH1	8.66	124.63	120.30
21	AA	522	C	N3-C2-O2	-8.66	115.84	121.90
21	AA	802	A	N1-C6-N6	-8.66	113.41	118.60
54	BA	204	A	C4-C5-C6	-8.65	112.67	117.00
21	AA	143	A	C5-C6-N1	8.65	122.03	117.70
21	AA	238	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	2003	A	C5-C6-N1	8.65	122.03	117.70
54	BA	2814	A	C5-C6-N1	8.64	122.02	117.70
56	B5	134	ARG	NE-CZ-NH1	8.64	124.62	120.30
54	BA	789	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	51	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	354	A	C5-C6-N1	8.64	122.02	117.70
54	BA	1504	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	354	G	O4'-C1'-N9	8.63	115.11	108.20
21	AA	1169	A	C5-C6-N1	8.63	122.02	117.70
21	AA	1360	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	1632	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	1871	A	C5-C6-N1	8.63	122.02	117.70
8	AI	105	ARG	NE-CZ-NH1	8.63	124.62	120.30
54	BA	1073	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	510	A	C5-C6-N1	8.63	122.02	117.70
54	BA	2868	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	915	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	238	A	C5-C6-N1	8.62	122.01	117.70
54	BA	1899	A	C5-C6-N1	8.62	122.01	117.70
54	BA	1700	A	C5-C6-N1	8.62	122.01	117.70
54	BA	1354	A	N1-C6-N6	-8.62	113.43	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	15	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	2448	A	C5-C6-N1	8.61	122.01	117.70
54	BA	2781	A	C5-C6-N1	8.61	122.01	117.70
21	AA	1167	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	2856	A	C5-C6-N1	8.61	122.00	117.70
21	AA	414	A	C5-C6-N1	8.60	122.00	117.70
54	BA	626	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1383	A	N1-C6-N6	-8.60	113.44	118.60
15	AP	5	ARG	NE-CZ-NH1	8.60	124.60	120.30
19	AT	59	ARG	NE-CZ-NH1	8.60	124.60	120.30
54	BA	1080	A	N1-C6-N6	-8.60	113.44	118.60
6	AG	118	ARG	NE-CZ-NH1	8.59	124.60	120.30
54	BA	1189	A	N1-C6-N6	-8.59	113.44	118.60
54	BA	1285	A	C5-C6-N1	8.59	122.00	117.70
54	BA	196	A	N1-C6-N6	-8.59	113.44	118.60
34	BL	41	ARG	NE-CZ-NH1	8.59	124.59	120.30
54	BA	719	C	N3-C2-O2	-8.59	115.89	121.90
54	BA	2009	A	N1-C6-N6	-8.59	113.45	118.60
25	BC	213	ARG	NE-CZ-NH1	8.59	124.59	120.30
54	BA	160	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	48	C	N3-C2-O2	-8.58	115.89	121.90
21	AA	781	A	C5-C6-N1	8.58	121.99	117.70
54	BA	750	A	C4-C5-C6	-8.58	112.71	117.00
9	AJ	37	ARG	NE-CZ-NH1	8.58	124.59	120.30
21	AA	1493	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	99	U	O4'-C1'-N1	8.58	115.06	108.20
54	BA	2451	A	C5-C6-N1	8.58	121.99	117.70
47	BY	29	ARG	NE-CZ-NH1	8.58	124.59	120.30
54	BA	204	A	C5-C6-N1	8.58	121.99	117.70
54	BA	1095	A	N1-C6-N6	-8.58	113.45	118.60
21	AA	274	A	N1-C6-N6	-8.57	113.45	118.60
21	AA	1362	A	C5-C6-N1	8.57	121.99	117.70
54	BA	1525	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	192	C	N3-C2-O2	-8.57	115.90	121.90
54	BA	1142	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	483	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	582	A	N1-C6-N6	-8.57	113.46	118.60
21	AA	831	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	371	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	766	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	1398	A	C5-C6-N1	8.55	121.98	117.70
54	BA	1757	A	C5-C6-N1	8.56	121.98	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1227	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	1698	A	C4-C5-C6	-8.55	112.72	117.00
55	BB	45	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	2060	A	C5-C6-N1	8.55	121.98	117.70
21	AA	640	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	2320	U	O4'-C1'-N1	8.55	115.04	108.20
21	AA	655	A	N1-C6-N6	-8.55	113.47	118.60
30	BH	50	ARG	NE-CZ-NH1	8.55	124.57	120.30
54	BA	371	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	1404	C	N1-C2-O2	8.55	124.03	118.90
54	BA	2851	A	C5-C6-N1	8.55	121.97	117.70
54	BA	739	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	1328	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	959	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	2886	A	C5-C6-N1	8.54	121.97	117.70
15	AP	28	ARG	NE-CZ-NH1	8.54	124.57	120.30
21	AA	983	A	C5-C6-N1	8.54	121.97	117.70
54	BA	64	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	104	A	C5-C6-N1	8.54	121.97	117.70
54	BA	1477	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	616	A	N1-C6-N6	-8.54	113.48	118.60
21	AA	8	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	1324	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	980	A	O4'-C1'-N9	8.53	115.02	108.20
54	BA	1321	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	497	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	1789	A	C4-C5-C6	-8.53	112.74	117.00
21	AA	994	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	643	A	C5-C6-N1	8.52	121.96	117.70
21	AA	1155	A	N1-C6-N6	-8.52	113.49	118.60
52	B3	29	ARG	NE-CZ-NH1	8.52	124.56	120.30
54	BA	1981	A	C5-C6-N1	8.52	121.96	117.70
54	BA	2211	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	14	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	181	A	N1-C6-N6	-8.52	113.49	118.60
48	BZ	30	ARG	NE-CZ-NH1	8.51	124.56	120.30
54	BA	56	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	730	A	O4'-C1'-N9	8.51	115.01	108.20
54	BA	804	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	1912	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	2459	A	C5-C6-N1	8.51	121.96	117.70
54	BA	1608	A	N1-C6-N6	-8.51	113.49	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	794	A	N1-C6-N6	-8.51	113.50	118.60
21	AA	80	A	C4-C5-C6	-8.51	112.75	117.00
24	A3	58	A	C5-C6-N1	8.50	121.95	117.70
54	BA	1451	C	O4'-C1'-N1	8.50	115.00	108.20
9	AJ	9	ARG	NE-CZ-NH2	-8.49	116.05	120.30
21	AA	1053	G	N3-C2-N2	-8.49	113.95	119.90
54	BA	492	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	996	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	172	A	C5-C6-N1	8.49	121.94	117.70
54	BA	1966	A	N1-C6-N6	-8.49	113.51	118.60
54	BA	2407	A	N1-C6-N6	-8.49	113.51	118.60
12	AM	91	ARG	NE-CZ-NH1	8.48	124.54	120.30
21	AA	1346	A	C4-C5-C6	-8.48	112.76	117.00
7	AH	14	ARG	NE-CZ-NH1	8.48	124.54	120.30
21	AA	197	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1803	A	C5-C6-N1	8.48	121.94	117.70
31	BI	64	ARG	NE-CZ-NH1	8.47	124.54	120.30
54	BA	320	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	374	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	716	A	C5-C6-N1	8.47	121.94	117.70
13	AN	53	ARG	NE-CZ-NH1	8.47	124.53	120.30
35	BM	66	ARG	NE-CZ-NH1	8.47	124.53	120.30
21	AA	143	A	C4-C5-C6	-8.47	112.77	117.00
54	BA	73	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	1722	A	C5-C6-N1	8.46	121.93	117.70
54	BA	2247	A	C4-C5-C6	-8.47	112.77	117.00
21	AA	298	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	1597	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	342	A	N1-C6-N6	-8.46	113.52	118.60
24	A3	74	A	C5-C6-N1	8.46	121.93	117.70
54	BA	1155	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	2411	A	C4-C5-C6	-8.46	112.77	117.00
54	BA	2600	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	51	A	C5-C6-N1	8.46	121.93	117.70
54	BA	1665	A	C5-C6-N1	8.45	121.93	117.70
54	BA	2513	A	C5-C6-N1	8.45	121.93	117.70
21	AA	790	A	C5-C6-N1	8.45	121.92	117.70
54	BA	368	A	C5-C6-N1	8.45	121.92	117.70
27	BE	21	ARG	NE-CZ-NH1	8.44	124.52	120.30
54	BA	1134	A	N1-C6-N6	-8.44	113.53	118.60
27	BE	61	ARG	NE-CZ-NH1	8.44	124.52	120.30
54	BA	1008	A	N1-C6-N6	-8.44	113.53	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	432	A	C5-C6-N1	8.44	121.92	117.70
54	BA	1241	A	C5-C6-N1	8.44	121.92	117.70
21	AA	171	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	196	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	1204	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	2439	A	O4'-C1'-N9	8.44	114.95	108.20
21	AA	1100	C	N3-C2-O2	-8.44	115.99	121.90
54	BA	582	A	C5-C6-N1	8.44	121.92	117.70
21	AA	790	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	28	A	N1-C6-N6	-8.43	113.54	118.60
23	A2	79	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	177	G	O4'-C1'-N9	8.43	114.94	108.20
2	AC	87	ARG	NE-CZ-NH1	8.43	124.51	120.30
52	B3	7	ARG	NE-CZ-NH1	8.43	124.52	120.30
54	BA	482	A	C4-C5-C6	-8.43	112.79	117.00
54	BA	2700	A	C4-C5-C6	-8.43	112.79	117.00
21	AA	1105	A	C4-C5-C6	-8.43	112.79	117.00
54	BA	2169	A	O4'-C1'-N9	8.43	114.94	108.20
54	BA	1580	A	N1-C6-N6	-8.42	113.55	118.60
21	AA	621	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	83	A	C5-C6-N1	8.42	121.91	117.70
54	BA	833	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2734	A	C5-C6-N1	8.42	121.91	117.70
54	BA	1111	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	1829	A	N1-C6-N6	-8.41	113.56	118.60
54	BA	1552	A	C5-C6-N1	8.41	121.90	117.70
21	AA	74	A	C5-C6-N1	8.40	121.90	117.70
21	AA	131	A	C4-C5-C6	-8.40	112.80	117.00
21	AA	16	A	C5-C6-N1	8.40	121.90	117.70
21	AA	1333	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	1913	A	O4'-C1'-N9	8.40	114.92	108.20
54	BA	244	A	N1-C6-N6	-8.40	113.56	118.60
16	AQ	61	ARG	NE-CZ-NH1	8.40	124.50	120.30
21	AA	694	A	N1-C6-N6	-8.39	113.56	118.60
21	AA	728	A	C4-C5-C6	-8.39	112.80	117.00
43	BU	21	ARG	NE-CZ-NH1	8.39	124.50	120.30
54	BA	1427	A	C5-C6-N1	8.39	121.90	117.70
54	BA	1794	A	C4-C5-C6	-8.39	112.80	117.00
54	BA	2412	A	C5-C6-N1	8.39	121.90	117.70
54	BA	2887	A	N1-C6-N6	-8.39	113.57	118.60
21	AA	1102	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	1965	C	N3-C2-O2	-8.39	116.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2451	A	C4-C5-C6	-8.39	112.81	117.00
29	BG	162	ARG	NE-CZ-NH1	8.38	124.49	120.30
54	BA	2137	U	N3-C2-O2	-8.38	116.33	122.20
54	BA	1900	A	C5-C6-N1	8.38	121.89	117.70
54	BA	792	A	C5-C6-N1	8.38	121.89	117.70
55	BB	87	U	O4'-C1'-N1	8.38	114.91	108.20
54	BA	2226	C	N3-C2-O2	-8.38	116.04	121.90
54	BA	2346	A	C5-C6-N1	8.38	121.89	117.70
54	BA	2129	C	N3-C2-O2	-8.37	116.04	121.90
21	AA	181	A	C5-C6-N1	8.37	121.88	117.70
54	BA	1419	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1000	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1717	A	N1-C6-N6	-8.37	113.58	118.60
49	B0	9	ARG	NE-CZ-NH1	8.37	124.48	120.30
54	BA	2755	C	N3-C2-O2	-8.36	116.05	121.90
21	AA	681	A	C5-C6-N1	8.35	121.88	117.70
24	A3	45	A	C4-C5-C6	-8.35	112.82	117.00
21	AA	1375	A	C5-C6-N1	8.35	121.88	117.70
54	BA	2430	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	535	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	1004	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	532	A	C5-C6-N1	8.34	121.87	117.70
54	BA	1689	A	C5-C6-N1	8.34	121.87	117.70
54	BA	2126	A	O4'-C1'-N9	8.34	114.88	108.20
21	AA	1267	C	N3-C2-O2	-8.34	116.06	121.90
19	AT	28	ARG	NE-CZ-NH1	8.34	124.47	120.30
21	AA	937	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	1848	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	2530	A	N1-C6-N6	-8.34	113.60	118.60
10	AK	52	ARG	NE-CZ-NH1	8.33	124.47	120.30
21	AA	1130	A	C4-C5-C6	-8.33	112.83	117.00
54	BA	5	A	C5-C6-N1	8.33	121.86	117.70
54	BA	223	A	C5-C6-N1	8.33	121.86	117.70
21	AA	33	A	C5-C6-N1	8.33	121.86	117.70
21	AA	77	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	253	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	640	A	C5-C6-N1	8.33	121.86	117.70
21	AA	780	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	2091	C	N3-C2-O2	-8.33	116.07	121.90
21	AA	1513	A	C5-C6-N1	8.32	121.86	117.70
21	AA	1428	A	C4-C5-C6	-8.32	112.84	117.00
21	AA	510	A	N1-C6-N6	-8.32	113.61	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1188	A	C5-C6-N1	8.32	121.86	117.70
21	AA	422	C	N3-C2-O2	-8.32	116.08	121.90
54	BA	2030	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	342	A	C5-C6-N1	8.31	121.86	117.70
54	BA	219	A	C4-C5-C6	-8.31	112.84	117.00
54	BA	2058	A	C4-C5-C6	-8.31	112.84	117.00
21	AA	188	C	N3-C2-O2	-8.31	116.08	121.90
54	BA	126	A	N1-C6-N6	-8.31	113.62	118.60
54	BA	453	A	N1-C6-N6	-8.31	113.62	118.60
54	BA	1969	A	C4-C5-C6	-8.31	112.85	117.00
54	BA	2126	A	C5-C6-N1	8.31	121.85	117.70
54	BA	233	A	C5-C6-N1	8.30	121.85	117.70
54	BA	1134	A	C5-C6-N1	8.31	121.85	117.70
21	AA	498	A	N1-C6-N6	-8.30	113.62	118.60
21	AA	1238	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	2771	C	N3-C2-O2	-8.30	116.09	121.90
54	BA	2411	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	1640	A	C5-C6-N1	8.29	121.85	117.70
54	BA	2758	A	C5-C6-N1	8.29	121.85	117.70
21	AA	7	A	N1-C6-N6	-8.29	113.62	118.60
21	AA	73	C	N3-C2-O2	-8.29	116.10	121.90
54	BA	849	A	N1-C6-N6	-8.29	113.62	118.60
56	B5	122	ARG	NE-CZ-NH1	8.29	124.45	120.30
21	AA	161	A	C5-C6-N1	8.29	121.84	117.70
21	AA	1363	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	613	A	O4'-C1'-N9	8.29	114.83	108.20
54	BA	2170	A	C4-C5-C6	-8.29	112.85	117.00
54	BA	2628	C	N3-C2-O2	-8.29	116.10	121.90
21	AA	264	C	O4'-C1'-N1	8.29	114.83	108.20
13	AN	75	ARG	NE-CZ-NH1	8.29	124.44	120.30
21	AA	958	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1347	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1603	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1606	C	O4'-C1'-N1	8.29	114.83	108.20
54	BA	503	A	C5-C6-N1	8.29	121.84	117.70
21	AA	448	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	532	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	792	A	N1-C6-N6	-8.28	113.63	118.60
21	AA	16	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	1981	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	1522	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	1789	A	C5-C6-N1	8.28	121.84	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	73	A	C5-C6-N1	8.28	121.84	117.70
54	BA	2062	A	O4'-C1'-N9	8.27	114.82	108.20
54	BA	222	A	C5-C6-N1	8.27	121.83	117.70
21	AA	768	A	C5-C6-N1	8.27	121.83	117.70
54	BA	1614	A	C5-C6-N1	8.27	121.83	117.70
7	AH	12	ARG	NE-CZ-NH1	8.27	124.43	120.30
36	BN	8	ARG	NE-CZ-NH1	8.27	124.43	120.30
54	BA	64	A	C5-C6-N1	8.27	121.83	117.70
54	BA	1672	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	2900	A	C5-C6-N1	8.27	121.83	117.70
56	B5	12	ARG	NE-CZ-NH1	8.27	124.43	120.30
54	BA	1819	A	C5-C6-N1	8.26	121.83	117.70
8	AI	98	ARG	NE-CZ-NH1	8.26	124.43	120.30
54	BA	1918	A	N1-C6-N6	-8.26	113.64	118.60
55	BB	109	A	C4-C5-C6	-8.26	112.87	117.00
54	BA	2369	A	C5-C6-N1	8.26	121.83	117.70
21	AA	325	A	N1-C6-N6	-8.26	113.65	118.60
21	AA	1507	A	C5-C6-N1	8.26	121.83	117.70
54	BA	447	A	C5-C6-N1	8.26	121.83	117.70
21	AA	787	A	N1-C6-N6	-8.26	113.65	118.60
21	AA	935	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2757	A	C5-C6-N1	8.25	121.83	117.70
26	BD	77	ARG	NE-CZ-NH1	8.25	124.42	120.30
54	BA	156	A	C4-C5-C6	-8.25	112.88	117.00
54	BA	218	A	C5-C6-N1	8.25	121.82	117.70
21	AA	1042	A	N1-C6-N6	-8.25	113.65	118.60
21	AA	1145	A	C5-C6-N1	8.25	121.82	117.70
54	BA	42	A	C5-C6-N1	8.25	121.82	117.70
54	BA	1439	A	O4'-C1'-N9	8.25	114.80	108.20
51	B2	14	ARG	NE-CZ-NH1	8.24	124.42	120.30
54	BA	49	A	C5-C6-N1	8.24	121.82	117.70
54	BA	1609	A	N1-C6-N6	-8.24	113.65	118.60
54	BA	2005	A	N1-C6-N6	-8.24	113.65	118.60
54	BA	441	U	O4'-C1'-N1	8.24	114.79	108.20
21	AA	702	A	C5-C6-N1	8.24	121.82	117.70
39	BQ	27	ARG	NE-CZ-NH1	8.24	124.42	120.30
54	BA	497	A	C5-C6-N1	8.24	121.82	117.70
54	BA	1354	A	C5-C6-N1	8.24	121.82	117.70
54	BA	2725	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	432	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	223	A	C4-C5-C6	-8.23	112.88	117.00
55	BB	70	C	N3-C2-O2	-8.23	116.14	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	335	C	N3-C2-O2	-8.23	116.14	121.90
54	BA	1969	A	C5-C6-N1	8.23	121.82	117.70
54	BA	21	A	C4-C5-C6	-8.23	112.89	117.00
54	BA	505	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	1392	A	C4-C5-C6	-8.23	112.89	117.00
54	BA	161	A	C5-C6-N1	8.23	121.81	117.70
54	BA	103	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2333	A	C4-C5-C6	-8.23	112.89	117.00
54	BA	1552	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	1299	A	C5-C6-N1	8.22	121.81	117.70
54	BA	322	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1304	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	71	A	N1-C6-N6	-8.22	113.67	118.60
31	BI	102	ARG	NE-CZ-NH1	8.22	124.41	120.30
54	BA	142	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	526	A	C5-C6-N1	8.22	121.81	117.70
54	BA	661	A	N1-C6-N6	-8.22	113.67	118.60
22	A1	60	C	N3-C2-O2	-8.22	116.15	121.90
54	BA	1470	A	N1-C6-N6	-8.22	113.67	118.60
6	AG	137	ARG	NE-CZ-NH1	8.22	124.41	120.30
55	BB	108	A	N1-C6-N6	-8.21	113.67	118.60
54	BA	1616	A	C5-C6-N1	8.21	121.81	117.70
54	BA	2386	A	C5-C6-N1	8.21	121.81	117.70
21	AA	1110	A	N1-C6-N6	-8.21	113.68	118.60
54	BA	241	A	C5-C6-N1	8.21	121.80	117.70
54	BA	529	A	N1-C6-N6	-8.21	113.68	118.60
54	BA	1072	C	N3-C2-O2	-8.21	116.16	121.90
4	AE	19	ARG	NE-CZ-NH1	8.20	124.40	120.30
54	BA	1317	G	O4'-C1'-N9	8.21	114.76	108.20
21	AA	781	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	454	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	2418	A	N1-C6-N6	-8.20	113.68	118.60
46	BX	27	ARG	NE-CZ-NH1	8.19	124.40	120.30
19	AT	9	ARG	NE-CZ-NH1	8.19	124.40	120.30
21	AA	1256	A	N1-C6-N6	-8.19	113.69	118.60
3	AD	50	TYR	CB-CG-CD1	-8.19	116.09	121.00
21	AA	977	A	C5-C6-N1	8.19	121.79	117.70
21	AA	777	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	889	A	C5-C6-N1	8.19	121.79	117.70
21	AA	1375	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	655	A	C5-C6-N1	8.19	121.79	117.70
41	BS	18	ARG	NE-CZ-NH1	8.18	124.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	828	U	O4'-C1'-N1	8.18	114.75	108.20
54	BA	2700	A	N1-C6-N6	-8.18	113.69	118.60
55	BB	115	A	N1-C6-N6	-8.18	113.69	118.60
21	AA	136	C	N3-C2-O2	-8.18	116.17	121.90
54	BA	889	C	N3-C2-O2	-8.18	116.17	121.90
54	BA	1275	A	C5-C6-N1	8.18	121.79	117.70
54	BA	2164	C	N3-C2-O2	-8.18	116.18	121.90
21	AA	715	A	C5-C6-N1	8.18	121.79	117.70
21	AA	795	C	N3-C2-O2	-8.18	116.18	121.90
22	A1	35	A	N1-C6-N6	-8.18	113.69	118.60
22	A1	38	A	C4-C5-C6	-8.18	112.91	117.00
54	BA	1690	A	C4-C5-C6	-8.18	112.91	117.00
5	AF	91	ARG	NE-CZ-NH1	8.17	124.39	120.30
6	AG	108	ARG	NE-CZ-NH1	8.17	124.39	120.30
21	AA	889	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2281	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2288	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2887	A	C5-C6-N1	8.17	121.78	117.70
21	AA	784	A	C5-C6-N1	8.17	121.78	117.70
54	BA	249	C	C1'-O4'-C4'	-8.17	103.37	109.90
54	BA	928	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	430	A	C5-C6-N1	8.17	121.78	117.70
54	BA	787	C	N3-C2-O2	-8.17	116.18	121.90
21	AA	139	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	764	A	C5-C6-N1	8.16	121.78	117.70
54	BA	715	A	C5-C6-N1	8.16	121.78	117.70
54	BA	1987	A	N1-C6-N6	-8.16	113.70	118.60
21	AA	1410	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	2176	A	O4'-C1'-N9	8.16	114.73	108.20
21	AA	1213	A	C5-C6-N1	8.16	121.78	117.70
54	BA	119	A	C4-C5-C6	-8.15	112.92	117.00
54	BA	911	A	C5-C6-N1	8.15	121.78	117.70
54	BA	1090	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	374	A	C4-C5-C6	-8.15	112.92	117.00
21	AA	459	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	759	A	C5-C6-N1	8.15	121.78	117.70
54	BA	2142	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	356	A	C4-C5-C6	-8.14	112.93	117.00
21	AA	1197	A	C5-C6-N1	8.14	121.77	117.70
54	BA	1096	A	N1-C6-N6	-8.14	113.71	118.60
54	BA	1288	G	O4'-C1'-N9	8.14	114.71	108.20
54	BA	1571	A	N1-C6-N6	-8.14	113.72	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	529	A	C5-C6-N1	8.14	121.77	117.70
21	AA	421	U	N3-C2-O2	-8.14	116.50	122.20
54	BA	1427	A	C4-C5-C6	-8.14	112.93	117.00
21	AA	1054	C	N3-C2-O2	-8.13	116.21	121.90
39	BQ	49	ARG	NE-CZ-NH1	8.13	124.37	120.30
54	BA	749	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	721	A	C4-C5-C6	-8.13	112.93	117.00
54	BA	1021	A	C5-C6-N1	8.13	121.77	117.70
54	BA	1566	A	C5-C6-N1	8.13	121.77	117.70
54	BA	2564	A	C5-C6-N1	8.13	121.77	117.70
54	BA	2147	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	371	A	C4-C5-C6	-8.13	112.94	117.00
21	AA	1341	U	O4'-C1'-N1	8.13	114.70	108.20
54	BA	1336	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1433	A	C4-C5-C6	-8.13	112.94	117.00
54	BA	2070	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1741	C	N3-C2-O2	-8.12	116.21	121.90
54	BA	2158	A	C5-C6-N1	8.12	121.76	117.70
21	AA	1360	A	C4-C5-C6	-8.12	112.94	117.00
54	BA	460	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1403	A	C4-C5-C6	-8.12	112.94	117.00
21	AA	80	A	C5-C6-N1	8.12	121.76	117.70
21	AA	279	A	C5-C6-N1	8.12	121.76	117.70
21	AA	629	A	C4-C5-C6	-8.11	112.94	117.00
21	AA	1322	C	N3-C2-O2	-8.12	116.22	121.90
21	AA	1508	A	C5-C6-N1	8.11	121.76	117.70
54	BA	1135	C	N3-C2-O2	-8.11	116.22	121.90
54	BA	1009	A	C5-C6-N1	8.11	121.76	117.70
54	BA	2268	A	C5-C6-N1	8.11	121.75	117.70
21	AA	609	A	C5-C6-N1	8.11	121.75	117.70
54	BA	1054	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	1175	A	O4'-C1'-N9	8.11	114.69	108.20
54	BA	2058	A	C5-C6-N1	8.11	121.75	117.70
54	BA	2212	A	C5-C6-N1	8.11	121.75	117.70
21	AA	441	A	C4-C5-C6	-8.11	112.95	117.00
21	AA	313	A	C5-C6-N1	8.11	121.75	117.70
54	BA	2740	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	2860	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	2426	A	N1-C6-N6	-8.10	113.74	118.60
9	AJ	72	ARG	NE-CZ-NH1	8.10	124.35	120.30
7	AH	113	ARG	NE-CZ-NH1	8.10	124.35	120.30
54	BA	227	A	N1-C6-N6	-8.10	113.74	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	620	G	C8-N9-C4	-8.10	103.16	106.40
54	BA	1508	A	N1-C6-N6	-8.09	113.74	118.60
2	AC	53	ARG	NE-CZ-NH1	8.09	124.35	120.30
54	BA	480	A	N1-C6-N6	-8.09	113.75	118.60
21	AA	397	A	C5-C6-N1	8.09	121.75	117.70
26	BD	33	ARG	NE-CZ-NH2	-8.09	116.25	120.30
21	AA	366	A	C5-C6-N1	8.09	121.74	117.70
21	AA	814	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	1808	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	144	A	C5-C6-N1	8.08	121.74	117.70
54	BA	941	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	1938	A	C5-C6-N1	8.08	121.74	117.70
36	BN	64	ARG	NE-CZ-NH1	8.08	124.34	120.30
54	BA	2407	A	C5-C6-N1	8.08	121.74	117.70
21	AA	167	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	783	A	C5-C6-N1	8.08	121.74	117.70
21	AA	743	A	N1-C6-N6	-8.08	113.75	118.60
36	BN	63	ARG	NE-CZ-NH1	8.08	124.34	120.30
54	BA	456	C	N3-C2-O2	-8.08	116.25	121.90
54	BA	2598	A	C5-C6-N1	8.08	121.74	117.70
21	AA	493	A	N1-C6-N6	-8.07	113.75	118.60
54	BA	2171	A	N1-C6-N6	-8.07	113.75	118.60
40	BR	68	ARG	NE-CZ-NH1	8.07	124.34	120.30
21	AA	750	C	N3-C2-O2	-8.07	116.25	121.90
54	BA	119	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	197	A	C5-C6-N1	8.07	121.74	117.70
54	BA	613	A	C5-C6-N1	8.07	121.73	117.70
54	BA	1503	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	1012	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	460	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	783	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	918	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	642	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	981	A	C4-C5-C6	-8.06	112.97	117.00
54	BA	322	A	C4-C5-C6	-8.06	112.97	117.00
54	BA	2267	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	2886	A	N1-C6-N6	-8.06	113.76	118.60
21	AA	1105	A	C5-C6-N1	8.06	121.73	117.70
54	BA	428	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	2476	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	984	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	2322	A	N1-C6-N6	-8.06	113.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BF	149	ARG	NE-CZ-NH1	8.06	124.33	120.30
54	BA	2377	A	N1-C6-N6	-8.06	113.77	118.60
54	BA	730	A	C5-C6-N1	8.06	121.73	117.70
54	BA	119	A	C5-C6-N1	8.05	121.73	117.70
21	AA	374	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	1180	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	918	A	C5-C6-N1	8.05	121.73	117.70
55	BB	57	A	C5-C6-N1	8.05	121.73	117.70
21	AA	1130	A	C5-C6-N1	8.05	121.72	117.70
21	AA	329	A	C5-C6-N1	8.05	121.72	117.70
21	AA	469	C	N3-C2-O2	-8.05	116.27	121.90
54	BA	118	A	C5-C6-N1	8.05	121.72	117.70
54	BA	1264	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	146	A	C5-C6-N1	8.05	121.72	117.70
54	BA	2687	U	O4'-C1'-N1	8.05	114.64	108.20
21	AA	860	A	C5-C6-N1	8.04	121.72	117.70
54	BA	1143	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	2727	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	779	C	N3-C2-O2	-8.04	116.28	121.90
54	BA	131	A	C5-C6-N1	8.04	121.72	117.70
54	BA	515	A	C5-C6-N1	8.04	121.72	117.70
54	BA	2326	C	N3-C2-O2	-8.04	116.28	121.90
54	BA	2726	A	C5-C6-N1	8.04	121.72	117.70
43	BU	93	ARG	NE-CZ-NH1	8.03	124.32	120.30
54	BA	1952	A	C5-C6-N1	8.03	121.72	117.70
21	AA	190	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	1067	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	2322	A	C4-C5-C6	-8.03	112.98	117.00
54	BA	2887	A	C4-C5-C6	-8.03	112.98	117.00
27	BE	67	ARG	NE-CZ-NH1	8.03	124.31	120.30
54	BA	1916	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	2278	A	C4-C5-C6	-8.03	112.99	117.00
21	AA	1274	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	2335	A	C5-C6-N1	8.03	121.71	117.70
54	BA	2497	A	C5-C6-N1	8.03	121.71	117.70
1	AB	34	ARG	NE-CZ-NH1	8.02	124.31	120.30
21	AA	192	A	C5-C6-N1	8.02	121.71	117.70
54	BA	905	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	947	A	C5-C6-N1	8.02	121.71	117.70
45	BW	24	ARG	NE-CZ-NH1	8.02	124.31	120.30
54	BA	2448	A	C4-C5-C6	-8.02	112.99	117.00
21	AA	1204	A	C5-C6-N1	8.02	121.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	311	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	1057	A	C5-C6-N1	8.02	121.71	117.70
21	AA	600	A	C5-C6-N1	8.02	121.71	117.70
54	BA	1705	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	1035	A	C5-C6-N1	8.02	121.71	117.70
54	BA	990	A	C5-C6-N1	8.02	121.71	117.70
54	BA	2376	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	864	A	C5-C6-N1	8.01	121.71	117.70
54	BA	111	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	528	A	C5-C6-N1	8.01	121.71	117.70
21	AA	1248	A	C5-C6-N1	8.01	121.71	117.70
21	AA	1374	A	C5-C6-N1	8.01	121.71	117.70
21	AA	1437	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	447	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	2396	G	O4'-C1'-N9	8.01	114.61	108.20
44	BV	9	ARG	NE-CZ-NH1	8.01	124.31	120.30
21	AA	151	A	N1-C6-N6	-8.01	113.80	118.60
21	AA	560	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	2587	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	1535	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	2482	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	423	A	C5-C6-N1	8.00	121.70	117.70
54	BA	504	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1508	A	C5-C6-N1	8.00	121.70	117.70
54	BA	2284	A	C4-C5-C6	-8.00	113.00	117.00
54	BA	528	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1086	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	2753	A	C4-C5-C6	-8.00	113.00	117.00
54	BA	2810	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1572	A	C5-C6-N1	8.00	121.70	117.70
54	BA	1732	C	N3-C2-O2	-8.00	116.30	121.90
54	BA	1359	A	C5-C6-N1	8.00	121.70	117.70
54	BA	2758	A	N1-C6-N6	-7.99	113.80	118.60
54	BA	199	A	C4-C5-C6	-7.99	113.00	117.00
54	BA	415	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	1050	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	1847	A	C5-C6-N1	7.99	121.69	117.70
54	BA	2705	A	C4-C5-C6	-7.99	113.01	117.00
14	AO	57	ARG	NE-CZ-NH1	7.99	124.29	120.30
54	BA	2014	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	1429	A	C4-C5-C6	-7.98	113.01	117.00
54	BA	1392	A	C5-C6-N1	7.98	121.69	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	872	A	C5-C6-N1	7.98	121.69	117.70
54	BA	1987	A	C5-C6-N1	7.98	121.69	117.70
21	AA	702	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	696	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	348	A	C5-C6-N1	7.98	121.69	117.70
54	BA	2327	A	C4-C5-C6	-7.97	113.01	117.00
21	AA	303	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	600	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	938	A	C5-C6-N1	7.97	121.69	117.70
54	BA	2278	A	C5-C6-N1	7.97	121.69	117.70
21	AA	1531	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	2565	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	353	A	C5-C6-N1	7.96	121.68	117.70
21	AA	1179	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	633	A	N1-C6-N6	-7.96	113.82	118.60
21	AA	1250	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	2660	A	O4'-C1'-N9	7.96	114.57	108.20
54	BA	1744	A	C5-C6-N1	7.96	121.68	117.70
21	AA	355	C	N3-C2-O2	-7.96	116.33	121.90
54	BA	470	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1607	C	N3-C2-O2	-7.95	116.33	121.90
21	AA	101	A	C5-C6-N1	7.95	121.68	117.70
21	AA	864	A	C4-C5-C6	-7.95	113.02	117.00
21	AA	186	C	N3-C2-O2	-7.95	116.33	121.90
21	AA	282	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1127	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1794	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1008	A	C5-C6-N1	7.95	121.67	117.70
21	AA	1476	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	590	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1054	A	C5-C6-N1	7.95	121.67	117.70
54	BA	2792	A	N1-C6-N6	-7.95	113.83	118.60
46	BX	26	ARG	NE-CZ-NH1	7.94	124.27	120.30
21	AA	681	A	C4-C5-C6	-7.94	113.03	117.00
29	BG	169	ARG	NE-CZ-NH1	7.94	124.27	120.30
54	BA	740	C	N3-C2-O2	-7.94	116.34	121.90
54	BA	2752	C	N3-C2-O2	-7.94	116.34	121.90
21	AA	1219	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	2666	C	N3-C2-O2	-7.93	116.35	121.90
21	AA	583	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	1239	A	C5-C6-N1	7.93	121.66	117.70
54	BA	2856	A	N1-C6-N6	-7.93	113.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	12	ARG	NE-CZ-NH1	7.93	124.26	120.30
21	AA	32	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	949	A	C5-C6-N1	7.93	121.66	117.70
54	BA	742	A	C5-C6-N1	7.93	121.66	117.70
54	BA	890	C	N3-C2-O2	-7.92	116.35	121.90
54	BA	2191	A	C5-C6-N1	7.92	121.66	117.70
54	BA	2358	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1916	A	C5-C6-N1	7.92	121.66	117.70
54	BA	330	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1302	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1151	A	C5-C6-N1	7.92	121.66	117.70
21	AA	1479	C	N3-C2-O2	-7.91	116.36	121.90
37	BO	81	ARG	NE-CZ-NH1	7.91	124.25	120.30
54	BA	2755	C	O4'-C1'-N1	7.91	114.53	108.20
21	AA	246	A	C5-C6-N1	7.91	121.65	117.70
21	AA	451	A	C5-C6-N1	7.91	121.65	117.70
54	BA	28	A	C5-C6-N1	7.91	121.66	117.70
54	BA	2003	A	C4-C5-C6	-7.91	113.05	117.00
54	BA	644	A	C5-C6-N1	7.91	121.65	117.70
54	BA	2882	A	C4-C5-C6	-7.91	113.05	117.00
21	AA	1357	A	C4-C5-C6	-7.90	113.05	117.00
54	BA	1821	A	C5-C6-N1	7.90	121.65	117.70
30	BH	68	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	689	A	C5-C6-N1	7.90	121.65	117.70
54	BA	752	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	753	A	C5-C6-N1	7.90	121.65	117.70
54	BA	1528	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2346	A	C4-C5-C6	-7.90	113.05	117.00
54	BA	301	G	O4'-C1'-N9	7.90	114.52	108.20
54	BA	401	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	227	A	C5-C6-N1	7.90	121.65	117.70
54	BA	341	C	N3-C2-O2	-7.90	116.37	121.90
54	BA	1585	C	N3-C2-O2	-7.90	116.37	121.90
55	BB	53	A	C5-C6-N1	7.89	121.65	117.70
21	AA	1239	A	C4-C5-C6	-7.89	113.05	117.00
24	A3	44	A	N1-C6-N6	-7.89	113.87	118.60
54	BA	2432	A	C5-C6-N1	7.89	121.64	117.70
24	A3	39	A	C5-C6-N1	7.88	121.64	117.70
54	BA	478	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	1365	A	C5-C6-N1	7.88	121.64	117.70
22	A1	66	A	C5-C6-N1	7.88	121.64	117.70
54	BA	482	A	C5-C6-N1	7.88	121.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	927	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	1247	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	1265	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	2095	A	C4-C5-C6	-7.88	113.06	117.00
44	BV	19	ARG	NE-CZ-NH1	7.88	124.24	120.30
54	BA	1301	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1387	A	C5-C6-N1	7.88	121.64	117.70
55	BB	118	C	N3-C2-O2	-7.88	116.39	121.90
54	BA	1320	C	N1-C2-O2	7.87	123.62	118.90
54	BA	2311	A	C5-C6-N1	7.87	121.64	117.70
21	AA	487	A	N1-C6-N6	-7.87	113.88	118.60
53	B4	12	ARG	NE-CZ-NH1	7.87	124.24	120.30
54	BA	2220	U	O4'-C1'-N1	7.87	114.50	108.20
21	AA	901	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	460	A	C5-C6-N1	7.87	121.64	117.70
54	BA	2776	A	C5-C6-N1	7.87	121.64	117.70
54	BA	1321	A	C5-C6-N1	7.87	121.64	117.70
54	BA	1784	A	C4-C5-C6	-7.87	113.07	117.00
54	BA	1870	C	N3-C2-O2	-7.87	116.39	121.90
21	AA	152	A	C5-C6-N1	7.87	121.63	117.70
21	AA	502	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	665	A	C4-C5-C6	-7.87	113.07	117.00
54	BA	1598	A	C5-C6-N1	7.87	121.63	117.70
54	BA	2900	A	C4-C5-C6	-7.87	113.07	117.00
21	AA	621	A	C5-C6-N1	7.86	121.63	117.70
54	BA	31	C	N3-C2-O2	-7.86	116.39	121.90
54	BA	1919	A	N1-C6-N6	-7.86	113.88	118.60
21	AA	383	A	C5-C6-N1	7.86	121.63	117.70
54	BA	430	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	487	C	N3-C2-O2	-7.86	116.40	121.90
21	AA	164	G	O4'-C1'-N9	7.86	114.49	108.20
21	AA	532	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	1630	A	C5-C6-N1	7.86	121.63	117.70
21	AA	726	C	N3-C2-O2	-7.85	116.41	121.90
21	AA	1500	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	173	A	C5-C6-N1	7.85	121.62	117.70
54	BA	1579	A	N1-C6-N6	-7.85	113.89	118.60
2	AC	126	ARG	NE-CZ-NH1	7.85	124.22	120.30
21	AA	1204	A	C4-C5-C6	-7.85	113.08	117.00
54	BA	2381	A	C4-C5-C6	-7.85	113.08	117.00
54	BA	609	A	N1-C6-N6	-7.84	113.89	118.60
27	BE	69	ARG	NE-CZ-NH1	7.84	124.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	386	C	N3-C2-O2	-7.84	116.41	121.90
21	AA	706	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	2090	A	C4-C5-C6	-7.84	113.08	117.00
21	AA	1216	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2825	G	O4'-C1'-N9	7.84	114.47	108.20
22	A1	35	A	C5-C6-N1	7.84	121.62	117.70
54	BA	756	A	C5-C6-N1	7.83	121.62	117.70
54	BA	2564	A	N1-C6-N6	-7.83	113.90	118.60
24	A3	39	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1717	A	C4-C5-C6	-7.83	113.08	117.00
54	BA	422	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	547	A	C5-C6-N1	7.83	121.61	117.70
54	BA	173	A	C4-C5-C6	-7.83	113.08	117.00
54	BA	1816	C	N3-C2-O2	-7.83	116.42	121.90
54	BA	2171	A	C4-C5-C6	-7.83	113.09	117.00
54	BA	2406	A	C5-C6-N1	7.83	121.61	117.70
21	AA	50	A	C5-C6-N1	7.83	121.61	117.70
21	AA	448	A	C5-C6-N1	7.83	121.61	117.70
54	BA	1126	A	N1-C6-N6	-7.83	113.91	118.60
54	BA	1213	A	N1-C6-N6	-7.83	113.91	118.60
21	AA	655	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1226	A	C5-C6-N1	7.82	121.61	117.70
54	BA	2654	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	155	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1313	U	O4'-C1'-N1	7.82	114.45	108.20
54	BA	655	A	C4-C5-C6	-7.82	113.09	117.00
54	BA	734	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	1439	A	C5-C6-N1	7.82	121.61	117.70
21	AA	892	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	2705	A	C5-C6-N1	7.81	121.61	117.70
21	AA	1342	C	N3-C2-O2	-7.81	116.43	121.90
21	AA	716	A	C4-C5-C6	-7.81	113.09	117.00
21	AA	1269	A	C5-C6-N1	7.81	121.61	117.70
54	BA	2134	A	N1-C6-N6	-7.81	113.92	118.60
21	AA	511	C	N3-C2-O2	-7.81	116.43	121.90
54	BA	603	A	C5-C6-N1	7.81	121.60	117.70
54	BA	2314	A	N1-C6-N6	-7.81	113.92	118.60
54	BA	2774	C	N3-C2-O2	-7.81	116.44	121.90
54	BA	502	A	N1-C6-N6	-7.81	113.92	118.60
54	BA	1353	A	C5-C6-N1	7.81	121.60	117.70
21	AA	345	C	N3-C2-O2	-7.80	116.44	121.90
21	AA	110	C	N3-C2-O2	-7.80	116.44	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	431	A	C5-C6-N1	7.80	121.60	117.70
22	A1	58	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	780	A	C4-C5-C6	-7.80	113.10	117.00
54	BA	1676	A	C4-C5-C6	-7.80	113.10	117.00
54	BA	896	A	C5-C6-N1	7.79	121.60	117.70
54	BA	900	A	C5-C6-N1	7.79	121.60	117.70
54	BA	941	A	C5-C6-N1	7.79	121.60	117.70
54	BA	972	A	C5-C6-N1	7.79	121.60	117.70
55	BB	36	C	N3-C2-O2	-7.79	116.44	121.90
54	BA	1678	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	1167	A	C5-C6-N1	7.79	121.59	117.70
12	AM	56	ARG	NE-CZ-NH1	7.79	124.19	120.30
21	AA	649	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	1152	A	C5-C6-N1	7.79	121.59	117.70
54	BA	599	A	C5-C6-N1	7.79	121.59	117.70
21	AA	74	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	1289	C	N3-C2-O2	-7.79	116.45	121.90
54	BA	2388	A	C4-C5-C6	-7.79	113.11	117.00
54	BA	2548	U	O4'-C1'-N1	7.79	114.43	108.20
54	BA	507	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	563	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	219	A	C5-C6-N1	7.78	121.59	117.70
54	BA	960	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	1073	A	C5-C6-N1	7.78	121.59	117.70
21	AA	53	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	415	A	C5-C6-N1	7.78	121.59	117.70
44	BV	93	ARG	NE-CZ-NH1	7.78	124.19	120.30
54	BA	1359	A	O4'-C1'-N9	7.78	114.42	108.20
54	BA	1932	A	C4-C5-C6	-7.78	113.11	117.00
21	AA	1191	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	1067	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1302	C	N3-C2-O2	-7.77	116.46	121.90
21	AA	1377	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	2051	A	C5-C6-N1	7.77	121.59	117.70
21	AA	349	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	1832	C	N3-C2-O2	-7.77	116.46	121.90
54	BA	975	A	C5-C6-N1	7.77	121.58	117.70
54	BA	2498	C	N3-C2-O2	-7.77	116.46	121.90
6	AG	95	ARG	NE-CZ-NH1	7.77	124.18	120.30
21	AA	53	A	C4-C5-C6	-7.77	113.12	117.00
21	AA	554	A	C5-C6-N1	7.77	121.58	117.70
21	AA	1259	C	N3-C2-O2	-7.77	116.46	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	38	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	982	C	N1-C2-O2	7.77	123.56	118.90
54	BA	1336	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1773	A	C5-C6-N1	7.77	121.58	117.70
54	BA	91	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	2019	A	C4-C5-C6	-7.77	113.12	117.00
54	BA	2071	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	195	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	2639	A	N1-C6-N6	-7.76	113.94	118.60
21	AA	162	A	C5-C6-N1	7.76	121.58	117.70
21	AA	1103	C	N3-C2-O2	-7.76	116.47	121.90
54	BA	1912	A	C5-C6-N1	7.76	121.58	117.70
54	BA	526	A	N1-C6-N6	-7.76	113.95	118.60
54	BA	1537	G	O4'-C1'-N9	7.76	114.41	108.20
21	AA	482	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	938	A	C4-C5-C6	-7.75	113.12	117.00
21	AA	270	A	C4-C5-C6	-7.75	113.12	117.00
54	BA	404	A	N1-C6-N6	-7.75	113.95	118.60
8	AI	48	ARG	NE-CZ-NH1	7.75	124.17	120.30
54	BA	793	A	C5-C6-N1	7.75	121.57	117.70
54	BA	1287	A	C5-C6-N1	7.75	121.57	117.70
54	BA	2740	A	C5-C6-N1	7.75	121.58	117.70
21	AA	819	A	C5-C6-N1	7.75	121.57	117.70
21	AA	1238	A	C5-C6-N1	7.75	121.57	117.70
21	AA	1285	A	N1-C6-N6	-7.75	113.95	118.60
40	BR	13	ARG	NE-CZ-NH1	7.75	124.17	120.30
54	BA	1495	A	C5-C6-N1	7.75	121.57	117.70
54	BA	1916	A	C4-C5-C6	-7.75	113.13	117.00
21	AA	1201	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	1227	A	C5-C6-N1	7.75	121.57	117.70
54	BA	1439	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	564	C	N3-C2-O2	-7.74	116.48	121.90
21	AA	1191	A	C5-C6-N1	7.74	121.57	117.70
9	AJ	89	ARG	NE-CZ-NH1	7.74	124.17	120.30
54	BA	1960	A	C5-C6-N1	7.74	121.57	117.70
21	AA	1169	A	C4-C5-C6	-7.74	113.13	117.00
21	AA	1466	C	N3-C2-O2	-7.74	116.48	121.90
54	BA	477	A	N1-C6-N6	-7.74	113.96	118.60
21	AA	1217	C	N3-C2-O2	-7.74	116.48	121.90
54	BA	1784	A	C5-C6-N1	7.74	121.57	117.70
21	AA	430	A	C5-C6-N1	7.74	121.57	117.70
22	A1	9	A	N1-C6-N6	-7.73	113.96	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	74	A	C4-C5-C6	-7.73	113.13	117.00
54	BA	5	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	586	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	2758	A	C4-C5-C6	-7.73	113.13	117.00
28	BF	79	ARG	NE-CZ-NH1	7.73	124.17	120.30
43	BU	5	ARG	NE-CZ-NH1	7.73	124.17	120.30
54	BA	1286	A	C5-C6-N1	7.73	121.56	117.70
54	BA	2826	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	223	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	2434	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	382	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	1211	C	N3-C2-O2	-7.73	116.49	121.90
24	A3	44	A	C5-C6-N1	7.72	121.56	117.70
54	BA	443	A	C5-C6-N1	7.72	121.56	117.70
48	BZ	37	ARG	NE-CZ-NH1	7.72	124.16	120.30
21	AA	238	A	P-O3'-C3'	7.72	128.97	119.70
21	AA	321	A	C5-C6-N1	7.72	121.56	117.70
21	AA	1031	C	N3-C2-O2	-7.72	116.50	121.90
26	BD	13	ARG	NE-CZ-NH1	7.72	124.16	120.30
54	BA	1069	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1085	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1363	C	N3-C2-O2	-7.72	116.50	121.90
54	BA	2063	C	N3-C2-O2	-7.72	116.50	121.90
21	AA	845	A	C5-C6-N1	7.71	121.56	117.70
24	A3	59	A	C5-C6-N1	7.71	121.56	117.70
54	BA	226	A	C5-C6-N1	7.71	121.56	117.70
54	BA	863	A	C5-C6-N1	7.71	121.56	117.70
54	BA	1700	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	338	A	N1-C6-N6	-7.71	113.97	118.60
22	A1	9	A	C5-C6-N1	7.71	121.56	117.70
54	BA	2749	A	N1-C6-N6	-7.71	113.97	118.60
14	AO	83	ARG	NE-CZ-NH1	7.71	124.16	120.30
54	BA	2021	C	N3-C2-O2	-7.71	116.50	121.90
54	BA	2031	A	C5-C6-N1	7.71	121.56	117.70
54	BA	2278	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	60	A	C5-C6-N1	7.71	121.56	117.70
21	AA	595	A	C5-C6-N1	7.71	121.55	117.70
54	BA	1978	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	2013	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	1429	A	C5-C6-N1	7.71	121.55	117.70
24	A3	67	C	N3-C2-O2	-7.71	116.51	121.90
54	BA	1986	C	N3-C2-O2	-7.71	116.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1214	A	N1-C6-N6	-7.71	113.98	118.60
15	AP	28	ARG	NE-CZ-NH2	7.70	124.15	120.30
21	AA	1357	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	382	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1552	A	O4'-C1'-N9	7.70	114.36	108.20
54	BA	608	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1241	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	1938	A	C4-C5-C6	-7.70	113.15	117.00
9	AJ	5	ARG	NE-CZ-NH1	7.70	124.15	120.30
21	AA	149	A	C5-C6-N1	7.70	121.55	117.70
54	BA	84	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	1264	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	482	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1098	A	C5-C6-N1	7.70	121.55	117.70
55	BB	53	A	N1-C6-N6	-7.70	113.98	118.60
21	AA	288	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	1170	A	C4-C5-C6	-7.70	113.15	117.00
54	BA	265	A	O4'-C1'-N9	7.70	114.36	108.20
54	BA	2055	C	O4'-C1'-N1	7.70	114.36	108.20
21	AA	737	C	N3-C2-O2	-7.69	116.51	121.90
54	BA	1650	A	N1-C6-N6	-7.69	113.98	118.60
5	AF	2	ARG	NE-CZ-NH1	7.69	124.15	120.30
21	AA	1137	C	N3-C2-O2	-7.69	116.52	121.90
54	BA	2541	A	C5-C6-N1	7.69	121.55	117.70
54	BA	2080	A	C4-C5-C6	-7.69	113.16	117.00
54	BA	479	A	C4-C5-C6	-7.69	113.16	117.00
54	BA	2015	A	C5-C6-N1	7.69	121.54	117.70
54	BA	2288	A	C5-C6-N1	7.69	121.54	117.70
11	AL	30	ARG	NE-CZ-NH1	7.69	124.14	120.30
21	AA	539	A	C5-C6-N1	7.69	121.54	117.70
21	AA	1044	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	1672	A	C5-C6-N1	7.68	121.54	117.70
54	BA	2866	U	O4'-C1'-N1	7.68	114.35	108.20
8	AI	44	ARG	NE-CZ-NH1	7.68	124.14	120.30
54	BA	345	A	N1-C6-N6	-7.68	113.99	118.60
21	AA	808	C	N3-C2-O2	-7.68	116.52	121.90
54	BA	1808	A	C5-C6-N1	7.68	121.54	117.70
6	AG	110	ARG	NE-CZ-NH1	7.68	124.14	120.30
54	BA	2560	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	2700	A	C5-C6-N1	7.68	121.54	117.70
21	AA	1130	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	614	A	C5-C6-N1	7.68	121.54	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	969	A	C4-C5-C6	-7.67	113.16	117.00
21	AA	1101	A	C4-C5-C6	-7.67	113.16	117.00
54	BA	739	A	C5-C6-N1	7.67	121.54	117.70
54	BA	2184	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	2646	C	N3-C2-O2	-7.67	116.53	121.90
21	AA	370	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	324	A	C5-C6-N1	7.67	121.54	117.70
54	BA	2019	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	320	A	C5-C6-N1	7.67	121.54	117.70
21	AA	1197	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	240	C	N3-C2-O2	-7.67	116.53	121.90
34	BL	78	ARG	NE-CZ-NH1	7.67	124.14	120.30
54	BA	2327	A	N1-C6-N6	-7.67	114.00	118.60
3	AD	187	ARG	NE-CZ-NH1	7.67	124.13	120.30
21	AA	596	A	C5-C6-N1	7.67	121.53	117.70
22	A1	14	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	2480	C	O4'-C1'-N1	7.67	114.33	108.20
54	BA	2665	A	C5-C6-N1	7.67	121.53	117.70
21	AA	81	A	C5-C6-N1	7.67	121.53	117.70
54	BA	457	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	640	A	C4-C5-C6	-7.66	113.17	117.00
54	BA	655	A	N1-C6-N6	-7.66	114.00	118.60
54	BA	195	A	C5-C6-N1	7.66	121.53	117.70
12	AM	70	ARG	NE-CZ-NH1	7.66	124.13	120.30
55	BB	66	A	C5-C6-N1	7.66	121.53	117.70
54	BA	2317	A	C5-C6-N1	7.66	121.53	117.70
26	BD	169	ARG	NE-CZ-NH1	7.66	124.13	120.30
21	AA	630	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	613	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	2021	C	O4'-C1'-N1	7.66	114.32	108.20
54	BA	863	A	N1-C6-N6	-7.65	114.01	118.60
1	AB	62	ARG	NE-CZ-NH1	7.65	124.12	120.30
24	A3	57	C	N3-C2-O2	-7.65	116.55	121.90
21	AA	1101	A	P-O3'-C3'	7.65	128.88	119.70
21	AA	510	A	C4-C5-C6	-7.65	113.18	117.00
54	BA	2050	C	N3-C2-O2	-7.65	116.55	121.90
21	AA	189	A	C4-C5-C6	-7.64	113.18	117.00
54	BA	2051	A	N1-C6-N6	-7.64	114.02	118.60
21	AA	1092	A	N1-C6-N6	-7.64	114.02	118.60
21	AA	743	A	C5-C6-N1	7.64	121.52	117.70
54	BA	750	A	C5-C6-N1	7.63	121.52	117.70
54	BA	2030	A	C4-C5-C6	-7.63	113.18	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1157	A	N1-C6-N6	-7.63	114.02	118.60
21	AA	1213	A	C4-C5-C6	-7.63	113.18	117.00
54	BA	2222	C	N3-C2-O2	-7.63	116.56	121.90
55	BB	39	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	479	A	C5-C6-N1	7.63	121.52	117.70
5	AF	79	ARG	NE-CZ-NH1	7.63	124.11	120.30
8	AI	112	ARG	NE-CZ-NH1	7.63	124.11	120.30
21	AA	28	A	C5-C6-N1	7.63	121.51	117.70
21	AA	676	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	995	C	N3-C2-O2	-7.63	116.56	121.90
54	BA	2547	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	497	A	C4-C5-C6	-7.63	113.19	117.00
54	BA	1698	A	N1-C6-N6	-7.63	114.02	118.60
24	A3	77	A	C5-C6-N1	7.62	121.51	117.70
54	BA	819	A	C5-C6-N1	7.62	121.51	117.70
54	BA	947	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	2738	A	C5-C6-N1	7.62	121.51	117.70
54	BA	866	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2435	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1021	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	1640	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	2534	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	2666	C	N1-C2-O2	7.62	123.47	118.90
54	BA	2682	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	905	A	C5-C6-N1	7.62	121.51	117.70
54	BA	56	A	C4-C5-C6	-7.62	113.19	117.00
21	AA	528	C	N3-C2-O2	-7.61	116.57	121.90
54	BA	1927	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	1264	A	C5-C6-N1	7.61	121.51	117.70
54	BA	270	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1090	A	C5-C6-N1	7.61	121.51	117.70
21	AA	1397	C	O4'-C1'-N1	7.61	114.29	108.20
54	BA	1686	C	N3-C2-O2	-7.61	116.57	121.90
54	BA	2764	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1551	A	C4-C5-C6	-7.61	113.20	117.00
11	AL	55	ARG	NE-CZ-NH1	7.61	124.10	120.30
17	AR	42	ARG	NE-CZ-NH1	7.61	124.10	120.30
21	AA	984	C	N3-C2-O2	-7.61	116.58	121.90
21	AA	1434	A	C5-C6-N1	7.61	121.50	117.70
21	AA	1507	A	N1-C6-N6	-7.61	114.04	118.60
54	BA	1308	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1610	A	C5-C6-N1	7.61	121.50	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2241	A	C4-C5-C6	-7.61	113.20	117.00
16	AQ	63	CYS	C-N-CA	7.60	140.71	121.70
21	AA	435	A	C4-C5-C6	-7.60	113.20	117.00
21	AA	819	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	1508	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	173	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	603	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	116	A	C5-C6-N1	7.60	121.50	117.70
21	AA	906	A	C5-C6-N1	7.60	121.50	117.70
54	BA	255	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	776	G	N3-C2-N2	-7.60	114.58	119.90
54	BA	784	G	O4'-C1'-N9	7.60	114.28	108.20
54	BA	1785	A	C4-C5-C6	-7.60	113.20	117.00
54	BA	2198	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	131	A	C5-C6-N1	7.60	121.50	117.70
54	BA	980	A	C4-C5-C6	-7.60	113.20	117.00
21	AA	162	A	N1-C6-N6	-7.59	114.04	118.60
54	BA	2381	A	C5-C6-N1	7.59	121.50	117.70
21	AA	321	A	C4-C5-C6	-7.59	113.20	117.00
21	AA	865	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	1254	A	C4-C5-C6	-7.59	113.21	117.00
21	AA	414	A	C4-C5-C6	-7.59	113.21	117.00
21	AA	996	A	C5-C6-N1	7.59	121.49	117.70
55	BB	37	C	N3-C2-O2	-7.59	116.59	121.90
14	AO	88	ARG	NE-CZ-NH1	7.58	124.09	120.30
21	AA	199	A	N1-C6-N6	-7.58	114.05	118.60
21	AA	780	A	C5-C6-N1	7.58	121.49	117.70
41	BS	25	ARG	NE-CZ-NH1	7.58	124.09	120.30
21	AA	1328	C	N3-C2-O2	-7.58	116.59	121.90
54	BA	1531	C	O4'-C1'-N1	7.58	114.27	108.20
54	BA	1247	A	C5-C6-N1	7.58	121.49	117.70
54	BA	937	C	O4'-C1'-N1	7.58	114.26	108.20
54	BA	941	A	C4-C5-C6	-7.58	113.21	117.00
54	BA	1793	C	N3-C2-O2	-7.58	116.59	121.90
21	AA	393	A	C4-C5-C6	-7.58	113.21	117.00
54	BA	1953	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2434	A	C5-C6-N1	7.58	121.49	117.70
47	BY	47	ARG	NE-CZ-NH1	7.57	124.09	120.30
54	BA	149	A	C5-C6-N1	7.57	121.49	117.70
54	BA	265	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	2116	G	N3-C2-N2	-7.57	114.60	119.90
15	AP	28	ARG	NH1-CZ-NH2	-7.57	111.07	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	706	A	C4-C5-C6	-7.57	113.21	117.00
21	AA	59	A	C5-C6-N1	7.57	121.48	117.70
21	AA	74	A	C4-C5-C6	-7.57	113.21	117.00
24	A3	73	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1385	A	C5-C6-N1	7.57	121.48	117.70
21	AA	1317	C	N3-C2-O2	-7.57	116.60	121.90
54	BA	1668	A	C4-C5-C6	-7.57	113.22	117.00
21	AA	523	A	C4-C5-C6	-7.56	113.22	117.00
54	BA	2030	A	C5-C6-N1	7.56	121.48	117.70
54	BA	429	A	C5-C6-N1	7.56	121.48	117.70
20	AU	17	ARG	NE-CZ-NH1	7.56	124.08	120.30
21	AA	1287	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2392	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	892	A	C5-C6-N1	7.56	121.48	117.70
21	AA	1005	A	C4-C5-C6	-7.56	113.22	117.00
24	A3	69	C	P-O3'-C3'	7.56	128.77	119.70
54	BA	1128	G	O4'-C1'-N9	7.56	114.25	108.20
54	BA	2264	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	2433	A	C5-C6-N1	7.56	121.48	117.70
21	AA	246	A	C4-C5-C6	-7.55	113.22	117.00
54	BA	368	A	C4-C5-C6	-7.55	113.22	117.00
54	BA	1299	G	O4'-C1'-N9	7.55	114.24	108.20
21	AA	466	A	C4-C5-C6	-7.55	113.22	117.00
54	BA	973	A	C5-C6-N1	7.55	121.48	117.70
54	BA	2114	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	645	C	N3-C2-O2	-7.55	116.61	121.90
54	BA	920	A	C5-C6-N1	7.55	121.48	117.70
21	AA	706	A	C5-C6-N1	7.55	121.47	117.70
21	AA	1082	A	C5-C6-N1	7.55	121.47	117.70
54	BA	457	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2328	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	2368	C	N3-C2-O2	-7.55	116.61	121.90
21	AA	600	A	C4-C5-C6	-7.55	113.23	117.00
21	AA	718	A	C5-C6-N1	7.55	121.47	117.70
21	AA	1350	A	C4-C5-C6	-7.55	113.23	117.00
54	BA	1114	C	N3-C2-O2	-7.55	116.62	121.90
55	BB	52	A	C5-C6-N1	7.55	121.47	117.70
21	AA	1446	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	961	C	N3-C2-O2	-7.54	116.62	121.90
45	BW	54	ARG	NE-CZ-NH1	7.54	124.07	120.30
54	BA	199	A	C5-C6-N1	7.54	121.47	117.70
21	AA	167	A	C4-C5-C6	-7.54	113.23	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	532	A	C5-C6-N1	7.54	121.47	117.70
21	AA	1462	C	N3-C2-O2	-7.54	116.62	121.90
54	BA	1067	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	2037	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	2247	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	1197	A	C4-C5-C6	-7.53	113.23	117.00
54	BA	900	A	C4-C5-C6	-7.53	113.23	117.00
54	BA	1912	A	C4-C5-C6	-7.53	113.23	117.00
54	BA	2675	A	C5-C6-N1	7.53	121.47	117.70
21	AA	574	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	1810	A	C5-C6-N1	7.53	121.47	117.70
21	AA	465	A	C5-C6-N1	7.53	121.46	117.70
21	AA	1132	C	N3-C2-O2	-7.53	116.63	121.90
54	BA	1362	C	N3-C2-O2	-7.53	116.63	121.90
54	BA	2610	C	N3-C2-O2	-7.53	116.63	121.90
21	AA	408	A	C5-C6-N1	7.53	121.46	117.70
54	BA	1676	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	2327	A	C5-C6-N1	7.53	121.46	117.70
54	BA	1941	C	N3-C2-O2	-7.52	116.63	121.90
21	AA	16	A	C4-C5-C6	-7.52	113.24	117.00
54	BA	742	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2052	A	C5-C6-N1	7.52	121.46	117.70
21	AA	716	A	C5-C6-N1	7.52	121.46	117.70
23	A2	82	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1254	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	1676	A	C5-C6-N1	7.52	121.46	117.70
21	AA	320	A	C4-C5-C6	-7.51	113.24	117.00
21	AA	1256	A	C5-C6-N1	7.51	121.46	117.70
21	AA	1362	A	N1-C6-N6	-7.51	114.09	118.60
33	BK	105	ARG	NE-CZ-NH1	7.51	124.06	120.30
54	BA	1084	A	C4-C5-C6	-7.51	113.24	117.00
21	AA	248	C	N3-C2-O2	-7.51	116.64	121.90
54	BA	1634	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	2095	A	N1-C6-N6	-7.51	114.09	118.60
21	AA	1500	A	C4-C5-C6	-7.51	113.25	117.00
54	BA	2468	A	C5-C6-N1	7.51	121.45	117.70
21	AA	374	A	C5-C6-N1	7.51	121.45	117.70
21	AA	1431	A	C5-C6-N1	7.51	121.45	117.70
54	BA	2092	U	N3-C2-O2	-7.51	116.94	122.20
54	BA	1936	A	C4-C5-C6	-7.50	113.25	117.00
42	BT	6	ARG	NE-CZ-NH1	7.50	124.05	120.30
54	BA	749	A	C5-C6-N1	7.50	121.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2478	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	839	U	O4'-C1'-N1	7.50	114.20	108.20
54	BA	1876	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	1360	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1000	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1156	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1854	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2572	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2835	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2765	A	C5-C6-N1	7.50	121.45	117.70
54	BA	190	A	N1-C6-N6	-7.49	114.10	118.60
21	AA	300	A	C5-C6-N1	7.49	121.45	117.70
54	BA	959	A	C5-C6-N1	7.49	121.44	117.70
54	BA	981	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	1393	A	C4-C5-C6	-7.49	113.25	117.00
4	AE	149	PRO	CA-N-CD	-7.49	101.02	111.50
21	AA	1496	C	N3-C2-O2	-7.49	116.66	121.90
21	AA	327	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	1382	G	O4'-C1'-N9	7.49	114.19	108.20
54	BA	63	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	1489	C	N3-C2-O2	-7.48	116.66	121.90
54	BA	1801	A	C5-C6-N1	7.48	121.44	117.70
54	BA	5	A	C4-C5-C6	-7.48	113.26	117.00
54	BA	1243	C	N3-C2-O2	-7.48	116.67	121.90
54	BA	1603	A	C5-C6-N1	7.48	121.44	117.70
54	BA	2051	A	C4-C5-C6	-7.47	113.26	117.00
21	AA	1180	A	C4-C5-C6	-7.47	113.26	117.00
54	BA	49	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	895	U	O4'-C1'-N1	7.47	114.18	108.20
54	BA	981	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1433	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2886	A	C4-C5-C6	-7.47	113.27	117.00
3	AD	55	ARG	NE-CZ-NH1	7.47	124.03	120.30
21	AA	743	A	C4-C5-C6	-7.47	113.27	117.00
54	BA	1236	G	O4'-C1'-N9	7.47	114.17	108.20
54	BA	1669	A	N1-C6-N6	-7.47	114.12	118.60
21	AA	573	A	C4-C5-C6	-7.47	113.27	117.00
54	BA	1812	U	O4'-C1'-N1	7.47	114.17	108.20
8	AI	121	ARG	NE-CZ-NH1	7.47	124.03	120.30
21	AA	502	A	C5-C6-N1	7.47	121.43	117.70
21	AA	815	A	C5-C6-N1	7.47	121.43	117.70
54	BA	796	C	N3-C2-O2	-7.47	116.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2070	A	C4-C5-C6	-7.47	113.27	117.00
54	BA	2235	G	N1-C6-O6	-7.47	115.42	119.90
16	AQ	5	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	1354	A	C4-C5-C6	-7.46	113.27	117.00
54	BA	1050	A	C5-C6-N1	7.46	121.43	117.70
54	BA	2229	U	O4'-C1'-N1	7.46	114.17	108.20
54	BA	2749	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1493	A	C4-C5-C6	-7.46	113.27	117.00
55	BB	101	A	C5-C6-N1	7.46	121.43	117.70
54	BA	53	A	N1-C6-N6	-7.46	114.13	118.60
54	BA	1490	A	C5-C6-N1	7.46	121.43	117.70
54	BA	687	C	O4'-C1'-N1	7.45	114.16	108.20
54	BA	931	U	O4'-C1'-N1	7.45	114.16	108.20
55	BB	78	A	C4-C5-C6	-7.45	113.27	117.00
21	AA	609	A	C4-C5-C6	-7.45	113.27	117.00
21	AA	900	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	689	A	C4-C5-C6	-7.45	113.28	117.00
54	BA	1032	A	C5-C6-N1	7.45	121.42	117.70
54	BA	945	A	C5-C6-N1	7.45	121.42	117.70
54	BA	2317	A	C4-C5-C6	-7.45	113.28	117.00
24	A3	45	A	C5-C6-N1	7.45	121.42	117.70
54	BA	38	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	217	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	343	C	N3-C2-O2	-7.45	116.69	121.90
54	BA	2750	A	C5-C6-N1	7.44	121.42	117.70
3	AD	2	ARG	NE-CZ-NH1	7.44	124.02	120.30
19	AT	24	ARG	NE-CZ-NH1	7.44	124.02	120.30
21	AA	554	A	N1-C6-N6	-7.44	114.13	118.60
32	BJ	120	ARG	NE-CZ-NH1	7.44	124.02	120.30
54	BA	627	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2385	C	N3-C2-O2	-7.44	116.69	121.90
21	AA	900	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2044	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	2614	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	1146	C	N3-C2-O2	-7.44	116.69	121.90
21	AA	172	A	C5-C6-N1	7.44	121.42	117.70
54	BA	505	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	229	C	N3-C2-O2	-7.43	116.69	121.90
21	AA	223	A	C5-C6-N1	7.43	121.42	117.70
54	BA	9	G	O4'-C1'-N9	7.43	114.15	108.20
54	BA	1551	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	10	A	C5-C6-N1	7.43	121.41	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1229	A	C4-C5-C6	-7.43	113.28	117.00
54	BA	172	A	C4-C5-C6	-7.43	113.29	117.00
54	BA	631	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	2342	C	N3-C2-O2	-7.43	116.70	121.90
21	AA	968	A	C5-C6-N1	7.43	121.41	117.70
30	BH	27	ARG	NE-CZ-NH1	7.43	124.01	120.30
54	BA	1792	G	O4'-C1'-N9	7.43	114.14	108.20
21	AA	1000	A	N1-C6-N6	-7.42	114.14	118.60
54	BA	1967	C	N3-C2-O2	-7.42	116.70	121.90
21	AA	1005	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1363	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1783	A	C4-C5-C6	-7.42	113.29	117.00
21	AA	1145	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	563	A	C5-C6-N1	7.42	121.41	117.70
54	BA	2757	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	226	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	2564	A	C4-C5-C6	-7.42	113.29	117.00
54	BA	2781	A	C4-C5-C6	-7.42	113.29	117.00
54	BA	1788	C	N3-C2-O2	-7.41	116.71	121.90
21	AA	495	A	N1-C6-N6	-7.41	114.15	118.60
15	AP	70	ARG	NE-CZ-NH1	7.41	124.00	120.30
21	AA	1368	A	C5-C6-N1	7.41	121.40	117.70
21	AA	1055	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	689	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	1717	A	C5-C6-N1	7.41	121.40	117.70
22	A1	32	C	N3-C2-O2	-7.41	116.72	121.90
54	BA	522	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	1598	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	2335	A	N1-C6-N6	-7.41	114.16	118.60
21	AA	631	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	1499	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2443	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	499	A	C5-C6-N1	7.40	121.40	117.70
21	AA	576	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	1418	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	1690	A	C5-C6-N1	7.40	121.40	117.70
54	BA	742	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	2516	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	1254	A	C5-C6-N1	7.40	121.40	117.70
21	AA	182	A	C5-C6-N1	7.40	121.40	117.70
21	AA	1045	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	89	A	N1-C6-N6	-7.40	114.16	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1111	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	309	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	1230	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	1791	A	C5-C6-N1	7.39	121.40	117.70
54	BA	2377	A	C5-C6-N1	7.39	121.40	117.70
54	BA	2591	C	N3-C2-O2	-7.39	116.72	121.90
54	BA	2611	C	N3-C2-O2	-7.39	116.72	121.90
21	AA	20	U	O4'-C1'-N1	7.39	114.11	108.20
54	BA	143	C	N3-C2-O2	-7.39	116.73	121.90
54	BA	56	A	C5-C6-N1	7.39	121.39	117.70
21	AA	228	A	C4-C5-C6	-7.39	113.31	117.00
54	BA	718	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	1532	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1821	A	C4-C5-C6	-7.39	113.31	117.00
54	BA	1477	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1754	A	C4-C5-C6	-7.38	113.31	117.00
21	AA	263	A	C5-C6-N1	7.38	121.39	117.70
30	BH	116	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	754	C	N3-C2-O2	-7.38	116.73	121.90
24	A3	62	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	2205	A	N1-C6-N6	-7.38	114.17	118.60
6	AG	77	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	879	C	N3-C2-O2	-7.38	116.74	121.90
54	BA	1736	U	O4'-C1'-N1	7.38	114.10	108.20
4	AE	156	ARG	NE-CZ-NH1	7.37	123.99	120.30
21	AA	475	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	663	A	C5-C6-N1	7.37	121.39	117.70
21	AA	1158	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	765	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	1990	C	O4'-C1'-N1	7.37	114.10	108.20
54	BA	2810	A	C5-C6-N1	7.37	121.39	117.70
21	AA	264	C	N1-C2-O2	7.37	123.32	118.90
54	BA	794	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	920	A	C4-C5-C6	-7.37	113.31	117.00
21	AA	55	A	N1-C6-N6	-7.37	114.18	118.60
35	BM	51	ARG	NE-CZ-NH1	7.37	123.98	120.30
54	BA	2654	A	C5-C6-N1	7.37	121.38	117.70
21	AA	1170	A	N1-C6-N6	-7.37	114.18	118.60
21	AA	393	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1004	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1378	C	N3-C2-O2	-7.36	116.75	121.90
54	BA	128	C	N3-C2-O2	-7.36	116.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	478	A	C5-C6-N1	7.36	121.38	117.70
54	BA	556	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	610	C	O4'-C1'-N1	7.36	114.09	108.20
54	BA	632	A	C4-C5-C6	-7.36	113.32	117.00
54	BA	917	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2287	A	O4'-C1'-N9	7.36	114.09	108.20
21	AA	718	A	N1-C6-N6	-7.36	114.18	118.60
46	BX	2	ARG	NE-CZ-NH2	-7.36	116.62	120.30
54	BA	190	A	C5-C6-N1	7.36	121.38	117.70
54	BA	644	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	1276	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1829	A	C4-C5-C6	-7.36	113.32	117.00
21	AA	694	A	C5-C6-N1	7.36	121.38	117.70
54	BA	611	C	O4'-C1'-N1	7.36	114.08	108.20
54	BA	1453	A	O4'-C1'-N9	7.36	114.09	108.20
54	BA	1996	C	N3-C2-O2	-7.36	116.75	121.90
3	AD	62	ARG	NE-CZ-NH1	7.36	123.98	120.30
54	BA	1596	A	C4-C5-C6	-7.35	113.32	117.00
54	BA	2374	C	N3-C2-O2	-7.35	116.75	121.90
21	AA	749	A	C5-C6-N1	7.35	121.38	117.70
54	BA	181	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2829	A	C4-C5-C6	-7.35	113.32	117.00
40	BR	79	ARG	NE-CZ-NH1	7.35	123.98	120.30
46	BX	49	ARG	NE-CZ-NH1	7.35	123.98	120.30
54	BA	94	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	1641	A	C5-C6-N1	7.35	121.37	117.70
54	BA	2565	A	C5-C6-N1	7.35	121.38	117.70
54	BA	38	A	C4-C5-C6	-7.35	113.33	117.00
54	BA	2434	A	C4-C5-C6	-7.35	113.33	117.00
54	BA	2727	A	C5-C6-N1	7.35	121.37	117.70
25	BC	101	ARG	NE-CZ-NH1	7.34	123.97	120.30
54	BA	1102	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	2084	C	N3-C2-O2	-7.34	116.76	121.90
21	AA	1319	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	531	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	2104	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	2799	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	2809	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	1275	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	1606	C	N3-C2-O2	-7.34	116.77	121.90
54	BA	2587	A	C5-C6-N1	7.33	121.37	117.70
8	AI	32	ARG	NE-CZ-NH1	7.33	123.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	7	A	C5-C6-N1	7.33	121.37	117.70
54	BA	675	A	C5-C6-N1	7.33	121.37	117.70
54	BA	676	A	C5-C6-N1	7.33	121.37	117.70
54	BA	2388	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	294	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	1035	U	O4'-C1'-N1	7.33	114.06	108.20
54	BA	1585	C	O4'-C1'-N1	7.33	114.06	108.20
54	BA	2499	C	O4'-C1'-N1	7.33	114.06	108.20
21	AA	190	A	C4-C5-C6	-7.33	113.34	117.00
21	AA	513	C	N3-C2-O2	-7.33	116.77	121.90
21	AA	1413	A	C5-C6-N1	7.33	121.36	117.70
54	BA	1679	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2762	C	N3-C2-O2	-7.33	116.77	121.90
21	AA	1252	A	C5-C6-N1	7.32	121.36	117.70
54	BA	761	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2135	A	O4'-C1'-N9	7.32	114.06	108.20
54	BA	1419	A	C5-C6-N1	7.32	121.36	117.70
54	BA	315	G	O4'-C1'-N9	7.32	114.06	108.20
54	BA	391	A	C5-C6-N1	7.32	121.36	117.70
54	BA	471	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	2208	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	2212	A	N1-C6-N6	-7.32	114.21	118.60
12	AM	108	ARG	NE-CZ-NH1	7.32	123.96	120.30
21	AA	393	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	182	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	1096	A	C5-C6-N1	7.32	121.36	117.70
21	AA	695	A	C5-C6-N1	7.31	121.36	117.70
21	AA	501	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	2175	C	N3-C2-O2	-7.31	116.78	121.90
3	AD	127	ARG	NE-CZ-NH1	7.31	123.96	120.30
8	AI	84	ARG	NE-CZ-NH1	7.31	123.95	120.30
54	BA	984	A	C5-C6-N1	7.31	121.36	117.70
54	BA	1827	U	O4'-C1'-N1	7.31	114.05	108.20
21	AA	421	U	O4'-C1'-N1	7.31	114.05	108.20
54	BA	1613	G	N1-C6-O6	-7.31	115.52	119.90
54	BA	2829	A	N1-C6-N6	-7.31	114.22	118.60
21	AA	156	C	N3-C2-O2	-7.31	116.79	121.90
21	AA	1081	A	C5-C6-N1	7.31	121.35	117.70
54	BA	620	G	N3-C2-N2	-7.31	114.79	119.90
21	AA	189	A	C5-C6-N1	7.30	121.35	117.70
54	BA	471	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1533	C	N3-C2-O2	-7.30	116.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2062	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2740	A	C4-C5-C6	-7.30	113.35	117.00
21	AA	389	A	N1-C6-N6	-7.30	114.22	118.60
21	AA	1382	C	N3-C2-O2	-7.30	116.79	121.90
54	BA	751	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1954	G	N1-C6-O6	-7.30	115.52	119.90
54	BA	2899	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2114	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2861	U	O4'-C1'-N1	7.30	114.04	108.20
21	AA	1413	A	C4-C5-C6	-7.29	113.35	117.00
54	BA	910	A	C5-C6-N1	7.29	121.35	117.70
54	BA	2137	U	O4'-C1'-N1	7.29	114.04	108.20
54	BA	2428	G	C8-N9-C4	-7.29	103.48	106.40
12	AM	69	ARG	NE-CZ-NH1	7.29	123.95	120.30
21	AA	440	C	N3-C2-O2	-7.29	116.80	121.90
21	AA	878	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	880	C	N3-C2-O2	-7.29	116.80	121.90
21	AA	1319	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1040	A	N1-C6-N6	-7.29	114.22	118.60
54	BA	1045	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	505	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1618	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	2766	A	C5-C6-N1	7.29	121.34	117.70
54	BA	1787	A	N1-C6-N6	-7.29	114.23	118.60
21	AA	1411	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	776	G	O4'-C1'-N9	7.29	114.03	108.20
54	BA	1677	A	N1-C6-N6	-7.29	114.23	118.60
21	AA	382	A	C4-C5-C6	-7.29	113.36	117.00
21	AA	782	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	145	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	2386	A	C4-C5-C6	-7.29	113.36	117.00
22	A1	76	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	129	C	N3-C2-O2	-7.28	116.80	121.90
54	BA	2542	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2340	A	N1-C6-N6	-7.28	114.23	118.60
21	AA	130	A	C5-C6-N1	7.27	121.34	117.70
3	AD	50	TYR	CB-CG-CD2	7.27	125.36	121.00
21	AA	28	A	C4-C5-C6	-7.27	113.36	117.00
21	AA	59	A	C4-C5-C6	-7.27	113.36	117.00
21	AA	363	A	C5-C6-N1	7.27	121.34	117.70
54	BA	1165	A	N1-C6-N6	-7.27	114.24	118.60
54	BA	1966	A	C5-C6-N1	7.27	121.34	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2054	A	C5-C6-N1	7.27	121.34	117.70
54	BA	1431	A	O4'-C1'-N9	7.27	114.02	108.20
54	BA	2322	A	C5-C6-N1	7.27	121.34	117.70
56	B5	162	ARG	NE-CZ-NH1	7.27	123.94	120.30
54	BA	11	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	69	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	1285	A	C4-C5-C6	-7.27	113.37	117.00
54	BA	2022	U	O4'-C1'-N1	7.27	114.01	108.20
54	BA	2726	A	C4-C5-C6	-7.27	113.37	117.00
21	AA	182	A	N1-C6-N6	-7.27	114.24	118.60
21	AA	389	A	C5-C6-N1	7.26	121.33	117.70
21	AA	716	A	N1-C6-N6	-7.26	114.24	118.60
54	BA	1244	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1414	C	N3-C2-O2	-7.26	116.82	121.90
54	BA	2453	A	C4-C5-C6	-7.26	113.37	117.00
21	AA	1022	A	N1-C6-N6	-7.26	114.24	118.60
11	AL	13	ARG	NE-CZ-NH1	7.26	123.93	120.30
19	AT	73	ARG	NE-CZ-NH1	7.26	123.93	120.30
21	AA	238	A	C3'-C2'-C1'	-7.26	95.69	101.50
40	BR	84	ARG	NE-CZ-NH1	7.26	123.93	120.30
54	BA	1794	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2091	C	N1-C2-O2	7.26	123.25	118.90
54	BA	143	C	O4'-C1'-N1	7.26	114.01	108.20
54	BA	352	A	N1-C6-N6	-7.26	114.25	118.60
54	BA	988	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1085	A	C4-C5-C6	-7.26	113.37	117.00
54	BA	1550	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	32	A	C5-C6-N1	7.25	121.33	117.70
37	BO	25	ARG	NE-CZ-NH1	7.25	123.93	120.30
54	BA	2362	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	1404	C	N3-C2-O2	-7.25	116.82	121.90
54	BA	547	A	C5-C6-N1	7.25	121.33	117.70
54	BA	2298	A	C5-C6-N1	7.25	121.33	117.70
21	AA	768	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	1260	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	2665	A	O4'-C1'-N9	7.25	114.00	108.20
21	AA	1054	C	N1-C2-O2	7.25	123.25	118.90
21	AA	1480	A	C4-C5-C6	-7.25	113.38	117.00
39	BQ	57	ARG	NE-CZ-NH1	7.25	123.92	120.30
54	BA	1866	A	C5-C6-N1	7.25	121.32	117.70
54	BA	2104	C	O4'-C1'-N1	7.25	114.00	108.20
54	BA	2602	A	O4'-C1'-N9	7.25	114.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2676	C	N3-C2-O2	-7.25	116.83	121.90
21	AA	1357	A	C5-C6-N1	7.25	121.32	117.70
54	BA	391	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	1979	U	O4'-C1'-N1	7.25	114.00	108.20
54	BA	111	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1545	A	C5-C6-N1	7.24	121.32	117.70
21	AA	179	A	N1-C6-N6	-7.24	114.25	118.60
21	AA	1322	C	N1-C2-O2	7.24	123.24	118.90
54	BA	602	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1253	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	1808	A	O4'-C1'-N9	7.24	113.99	108.20
55	BB	60	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	10	A	C5-C6-N1	7.24	121.32	117.70
54	BA	225	C	O4'-C1'-N1	7.24	113.99	108.20
54	BA	2126	A	C4-C5-C6	-7.24	113.38	117.00
54	BA	2512	C	O4'-C1'-N1	7.24	113.99	108.20
21	AA	602	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	933	A	C5-C6-N1	7.24	121.32	117.70
21	AA	336	A	C5-C6-N1	7.23	121.32	117.70
54	BA	936	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	2738	A	N1-C6-N6	-7.23	114.26	118.60
21	AA	1274	A	C5-C6-N1	7.23	121.32	117.70
21	AA	1412	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	886	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	1757	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	2060	A	C4-C5-C6	-7.23	113.38	117.00
54	BA	1431	A	C5-C6-N1	7.23	121.31	117.70
5	AF	2	ARG	NE-CZ-NH2	-7.23	116.69	120.30
21	AA	52	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	1504	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2052	A	C4-C5-C6	-7.23	113.39	117.00
21	AA	58	C	N3-C2-O2	-7.23	116.84	121.90
21	AA	1503	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2541	A	N1-C6-N6	-7.22	114.27	118.60
21	AA	811	C	N3-C2-O2	-7.22	116.84	121.90
21	AA	85	U	O4'-C1'-N1	7.22	113.98	108.20
21	AA	262	A	C5-C6-N1	7.22	121.31	117.70
21	AA	535	A	C5-C6-N1	7.22	121.31	117.70
21	AA	622	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	669	G	O4'-C1'-N9	7.22	113.98	108.20
54	BA	1357	C	N3-C2-O2	-7.22	116.85	121.90
21	AA	978	A	C5-C6-N1	7.22	121.31	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1553	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	347	A	C5-C6-N1	7.21	121.31	117.70
54	BA	470	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1205	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1735	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1913	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	2288	A	C4-C5-C6	-7.21	113.39	117.00
54	BA	2821	A	N1-C6-N6	-7.21	114.27	118.60
21	AA	162	A	C4-C5-C6	-7.21	113.39	117.00
21	AA	1163	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1151	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	2378	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	2403	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	281	C	N3-C2-O2	-7.21	116.86	121.90
54	BA	849	A	C5-C6-N1	7.21	121.30	117.70
54	BA	146	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	1251	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	1454	C	N3-C2-O2	-7.20	116.86	121.90
21	AA	554	A	C4-C5-C6	-7.20	113.40	117.00
21	AA	924	C	N3-C2-O2	-7.20	116.86	121.90
21	AA	736	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	299	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	2546	U	O4'-C1'-N1	7.20	113.96	108.20
21	AA	1209	C	N3-C2-O2	-7.19	116.86	121.90
54	BA	167	A	C5-C6-N1	7.19	121.30	117.70
54	BA	1952	A	N1-C6-N6	-7.19	114.28	118.60
54	BA	909	A	C5-C6-N1	7.19	121.29	117.70
54	BA	2761	A	C5-C6-N1	7.19	121.29	117.70
54	BA	453	A	C5-C6-N1	7.19	121.29	117.70
54	BA	445	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	1632	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2380	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	2778	A	N1-C6-N6	-7.18	114.29	118.60
18	AS	2	ARG	NE-CZ-NH1	7.18	123.89	120.30
21	AA	169	C	C1'-O4'-C4'	-7.18	104.16	109.90
21	AA	312	C	N3-C2-O2	-7.18	116.87	121.90
21	AA	1016	A	C5-C6-N1	7.18	121.29	117.70
52	B3	12	ARG	NE-CZ-NH1	7.18	123.89	120.30
54	BA	2108	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2175	C	O4'-C1'-N1	7.18	113.95	108.20
21	AA	465	A	O4'-C1'-N9	7.18	113.94	108.20
21	AA	1275	A	N1-C6-N6	-7.18	114.29	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1098	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	1126	A	C5-C6-N1	7.18	121.29	117.70
21	AA	509	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	1250	A	C5-C6-N1	7.18	121.29	117.70
54	BA	572	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	792	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	1502	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	2450	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	2634	A	C5-C6-N1	7.18	121.29	117.70
21	AA	411	A	N1-C6-N6	-7.17	114.30	118.60
21	AA	1236	A	C5-C6-N1	7.17	121.29	117.70
21	AA	1248	A	C4-C5-C6	-7.17	113.41	117.00
54	BA	833	A	C4-C5-C6	-7.17	113.41	117.00
54	BA	1010	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1088	A	C4-C5-C6	-7.17	113.41	117.00
54	BA	1928	A	C5-C6-N1	7.17	121.29	117.70
54	BA	2412	A	N1-C6-N6	-7.17	114.30	118.60
21	AA	78	A	C5-C6-N1	7.17	121.29	117.70
21	AA	215	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	767	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	1496	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	1981	A	C4-C5-C6	-7.17	113.42	117.00
21	AA	913	A	P-O3'-C3'	7.17	128.30	119.70
21	AA	1339	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	323	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	422	C	N1-C2-O2	7.17	123.20	118.90
54	BA	985	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	1990	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	1110	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	911	A	C4-C5-C6	-7.17	113.42	117.00
23	A2	91	A	N1-C6-N6	-7.16	114.30	118.60
54	BA	587	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	2781	A	N1-C6-N6	-7.16	114.30	118.60
54	BA	2045	C	N3-C2-O2	-7.16	116.89	121.90
21	AA	1159	U	C1'-O4'-C4'	-7.16	104.17	109.90
46	BX	44	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	2868	A	C5-C6-N1	7.16	121.28	117.70
6	AG	118	ARG	NE-CZ-NH2	-7.16	116.72	120.30
21	AA	860	A	C4-C5-C6	-7.16	113.42	117.00
25	BC	47	ARG	NE-CZ-NH1	7.16	123.88	120.30
21	AA	217	C	N3-C2-O2	-7.16	116.89	121.90
21	AA	853	C	N3-C2-O2	-7.16	116.89	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	BP	61	ARG	NE-CZ-NH2	-7.16	116.72	120.30
54	BA	2734	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	1011	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	504	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2755	C	C3'-C2'-C1'	7.15	107.22	101.50
8	AI	17	ARG	NE-CZ-NH2	-7.15	116.72	120.30
21	AA	729	A	C4-C5-C6	-7.15	113.42	117.00
21	AA	765	G	O4'-C1'-N9	7.15	113.92	108.20
54	BA	603	A	C4-C5-C6	-7.15	113.42	117.00
54	BA	960	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2761	A	O4'-C1'-N9	7.15	113.92	108.20
22	A1	26	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	1447	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	671	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	1367	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	2439	A	C5-C6-N1	7.15	121.27	117.70
21	AA	1377	A	C5-C6-N1	7.14	121.27	117.70
26	BD	46	ARG	NE-CZ-NH1	7.14	123.87	120.30
54	BA	1953	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	2764	A	C4-C5-C6	-7.14	113.43	117.00
22	A1	28	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	131	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	1070	A	N1-C6-N6	-7.14	114.31	118.60
54	BA	1472	C	N3-C2-O2	-7.14	116.90	121.90
55	BB	3	C	N3-C2-O2	-7.14	116.90	121.90
21	AA	826	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1383	A	C5-C6-N1	7.14	121.27	117.70
54	BA	735	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1549	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	1652	A	N1-C6-N6	-7.14	114.32	118.60
54	BA	1947	C	N3-C2-O2	-7.14	116.90	121.90
21	AA	308	C	N3-C2-O2	-7.14	116.90	121.90
46	BX	17	ARG	NE-CZ-NH1	7.14	123.87	120.30
21	AA	109	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1183	U	O4'-C1'-N1	7.14	113.91	108.20
41	BS	110	ARG	NE-CZ-NH1	7.14	123.87	120.30
54	BA	2267	A	C5-C6-N1	7.14	121.27	117.70
21	AA	40	C	N3-C2-O2	-7.13	116.91	121.90
21	AA	995	C	N3-C2-O2	-7.13	116.91	121.90
22	A1	23	A	C5-C6-N1	7.13	121.27	117.70
54	BA	979	A	N1-C6-N6	-7.13	114.32	118.60
54	BA	2263	C	N3-C2-O2	-7.13	116.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1172	C	N3-C2-O2	-7.13	116.91	121.90
46	BX	56	ARG	NE-CZ-NH1	7.13	123.87	120.30
21	AA	783	C	N3-C2-O2	-7.13	116.91	121.90
21	AA	1226	C	N3-C2-O2	-7.13	116.91	121.90
55	BB	109	A	C5-C6-N1	7.13	121.27	117.70
21	AA	523	A	N1-C6-N6	-7.13	114.32	118.60
54	BA	1877	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	98	A	C4-C5-C6	-7.13	113.44	117.00
21	AA	321	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	1499	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	439	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	1020	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1352	U	N3-C2-O2	-7.13	117.21	122.20
54	BA	1580	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1885	A	C5-C6-N1	7.13	121.26	117.70
21	AA	1203	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	83	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	104	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	1496	A	C5-C6-N1	7.13	121.26	117.70
54	BA	115	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	590	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	820	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2471	A	N1-C6-N6	-7.12	114.33	118.60
51	B2	34	ARG	NE-CZ-NH1	7.12	123.86	120.30
54	BA	528	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	734	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2352	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	76	C	N3-C2-O2	-7.12	116.92	121.90
54	BA	332	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	609	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1304	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1637	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1925	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	996	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1654	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	155	A	C5-C6-N1	7.11	121.26	117.70
21	AA	478	A	N1-C6-N6	-7.11	114.33	118.60
21	AA	792	A	C4-C5-C6	-7.11	113.44	117.00
54	BA	2477	U	O4'-C1'-N1	7.11	113.89	108.20
54	BA	2879	A	N1-C6-N6	-7.11	114.33	118.60
54	BA	456	C	N1-C2-O2	7.11	123.17	118.90
54	BA	2377	A	C4-C5-C6	-7.11	113.44	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1237	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	213	A	C5-C6-N1	7.11	121.25	117.70
54	BA	279	A	N1-C6-N6	-7.11	114.33	118.60
21	AA	1140	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	2309	A	N1-C6-N6	-7.11	114.34	118.60
21	AA	1394	A	C4-C5-C6	-7.11	113.45	117.00
54	BA	118	A	C4-C5-C6	-7.11	113.45	117.00
24	A3	59	A	C4-C5-C6	-7.10	113.45	117.00
21	AA	651	C	N3-C2-O2	-7.10	116.93	121.90
25	BC	237	ARG	NE-CZ-NH1	7.10	123.85	120.30
33	BK	78	ARG	NE-CZ-NH1	7.10	123.85	120.30
21	AA	411	A	C4-C5-C6	-7.10	113.45	117.00
21	AA	1066	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	1554	U	O4'-C1'-N1	7.10	113.88	108.20
24	A3	68	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	632	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	2073	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	699	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	2820	A	C5-C6-N1	7.10	121.25	117.70
21	AA	431	A	N1-C6-N6	-7.09	114.34	118.60
21	AA	1261	A	C5-C6-N1	7.09	121.25	117.70
25	BC	12	ARG	NE-CZ-NH1	7.09	123.85	120.30
54	BA	1801	A	N1-C6-N6	-7.09	114.34	118.60
9	AJ	68	ARG	NE-CZ-NH2	-7.09	116.75	120.30
21	AA	5	U	O4'-C1'-N1	7.09	113.87	108.20
54	BA	1591	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	2336	A	N1-C6-N6	-7.09	114.35	118.60
55	BB	104	A	N1-C6-N6	-7.09	114.35	118.60
1	AB	221	ARG	NE-CZ-NH1	7.09	123.84	120.30
21	AA	994	A	C5-C6-N1	7.09	121.24	117.70
56	B5	164	ARG	NE-CZ-NH1	7.09	123.84	120.30
34	BL	21	ARG	NE-CZ-NH1	7.08	123.84	120.30
54	BA	1469	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	2634	A	N1-C6-N6	-7.08	114.35	118.60
55	BB	66	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	1833	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	2552	U	O4'-C1'-N1	7.08	113.86	108.20
21	AA	1146	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1579	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2705	A	N1-C6-N6	-7.08	114.35	118.60
21	AA	277	C	N3-C2-O2	-7.08	116.94	121.90
51	B2	21	ARG	NE-CZ-NH1	7.08	123.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	9	G	N1-C6-O6	-7.08	115.65	119.90
54	BA	1787	A	C5-C6-N1	7.08	121.24	117.70
21	AA	120	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	233	C	N3-C2-O2	-7.08	116.95	121.90
21	AA	279	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	583	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	1042	A	C5-C6-N1	7.08	121.24	117.70
24	A3	22	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1879	C	N3-C2-O2	-7.08	116.95	121.90
54	BA	2527	C	N3-C2-O2	-7.08	116.95	121.90
54	BA	2679	A	N1-C6-N6	-7.08	114.35	118.60
21	AA	98	A	C5-C6-N1	7.07	121.24	117.70
54	BA	439	A	C5-C6-N1	7.07	121.24	117.70
54	BA	1181	U	O4'-C1'-N1	7.07	113.86	108.20
55	BB	73	A	C4-C5-C6	-7.07	113.46	117.00
21	AA	119	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	174	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	435	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	660	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	2794	C	N3-C2-O2	-7.07	116.95	121.90
24	A3	36	A	N1-C6-N6	-7.07	114.36	118.60
25	BC	68	ARG	NE-CZ-NH1	7.07	123.83	120.30
54	BA	299	A	C4-C5-C6	-7.07	113.47	117.00
54	BA	502	A	C5-C6-N1	7.07	121.23	117.70
21	AA	816	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	1575	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	2715	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	815	A	C4-C5-C6	-7.06	113.47	117.00
21	AA	1318	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2710	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	456	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	140	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	1452	C	P-O3'-C3'	7.06	128.17	119.70
54	BA	861	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1142	A	C4-C5-C6	-7.06	113.47	117.00
55	BB	47	C	O4'-C1'-N1	7.06	113.85	108.20
54	BA	1815	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2716	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	344	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1553	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	165	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	1244	A	N1-C6-N6	-7.05	114.37	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1655	A	C5-C6-N1	7.05	121.23	117.70
21	AA	559	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1822	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	731	C	N3-C2-O2	-7.05	116.97	121.90
55	BB	45	A	C5-C6-N1	7.05	121.22	117.70
21	AA	919	A	C5-C6-N1	7.05	121.22	117.70
54	BA	244	A	C5-C6-N1	7.05	121.22	117.70
54	BA	461	C	O4'-C1'-N1	7.05	113.84	108.20
54	BA	2518	A	N1-C6-N6	-7.05	114.37	118.60
9	AJ	31	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	1095	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2297	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2338	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	106	C	N3-C2-O2	-7.04	116.97	121.90
33	BK	31	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	272	A	C5-C6-N1	7.04	121.22	117.70
21	AA	509	A	C5-C6-N1	7.03	121.22	117.70
21	AA	907	A	C5-C6-N1	7.03	121.22	117.70
21	AA	1035	A	N1-C6-N6	-7.03	114.38	118.60
24	A3	14	A	N1-C6-N6	-7.03	114.38	118.60
35	BM	18	ARG	NE-CZ-NH1	7.03	123.82	120.30
54	BA	1434	A	O4'-C1'-N9	7.03	113.83	108.20
54	BA	1606	C	N1-C2-O2	7.03	123.12	118.90
28	BF	109	ARG	NE-CZ-NH1	7.03	123.82	120.30
54	BA	2173	A	C4-C5-C6	-7.03	113.48	117.00
21	AA	1191	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	1749	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	2654	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	840	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1383	A	C4-C5-C6	-7.03	113.49	117.00
21	AA	175	C	N3-C2-O2	-7.02	116.98	121.90
54	BA	838	C	N3-C2-O2	-7.02	116.98	121.90
21	AA	915	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	218	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	699	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	1866	A	N1-C6-N6	-7.02	114.39	118.60
21	AA	149	A	C4-C5-C6	-7.02	113.49	117.00
21	AA	109	A	N1-C6-N6	-7.02	114.39	118.60
21	AA	937	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	928	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1085	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	2006	C	N3-C2-O2	-7.02	116.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	886	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1977	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	2406	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	523	C	N3-C2-O2	-7.02	116.99	121.90
30	BH	123	ARG	NE-CZ-NH1	7.01	123.81	120.30
54	BA	1522	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1805	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2094	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1274	A	C5-C6-N1	7.01	121.21	117.70
54	BA	2433	A	C4-C5-C6	-7.01	113.49	117.00
21	AA	1195	C	N3-C2-O2	-7.01	116.99	121.90
24	A3	11	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1008	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2352	A	C4-C5-C6	-7.01	113.50	117.00
21	AA	1289	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	228	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	661	A	C5-C6-N1	7.01	121.20	117.70
54	BA	802	A	C4-C5-C6	-7.01	113.50	117.00
54	BA	2099	U	N3-C2-O2	-7.01	117.29	122.20
54	BA	2635	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2860	A	C4-C5-C6	-7.01	113.50	117.00
54	BA	1140	C	O4'-C1'-N1	7.01	113.81	108.20
21	AA	696	A	C5-C6-N1	7.01	121.20	117.70
21	AA	756	C	N3-C2-O2	-7.01	117.00	121.90
34	BL	60	ARG	NE-CZ-NH1	7.01	123.80	120.30
54	BA	541	A	C4-C5-C6	-7.01	113.50	117.00
54	BA	942	G	N3-C2-N2	-7.01	115.00	119.90
54	BA	1571	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2247	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2275	C	N3-C2-O2	-7.01	117.00	121.90
21	AA	932	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2162	G	C8-N9-C4	-7.00	103.60	106.40
54	BA	1257	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2558	C	N3-C2-O2	-7.00	117.00	121.90
18	AS	77	ARG	NE-CZ-NH1	7.00	123.80	120.30
21	AA	1196	A	C5-C6-N1	7.00	121.20	117.70
54	BA	693	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1562	U	O4'-C1'-N1	7.00	113.80	108.20
3	AD	153	ARG	NE-CZ-NH1	7.00	123.80	120.30
54	BA	1804	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2183	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	2507	C	N3-C2-O2	-7.00	117.00	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	431	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	192	C	N1-C2-O2	7.00	123.10	118.90
55	BB	58	A	C5-C6-N1	7.00	121.20	117.70
21	AA	931	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	996	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	1046	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1937	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2295	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2531	A	C5-C6-N1	7.00	121.20	117.70
55	BB	80	U	O4'-C1'-N1	7.00	113.80	108.20
21	AA	715	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1655	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	2482	A	C5-C6-N1	7.00	121.20	117.70
8	AI	123	ARG	NE-CZ-NH1	6.99	123.80	120.30
21	AA	1271	A	C5-C6-N1	6.99	121.20	117.70
54	BA	433	C	N3-C2-O2	-6.99	117.00	121.90
54	BA	1700	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	2117	A	C5-C6-N1	6.99	121.20	117.70
54	BA	2520	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	1596	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1985	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	2094	A	N1-C6-N6	-6.99	114.41	118.60
21	AA	1219	A	C5-C6-N1	6.99	121.19	117.70
54	BA	602	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	1039	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1322	A	C5-C6-N1	6.99	121.19	117.70
54	BA	302	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	155	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	1393	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2019	A	C5-C6-N1	6.99	121.19	117.70
54	BA	126	A	C5-C6-N1	6.98	121.19	117.70
54	BA	844	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	800	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	1266	G	O4'-C1'-N9	6.98	113.78	108.20
54	BA	1268	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	2670	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2727	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	1714	U	O4'-C1'-N1	6.98	113.78	108.20
54	BA	41	C	N3-C2-O2	-6.98	117.02	121.90
54	BA	1711	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	2025	C	N1-C2-O2	6.98	123.09	118.90
54	BA	2503	A	N1-C6-N6	-6.98	114.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	699	A	C5-C6-N1	6.98	121.19	117.70
21	AA	65	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	207	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	629	A	C5-C6-N1	6.97	121.19	117.70
54	BA	131	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	262	A	C5-C6-N1	6.97	121.19	117.70
54	BA	721	A	C5-C6-N1	6.97	121.19	117.70
54	BA	743	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	1701	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2788	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	1179	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1439	A	C4-C5-C6	-6.97	113.51	117.00
54	BA	2020	A	C5-C6-N1	6.97	121.19	117.70
54	BA	821	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1472	C	N1-C2-O2	6.97	123.08	118.90
54	BA	1780	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	990	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	156	A	C5-C6-N1	6.97	121.19	117.70
54	BA	698	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2350	C	N3-C2-O2	-6.97	117.02	121.90
55	BB	110	C	N3-C2-O2	-6.97	117.02	121.90
5	AF	44	ARG	NE-CZ-NH1	6.97	123.78	120.30
12	AM	112	ARG	NE-CZ-NH1	6.97	123.78	120.30
21	AA	607	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	622	A	C5-C6-N1	6.97	121.18	117.70
54	BA	251	A	C5-C6-N1	6.97	121.18	117.70
54	BA	1304	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	192	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1054	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	2225	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	766	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1246	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	53	A	C5-C6-N1	6.96	121.18	117.70
54	BA	197	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	1251	A	C5-C6-N1	6.96	121.18	117.70
24	A3	72	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	299	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1269	A	N1-C6-N6	-6.96	114.43	118.60
3	AD	43	ARG	NE-CZ-NH1	6.96	123.78	120.30
21	AA	298	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	374	A	C5-C6-N1	6.96	121.18	117.70
54	BA	444	C	O4'-C1'-N1	6.96	113.76	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	474	G	O4'-C1'-N9	6.96	113.76	108.20
54	BA	1213	A	C5-C6-N1	6.96	121.18	117.70
21	AA	564	C	N3-C2-O2	-6.95	117.03	121.90
22	A1	71	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	63	A	C4-C5-C6	-6.95	113.52	117.00
54	BA	323	C	C3'-C2'-C1'	6.95	107.06	101.50
54	BA	2198	A	C5-C6-N1	6.95	121.18	117.70
20	AU	20	ARG	NE-CZ-NH1	6.95	123.78	120.30
21	AA	738	C	N3-C2-O2	-6.95	117.03	121.90
22	A1	72	C	N3-C2-O2	-6.95	117.03	121.90
50	B1	5	ARG	NE-CZ-NH1	6.95	123.78	120.30
54	BA	1020	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	1974	C	N3-C2-O2	-6.95	117.03	121.90
21	AA	325	A	C5-C6-N1	6.95	121.17	117.70
54	BA	791	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	1760	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	1927	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2698	U	O4'-C1'-N1	6.95	113.76	108.20
54	BA	886	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	381	C	N3-C2-O2	-6.95	117.04	121.90
21	AA	959	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2427	C	N3-C2-O2	-6.95	117.04	121.90
21	AA	1375	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	1327	A	C5-C6-N1	6.94	121.17	117.70
54	BA	587	C	N1-C2-O2	6.94	123.06	118.90
54	BA	1722	A	N1-C6-N6	-6.94	114.44	118.60
54	BA	2793	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	345	C	N1-C2-O2	6.94	123.06	118.90
48	BZ	44	ARG	NE-CZ-NH1	6.94	123.77	120.30
54	BA	71	A	C4-C5-C6	-6.94	113.53	117.00
1	AB	20	ARG	NE-CZ-NH1	6.94	123.77	120.30
21	AA	643	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	1037	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	472	A	C5-C6-N1	6.94	121.17	117.70
54	BA	591	U	O4'-C1'-N1	6.94	113.75	108.20
54	BA	983	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1675	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	1332	A	N1-C6-N6	-6.94	114.44	118.60
22	A1	14	A	C5-C6-N1	6.94	121.17	117.70
54	BA	2008	C	N3-C2-O2	-6.94	117.05	121.90
54	BA	2153	C	N3-C2-O2	-6.94	117.05	121.90
21	AA	353	A	O4'-C1'-N9	6.93	113.75	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	26	A	C5-C6-N1	6.93	121.17	117.70
21	AA	889	A	C4-C5-C6	-6.93	113.53	117.00
24	A3	14	A	C5-C6-N1	6.93	121.17	117.70
54	BA	806	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	1548	A	C5-C6-N1	6.93	121.17	117.70
54	BA	2629	U	O4'-C1'-N1	6.93	113.75	108.20
25	BC	155	ARG	NE-CZ-NH1	6.93	123.76	120.30
54	BA	1890	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	2767	C	N3-C2-O2	-6.93	117.05	121.90
38	BP	102	ARG	NE-CZ-NH1	6.93	123.76	120.30
54	BA	2883	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	1000	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2009	A	C5-C6-N1	6.92	121.16	117.70
21	AA	1012	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	819	A	N1-C6-N6	-6.92	114.45	118.60
21	AA	790	A	C4-C5-C6	-6.92	113.54	117.00
11	AL	98	ARG	NE-CZ-NH1	6.92	123.76	120.30
21	AA	901	A	C5-C6-N1	6.92	121.16	117.70
21	AA	1427	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	878	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	1832	C	N1-C2-O2	6.92	123.05	118.90
21	AA	746	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	908	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	1155	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1307	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2225	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2418	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2420	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	599	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	1689	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	1805	A	C5-C6-N1	6.92	121.16	117.70
54	BA	294	A	C4-C5-C6	-6.91	113.54	117.00
54	BA	1373	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	1626	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1956	U	C5-C6-N1	-6.91	119.24	122.70
55	BB	59	A	C5-C6-N1	6.91	121.16	117.70
54	BA	685	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	1586	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1944	U	O4'-C1'-N1	6.91	113.73	108.20
54	BA	1998	A	C5-C6-N1	6.91	121.16	117.70
54	BA	2499	C	N1-C2-O2	6.91	123.05	118.90
13	AN	13	ARG	NE-CZ-NH1	6.91	123.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2471	A	C5-C6-N1	6.91	121.15	117.70
21	AA	936	C	N3-C2-O2	-6.91	117.07	121.90
54	BA	2227	A	C4-C5-C6	-6.91	113.55	117.00
21	AA	767	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1092	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	1140	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	2117	A	O4'-C1'-N9	6.90	113.72	108.20
54	BA	1997	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	2635	A	C4-C5-C6	-6.90	113.55	117.00
55	BB	113	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	404	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1143	A	C5-C6-N1	6.90	121.15	117.70
21	AA	315	A	N1-C6-N6	-6.90	114.46	118.60
54	BA	1169	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2855	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	2799	A	O4'-C1'-N9	6.90	113.72	108.20
54	BA	2813	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1078	U	C1'-O4'-C4'	-6.89	104.39	109.90
55	BB	45	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	925	A	C5-C6-N1	6.89	121.15	117.70
54	BA	1331	G	N1-C6-O6	-6.89	115.77	119.90
21	AA	306	A	C5-C6-N1	6.89	121.15	117.70
21	AA	977	A	C4-C5-C6	-6.89	113.55	117.00
21	AA	1141	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	33	A	C4-C5-C6	-6.89	113.56	117.00
40	BR	80	ARG	NE-CZ-NH1	6.89	123.75	120.30
54	BA	1266	G	N3-C4-C5	-6.89	125.16	128.60
55	BB	19	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	2326	C	N1-C2-O2	6.89	123.03	118.90
54	BA	315	G	N1-C6-O6	-6.89	115.77	119.90
54	BA	1336	A	C4-C5-C6	-6.89	113.56	117.00
21	AA	1168	U	N3-C2-O2	-6.88	117.38	122.20
22	A1	11	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	1043	C	N1-C2-O2	6.88	123.03	118.90
54	BA	1605	C	N3-C2-O2	-6.88	117.08	121.90
12	AM	92	ARG	NE-CZ-NH1	6.88	123.74	120.30
21	AA	949	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	742	G	N1-C6-O6	-6.88	115.77	119.90
54	BA	1009	A	O4'-C1'-N9	6.88	113.70	108.20
54	BA	643	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2342	C	O4'-C1'-N1	6.88	113.70	108.20
54	BA	2432	A	O4'-C1'-N9	6.88	113.70	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2602	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2723	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	222	C	N3-C2-O2	-6.88	117.09	121.90
21	AA	448	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	337	C	N3-C2-O2	-6.88	117.09	121.90
21	AA	1126	U	N3-C2-O2	-6.88	117.39	122.20
54	BA	2335	A	C4-C5-C6	-6.88	113.56	117.00
4	AE	137	ARG	NE-CZ-NH1	6.87	123.74	120.30
21	AA	1524	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	11	C	N1-C2-O2	6.87	123.02	118.90
54	BA	378	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1189	A	C5-C6-N1	6.87	121.14	117.70
54	BA	1357	C	O4'-C1'-N1	6.87	113.70	108.20
54	BA	1977	A	C5-C6-N1	6.87	121.14	117.70
54	BA	2255	G	N1-C6-O6	-6.87	115.78	119.90
54	BA	2300	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	1433	A	N1-C6-N6	-6.87	114.48	118.60
21	AA	1469	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1398	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	1344	C	N1-C2-O2	6.87	123.02	118.90
24	A3	11	A	N1-C6-N6	-6.87	114.48	118.60
54	BA	764	A	O4'-C1'-N9	6.87	113.69	108.20
21	AA	175	C	O4'-C1'-N1	6.87	113.69	108.20
54	BA	623	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1328	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1889	A	C5-C6-N1	6.87	121.13	117.70
21	AA	563	A	C5-C6-N1	6.87	121.13	117.70
54	BA	2711	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	2733	A	C4-C5-C6	-6.87	113.57	117.00
21	AA	1208	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	1320	C	N1-C2-O2	6.86	123.02	118.90
28	BF	147	ARG	NE-CZ-NH1	6.86	123.73	120.30
36	BN	96	ARG	NE-CZ-NH1	6.86	123.73	120.30
54	BA	164	C	N3-C2-O2	-6.86	117.10	121.90
25	BC	100	ARG	NE-CZ-NH1	6.86	123.73	120.30
55	BB	78	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1345	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2146	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	866	C	O4'-C1'-N1	6.86	113.68	108.20
54	BA	84	A	C5-C6-N1	6.86	121.13	117.70
54	BA	216	A	N1-C6-N6	-6.86	114.49	118.60
54	BA	1134	A	C4-C5-C6	-6.86	113.57	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2147	A	C5-C6-N1	6.86	121.13	117.70
21	AA	946	A	N1-C6-N6	-6.85	114.49	118.60
54	BA	2227	A	N1-C6-N6	-6.85	114.49	118.60
16	AQ	10	ARG	NE-CZ-NH1	6.85	123.73	120.30
21	AA	596	A	N1-C6-N6	-6.85	114.49	118.60
28	BF	177	ARG	NE-CZ-NH2	6.85	123.73	120.30
51	B2	33	ARG	NE-CZ-NH1	6.85	123.73	120.30
54	BA	644	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	2174	C	N3-C2-O2	-6.85	117.10	121.90
2	AC	163	ARG	NE-CZ-NH1	6.85	123.72	120.30
21	AA	81	A	C4-C5-C6	-6.85	113.58	117.00
21	AA	840	C	N3-C2-O2	-6.85	117.10	121.90
22	A1	73	A	C4-C5-C6	-6.85	113.58	117.00
54	BA	899	A	C5-C6-N1	6.85	121.12	117.70
54	BA	345	A	C5-C6-N1	6.85	121.12	117.70
54	BA	412	A	C5-C6-N1	6.85	121.12	117.70
54	BA	2542	A	C4-C5-C6	-6.85	113.58	117.00
54	BA	2572	A	C4-C5-C6	-6.85	113.58	117.00
10	AK	12	ARG	NE-CZ-NH1	6.85	123.72	120.30
21	AA	962	C	N3-C2-O2	-6.85	117.11	121.90
21	AA	1441	A	C4-C5-C6	-6.85	113.58	117.00
24	A3	36	A	C4-C5-C6	-6.85	113.58	117.00
24	A3	59	A	N1-C6-N6	-6.85	114.49	118.60
21	AA	67	C	N3-C2-O2	-6.85	117.11	121.90
54	BA	710	U	O4'-C1'-N1	6.85	113.68	108.20
54	BA	1630	A	C4-C5-C6	-6.85	113.58	117.00
21	AA	267	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1147	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1689	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1890	A	C5-C6-N1	6.84	121.12	117.70
37	BO	33	ARG	NE-CZ-NH2	6.84	123.72	120.30
54	BA	449	A	N1-C6-N6	-6.84	114.49	118.60
21	AA	676	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1281	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	1289	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1332	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2498	C	N1-C2-O2	6.84	123.00	118.90
54	BA	2875	C	N3-C2-O2	-6.84	117.11	121.90
20	AU	30	GLU	C-N-CA	6.84	138.80	121.70
21	AA	539	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	641	U	O4'-C1'-N1	6.84	113.67	108.20
54	BA	2094	A	C4-C5-C6	-6.84	113.58	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	519	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	800	A	C5-C6-N1	6.84	121.12	117.70
54	BA	580	U	O4'-C1'-N1	6.83	113.67	108.20
54	BA	2469	A	C5-C6-N1	6.83	121.12	117.70
21	AA	523	A	C5-C6-N1	6.83	121.12	117.70
21	AA	753	A	C5-C6-N1	6.83	121.11	117.70
21	AA	1036	A	C4-C5-C6	-6.83	113.58	117.00
24	A3	29	C	N3-C2-O2	-6.83	117.12	121.90
32	BJ	116	ARG	NE-CZ-NH1	6.83	123.72	120.30
54	BA	1762	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2738	A	C4-C5-C6	-6.83	113.58	117.00
21	AA	908	A	C5-C6-N1	6.83	121.11	117.70
21	AA	1186	G	N3-C2-N2	-6.83	115.12	119.90
54	BA	2581	G	O4'-C1'-N9	6.83	113.66	108.20
54	BA	2809	A	C5-C6-N1	6.83	121.11	117.70
21	AA	1278	G	N3-C2-N2	-6.83	115.12	119.90
54	BA	146	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	514	A	C5-C6-N1	6.83	121.11	117.70
54	BA	861	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	1226	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	2038	G	O4'-C1'-N9	6.83	113.66	108.20
54	BA	2576	G	N3-C2-N2	-6.83	115.12	119.90
21	AA	764	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	428	A	C5-C6-N1	6.82	121.11	117.70
54	BA	817	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	1044	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	1335	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	2176	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	2873	A	C5-C6-N1	6.82	121.11	117.70
4	AE	111	ARG	NE-CZ-NH1	6.82	123.71	120.30
21	AA	383	A	C4-C5-C6	-6.82	113.59	117.00
41	BS	8	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	16	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	582	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	917	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	2741	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	2282	G	N9-C4-C5	6.82	108.13	105.40
54	BA	2893	A	N1-C6-N6	-6.82	114.51	118.60
21	AA	280	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	992	U	O4'-C1'-N1	6.82	113.65	108.20
54	BA	2079	U	O4'-C1'-N1	6.82	113.65	108.20
21	AA	566	G	C5-C6-N1	6.82	114.91	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1071	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	1214	C	N1-C2-O2	6.82	122.99	118.90
21	AA	1344	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	2530	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1014	A	C5-C6-N1	6.81	121.11	117.70
6	AG	142	ARG	NE-CZ-NH1	6.81	123.71	120.30
21	AA	214	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	675	A	C5-C6-N1	6.81	121.11	117.70
21	AA	807	A	C5-C6-N1	6.81	121.11	117.70
21	AA	1229	A	N1-C6-N6	-6.81	114.51	118.60
22	A1	76	A	C5-C6-N1	6.81	121.11	117.70
54	BA	982	C	C6-N1-C2	-6.81	117.58	120.30
54	BA	2829	A	C5-C6-N1	6.81	121.10	117.70
8	AI	108	ARG	NE-CZ-NH1	6.81	123.70	120.30
23	A2	80	C	N3-C4-C5	6.81	124.62	121.90
54	BA	782	A	C5-C6-N1	6.81	121.10	117.70
54	BA	1323	C	N3-C2-O2	-6.81	117.14	121.90
54	BA	1453	A	N1-C6-N6	-6.81	114.52	118.60
54	BA	1556	C	N1-C2-O2	6.81	122.98	118.90
54	BA	2169	A	C5-C6-N1	6.81	121.10	117.70
54	BA	1558	C	N1-C2-O2	6.80	122.98	118.90
54	BA	1664	A	N1-C6-N6	-6.80	114.52	118.60
24	A3	17	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	160	A	C5-C6-N1	6.80	121.10	117.70
54	BA	217	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2059	A	C4-C5-C6	-6.80	113.60	117.00
55	BB	108	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	85	U	N3-C2-O2	-6.80	117.44	122.20
54	BA	116	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	182	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2324	U	O4'-C1'-N1	6.80	113.64	108.20
1	AB	73	ARG	NE-CZ-NH1	6.80	123.70	120.30
54	BA	1706	C	O4'-C1'-N1	6.80	113.64	108.20
21	AA	1394	A	C5-C6-N1	6.80	121.10	117.70
51	B2	19	ARG	NE-CZ-NH1	6.80	123.70	120.30
54	BA	330	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1725	U	O4'-C1'-N1	6.80	113.64	108.20
54	BA	866	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	1558	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	1237	A	C5-C6-N1	6.79	121.10	117.70
54	BA	2009	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	2416	C	N3-C2-O2	-6.79	117.14	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	964	A	C5-C6-N1	6.79	121.10	117.70
18	AS	80	ARG	NE-CZ-NH1	6.79	123.69	120.30
54	BA	1583	A	N1-C6-N6	-6.79	114.53	118.60
54	BA	1578	U	O4'-C1'-N1	6.79	113.63	108.20
21	AA	396	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	533	A	C5-C6-N1	6.79	121.09	117.70
54	BA	398	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	1039	A	N1-C6-N6	-6.79	114.53	118.60
54	BA	1932	A	C5-C6-N1	6.79	121.09	117.70
21	AA	1377	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	52	A	C5-C6-N1	6.78	121.09	117.70
54	BA	634	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	1685	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	1340	A	N1-C6-N6	-6.78	114.53	118.60
52	B3	44	ARG	NE-CZ-NH1	6.78	123.69	120.30
54	BA	218	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2082	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	1397	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	213	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	343	C	N1-C2-O2	6.78	122.97	118.90
54	BA	1086	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2266	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2789	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	1329	A	C5-C6-N1	6.78	121.09	117.70
54	BA	554	U	O4'-C1'-N1	6.78	113.62	108.20
54	BA	556	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1183	U	O4'-C1'-N1	6.78	113.62	108.20
54	BA	1672	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2856	A	C4-C5-C6	-6.78	113.61	117.00
55	BB	99	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1014	A	N1-C6-N6	-6.78	114.53	118.60
54	BA	2070	A	C5-C6-N1	6.78	121.09	117.70
21	AA	250	A	C5-C6-N1	6.77	121.09	117.70
54	BA	67	U	O4'-C1'-N1	6.77	113.62	108.20
54	BA	2814	A	C4-C5-C6	-6.77	113.61	117.00
21	AA	120	A	C5-C6-N1	6.77	121.08	117.70
21	AA	592	G	O4'-C1'-N9	6.77	113.62	108.20
21	AA	1036	A	C5-C6-N1	6.77	121.08	117.70
54	BA	2433	A	N1-C6-N6	-6.77	114.54	118.60
54	BA	626	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	2660	A	N1-C6-N6	-6.77	114.54	118.60
21	AA	1363	A	C4-C5-C6	-6.77	113.62	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	334	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	421	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	892	A	C4-C5-C6	-6.77	113.62	117.00
21	AA	1285	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1485	U	O4'-C1'-N1	6.77	113.61	108.20
54	BA	2566	A	C5-C6-N1	6.77	121.08	117.70
3	AD	103	ARG	NE-CZ-NH1	6.76	123.68	120.30
21	AA	147	G	C5-C6-N1	6.76	114.88	111.50
21	AA	451	A	P-O3'-C3'	6.76	127.82	119.70
54	BA	1532	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1595	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	2547	A	C5-C6-N1	6.76	121.08	117.70
21	AA	392	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	2632	A	N1-C6-N6	-6.76	114.54	118.60
40	BR	21	ARG	NE-CZ-NH1	6.76	123.68	120.30
54	BA	1043	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	28	A	N1-C6-N6	-6.76	114.55	118.60
34	BL	59	ARG	NE-CZ-NH1	6.76	123.68	120.30
56	B5	7	ARG	NE-CZ-NH1	6.76	123.68	120.30
6	AG	78	ARG	NE-CZ-NH1	6.76	123.68	120.30
21	AA	435	A	C5-C6-N1	6.76	121.08	117.70
54	BA	575	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1027	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1367	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1210	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	1363	A	O4'-C1'-N9	6.75	113.60	108.20
54	BA	95	A	C5-C6-N1	6.75	121.08	117.70
54	BA	130	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	2827	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	1586	A	N1-C6-N6	-6.75	114.55	118.60
54	BA	221	A	C5-C6-N1	6.75	121.07	117.70
54	BA	581	C	N3-C2-O2	-6.75	117.18	121.90
54	BA	1480	C	O4'-C1'-N1	6.75	113.60	108.20
54	BA	300	A	C4-C5-C6	-6.75	113.63	117.00
54	BA	595	C	N3-C2-O2	-6.75	117.18	121.90
54	BA	899	A	N1-C6-N6	-6.75	114.55	118.60
9	AJ	16	ARG	NE-CZ-NH1	6.75	123.67	120.30
24	A3	60	A	C5-C6-N1	6.75	121.07	117.70
54	BA	885	C	N3-C2-O2	-6.75	117.18	121.90
17	AR	52	ARG	NE-CZ-NH1	6.74	123.67	120.30
54	BA	1870	C	N1-C2-O2	6.74	122.94	118.90
21	AA	489	C	N3-C2-O2	-6.74	117.18	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2331	G	C5-C6-N1	6.74	114.87	111.50
55	BB	113	C	N1-C2-O2	6.74	122.94	118.90
20	AU	16	ARG	NE-CZ-NH1	6.74	123.67	120.30
21	AA	8	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1180	A	C5-C6-N1	6.74	121.07	117.70
54	BA	492	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1551	A	C5-C6-N1	6.74	121.07	117.70
54	BA	208	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	2014	A	C5-C6-N1	6.73	121.07	117.70
54	BA	2353	G	N3-C2-N2	-6.73	115.19	119.90
54	BA	2422	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1070	A	C5-C6-N1	6.73	121.07	117.70
55	BB	71	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2396	G	C8-N9-C4	-6.73	103.71	106.40
54	BA	2649	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	670	A	P-O3'-C3'	6.73	127.77	119.70
54	BA	1635	A	C5-C6-N1	6.73	121.06	117.70
54	BA	2268	A	N1-C6-N6	-6.73	114.56	118.60
55	BB	8	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	1179	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	680	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1118	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1638	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2298	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	2478	A	C5-C6-N1	6.73	121.06	117.70
54	BA	2883	A	C4-C5-C6	-6.73	113.64	117.00
30	BH	97	ARG	NE-CZ-NH1	6.73	123.66	120.30
21	AA	784	A	C4-C5-C6	-6.72	113.64	117.00
40	BR	78	ARG	NE-CZ-NH1	6.72	123.66	120.30
54	BA	1525	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	2173	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2712	C	N3-C2-O2	-6.72	117.19	121.90
21	AA	545	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	1520	U	O4'-C1'-N1	6.72	113.58	108.20
21	AA	401	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	201	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	1362	C	O4'-C1'-N1	6.72	113.58	108.20
21	AA	635	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	574	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	2165	C	N3-C2-O2	-6.72	117.20	121.90
38	BP	100	ARG	NE-CZ-NH1	6.71	123.66	120.30
54	BA	919	U	O4'-C1'-N1	6.71	113.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1194	A	C5-C6-N1	6.71	121.06	117.70
54	BA	2339	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	621	A	N1-C6-N6	-6.71	114.57	118.60
54	BA	793	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	1330	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1793	C	N1-C2-O2	6.71	122.93	118.90
54	BA	2776	A	C4-C5-C6	-6.71	113.64	117.00
56	B5	53	ARG	NE-CZ-NH1	6.71	123.66	120.30
54	BA	896	A	O4'-C1'-N9	6.71	113.57	108.20
54	BA	2430	A	C5-C6-N1	6.71	121.06	117.70
21	AA	129	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	1201	A	C5-C6-N1	6.71	121.06	117.70
21	AA	1483	A	N1-C6-N6	-6.71	114.58	118.60
54	BA	6	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1370	C	N3-C4-C5	6.71	124.58	121.90
54	BA	1387	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	1962	C	N3-C2-O2	-6.71	117.20	121.90
34	BL	48	ARG	NE-CZ-NH2	-6.71	116.95	120.30
54	BA	1366	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1808	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	205	G	O4'-C1'-N9	6.70	113.56	108.20
54	BA	1189	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2388	A	C5-C6-N1	6.70	121.05	117.70
21	AA	923	A	C5-C6-N1	6.70	121.05	117.70
21	AA	325	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1113	U	O4'-C1'-N1	6.70	113.56	108.20
21	AA	533	A	N1-C6-N6	-6.70	114.58	118.60
54	BA	670	A	C5-C6-N1	6.70	121.05	117.70
21	AA	1254	A	C5-C6-N1	6.70	121.05	117.70
54	BA	323	C	N1-C2-O2	6.70	122.92	118.90
13	AN	9	ARG	NE-CZ-NH1	6.70	123.65	120.30
21	AA	985	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	118	A	N1-C6-N6	-6.70	114.58	118.60
54	BA	125	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1772	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2281	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2632	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2134	A	C4-C5-C6	-6.69	113.65	117.00
54	BA	2204	G	C5-C6-N1	6.69	114.85	111.50
54	BA	2518	A	C5-C6-N1	6.69	121.05	117.70
21	AA	342	C	N1-C2-O2	6.69	122.92	118.90
21	AA	732	C	N3-C2-O2	-6.69	117.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	135	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	348	G	O4'-C1'-N9	6.69	113.55	108.20
21	AA	1479	C	N1-C2-O2	6.69	122.91	118.90
54	BA	125	A	P-O3'-C3'	6.69	127.73	119.70
54	BA	196	A	O4'-C1'-N9	6.69	113.55	108.20
54	BA	503	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	506	G	O4'-C1'-N9	6.69	113.55	108.20
54	BA	1893	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2352	A	C5-C6-N1	6.69	121.05	117.70
54	BA	2799	A	C5-C6-N1	6.69	121.05	117.70
54	BA	96	C	O4'-C1'-N1	6.69	113.55	108.20
21	AA	1277	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	1413	A	N1-C6-N6	-6.69	114.59	118.60
54	BA	2421	G	N3-C2-N2	-6.69	115.22	119.90
21	AA	1019	A	C5-C6-N1	6.69	121.04	117.70
54	BA	461	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	1652	A	C5-C6-N1	6.69	121.04	117.70
21	AA	1368	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	654	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	1115	G	C5-C6-N1	6.68	114.84	111.50
54	BA	2753	A	C5-C6-N1	6.68	121.04	117.70
21	AA	913	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1093	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	2619	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	694	U	N3-C2-O2	-6.68	117.52	122.20
54	BA	1664	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1306	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	2088	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	2332	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	2506	U	O4'-C1'-N1	6.68	113.54	108.20
55	BB	66	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	1029	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1359	C	N3-C2-O2	-6.68	117.23	121.90
39	BQ	91	ARG	NE-CZ-NH2	-6.68	116.96	120.30
54	BA	611	C	N3-C2-O2	-6.68	117.23	121.90
54	BA	909	A	C4-C5-C6	-6.68	113.66	117.00
19	AT	23	ARG	NE-CZ-NH1	6.67	123.64	120.30
21	AA	1251	A	C4-C5-C6	-6.67	113.66	117.00
22	A1	73	A	C5-C6-N1	6.67	121.04	117.70
24	A3	24	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	399	U	O4'-C1'-N1	6.67	113.54	108.20
54	BA	668	A	C5-C6-N1	6.67	121.04	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2215	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2266	A	C5-C6-N1	6.67	121.04	117.70
54	BA	2660	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1989	G	C8-N9-C4	-6.67	103.73	106.40
54	BA	72	U	O4'-C1'-N1	6.67	113.54	108.20
54	BA	421	C	P-O3'-C3'	6.67	127.70	119.70
54	BA	821	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	1194	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	1335	C	O4'-C1'-N1	6.67	113.54	108.20
54	BA	1493	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	190	A	C5-C6-N1	6.67	121.03	117.70
21	AA	409	U	C5-C6-N1	-6.67	119.36	122.70
21	AA	1447	A	N1-C6-N6	-6.67	114.60	118.60
37	BO	13	ARG	NE-CZ-NH1	6.67	123.64	120.30
54	BA	1268	A	C5-C6-N1	6.67	121.03	117.70
21	AA	1234	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	1268	A	N1-C6-N6	-6.67	114.60	118.60
54	BA	1413	A	C5-C6-N1	6.67	121.03	117.70
54	BA	1748	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	1615	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1847	A	O4'-C1'-N9	6.66	113.53	108.20
21	AA	1117	A	C5-C6-N1	6.66	121.03	117.70
54	BA	635	C	N3-C2-O2	-6.66	117.24	121.90
10	AK	126	ARG	NE-CZ-NH1	6.66	123.63	120.30
21	AA	400	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	1340	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1408	G	N1-C6-O6	-6.66	115.90	119.90
54	BA	2199	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	583	A	C5-C6-N1	6.66	121.03	117.70
54	BA	899	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2803	G	N1-C6-O6	-6.66	115.91	119.90
21	AA	1070	U	O4'-C1'-N1	6.66	113.53	108.20
54	BA	781	A	C5-C6-N1	6.66	121.03	117.70
54	BA	898	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	498	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	447	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	480	A	C5-C6-N1	6.65	121.03	117.70
21	AA	298	A	C5-C6-N1	6.65	121.03	117.70
54	BA	330	A	O4'-C1'-N9	6.65	113.52	108.20
54	BA	572	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	852	G	N1-C6-O6	-6.65	115.91	119.90
54	BA	802	A	C5-C6-N1	6.65	121.03	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1320	C	O4'-C1'-N1	6.65	113.52	108.20
54	BA	1246	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	2369	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	2778	A	C5-C6-N1	6.65	121.02	117.70
16	AQ	64	ARG	NE-CZ-NH1	6.65	123.62	120.30
21	AA	389	A	C4-C5-C6	-6.65	113.68	117.00
54	BA	477	A	C5-C6-N1	6.65	121.02	117.70
32	BJ	69	ARG	NE-CZ-NH1	6.65	123.62	120.30
21	AA	345	C	O4'-C1'-N1	6.64	113.52	108.20
21	AA	553	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2560	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2577	A	C5-C6-N1	6.64	121.02	117.70
21	AA	395	C	N3-C2-O2	-6.64	117.25	121.90
39	BQ	47	ARG	NE-CZ-NH1	6.64	123.62	120.30
54	BA	127	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2007	U	O4'-C1'-N1	6.64	113.51	108.20
54	BA	2882	A	C5-C6-N1	6.64	121.02	117.70
54	BA	484	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1070	A	C4-C5-C6	-6.64	113.68	117.00
55	BB	24	G	N9-C4-C5	6.64	108.06	105.40
55	BB	99	A	N1-C6-N6	-6.64	114.62	118.60
20	AU	20	ARG	NE-CZ-NH2	-6.63	116.98	120.30
54	BA	1366	A	C4-C5-C6	-6.63	113.68	117.00
21	AA	1022	A	C5-C6-N1	6.63	121.02	117.70
43	BU	81	ARG	NE-CZ-NH1	6.63	123.61	120.30
54	BA	888	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1524	G	C5-C6-N1	6.63	114.82	111.50
55	BB	26	C	N1-C2-O2	6.63	122.88	118.90
54	BA	2827	C	O4'-C1'-N1	6.63	113.50	108.20
21	AA	747	A	N1-C6-N6	-6.63	114.62	118.60
54	BA	1792	G	N1-C6-O6	-6.63	115.92	119.90
54	BA	2191	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	1366	A	N1-C6-N6	-6.62	114.62	118.60
21	AA	766	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	980	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	982	C	C2-N1-C1'	6.62	126.08	118.80
55	BB	94	A	C5-C6-N1	6.62	121.01	117.70
21	AA	196	A	C5-C6-N1	6.62	121.01	117.70
21	AA	754	C	N1-C2-O2	6.62	122.87	118.90
43	BU	6	ARG	NE-CZ-NH1	6.62	123.61	120.30
54	BA	1454	C	N1-C2-O2	6.62	122.87	118.90
5	AF	24	ARG	NE-CZ-NH1	6.62	123.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	946	A	C5-C6-N1	6.62	121.01	117.70
21	AA	1288	A	C5-C6-N1	6.62	121.01	117.70
21	AA	1518	A	C5-C6-N1	6.62	121.01	117.70
22	A1	41	A	C5-C6-N1	6.62	121.01	117.70
54	BA	538	A	N1-C6-N6	-6.62	114.63	118.60
54	BA	1967	C	N1-C2-O2	6.62	122.87	118.90
54	BA	2393	U	O4'-C1'-N1	6.62	113.49	108.20
54	BA	2828	G	C5-C6-N1	6.62	114.81	111.50
21	AA	1281	C	N1-C2-O2	6.61	122.87	118.90
54	BA	849	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	2879	A	C5-C6-N1	6.61	121.01	117.70
21	AA	680	C	N3-C2-O2	-6.61	117.27	121.90
22	A1	61	C	N3-C2-O2	-6.61	117.27	121.90
29	BG	152	ARG	NE-CZ-NH1	6.61	123.61	120.30
54	BA	2258	C	N3-C2-O2	-6.61	117.27	121.90
11	AL	11	ARG	NE-CZ-NH1	6.61	123.61	120.30
21	AA	758	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	1014	A	C5-C6-N1	6.61	121.00	117.70
21	AA	1170	A	C5-C6-N1	6.61	121.01	117.70
33	BK	18	ARG	NE-CZ-NH1	6.61	123.61	120.30
54	BA	6	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	255	A	C5-C6-N1	6.61	121.00	117.70
54	BA	620	G	N9-C4-C5	6.61	108.04	105.40
22	A1	56	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	241	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	990	A	C4-C5-C6	-6.61	113.69	117.00
25	BC	62	ARG	NE-CZ-NH1	6.61	123.60	120.30
48	BZ	29	ARG	NE-CZ-NH1	6.61	123.60	120.30
54	BA	1980	G	N1-C6-O6	-6.61	115.94	119.90
54	BA	2183	A	C4-C5-C6	-6.61	113.70	117.00
21	AA	1408	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	902	C	O4'-C1'-N1	6.60	113.48	108.20
54	BA	994	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	1054	C	N3-C4-C5	6.60	124.54	121.90
54	BA	444	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	632	A	C5-C6-N1	6.60	121.00	117.70
21	AA	279	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	1013	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	364	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	96	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	101	A	C5-C6-N1	6.60	121.00	117.70
21	AA	266	G	C1'-O4'-C4'	-6.60	104.62	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	493	A	C5-C6-N1	6.59	121.00	117.70
21	AA	841	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	1484	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	1848	A	C5-C6-N1	6.59	121.00	117.70
54	BA	1991	U	O4'-C1'-N1	6.59	113.47	108.20
21	AA	1533	C	P-O3'-C3'	6.59	127.61	119.70
36	BN	46	ARG	NE-CZ-NH1	6.59	123.59	120.30
54	BA	2703	C	N3-C2-O2	-6.59	117.29	121.90
24	A3	76	C	C6-N1-C2	-6.59	117.67	120.30
54	BA	2668	G	P-O3'-C3'	6.59	127.60	119.70
21	AA	536	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	689	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	531	C	C1'-O4'-C4'	-6.58	104.63	109.90
54	BA	2114	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2822	G	O4'-C1'-N9	6.58	113.47	108.20
54	BA	1538	G	N1-C6-O6	-6.58	115.95	119.90
54	BA	2059	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	2612	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	1885	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	1158	C	N1-C2-O2	6.58	122.85	118.90
21	AA	1336	C	C1'-O4'-C4'	-6.58	104.64	109.90
24	A3	75	C	N3-C4-N4	-6.58	113.39	118.00
54	BA	784	G	N3-C4-C5	-6.58	125.31	128.60
54	BA	1616	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2321	U	O4'-C1'-N1	6.58	113.46	108.20
21	AA	373	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1040	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1920	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	1970	A	C5-C6-N1	6.58	120.99	117.70
21	AA	303	A	C5-C6-N1	6.57	120.99	117.70
22	A1	58	A	C5-C6-N1	6.57	120.99	117.70
21	AA	432	A	C5-C6-N1	6.57	120.99	117.70
54	BA	282	A	N1-C6-N6	-6.57	114.66	118.60
54	BA	964	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1147	A	C5-C6-N1	6.57	120.98	117.70
54	BA	2618	G	N3-C4-C5	-6.57	125.31	128.60
11	AL	8	ARG	NE-CZ-NH1	6.57	123.58	120.30
21	AA	1051	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	1446	A	C5-C6-N1	6.57	120.98	117.70
54	BA	282	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	2741	A	C5-C6-N1	6.57	120.98	117.70
54	BA	292	U	C5-C6-N1	-6.57	119.42	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1005	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	2704	C	N3-C2-O2	-6.57	117.30	121.90
24	A3	42	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1060	U	O4'-C1'-N1	6.57	113.45	108.20
54	BA	1924	C	N3-C2-O2	-6.57	117.31	121.90
54	BA	2117	A	N1-C6-N6	-6.57	114.66	118.60
54	BA	371	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2359	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2717	C	N3-C2-O2	-6.56	117.31	121.90
36	BN	71	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	2632	A	C5-C6-N1	6.56	120.98	117.70
21	AA	250	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	466	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	1104	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1175	A	N1-C6-N6	-6.56	114.66	118.60
54	BA	2082	A	C5-C6-N1	6.56	120.98	117.70
54	BA	372	G	C1'-O4'-C4'	-6.56	104.66	109.90
54	BA	549	G	N3-C4-C5	-6.56	125.32	128.60
54	BA	1274	A	C4-C5-C6	-6.55	113.72	117.00
21	AA	1259	C	N1-C2-O2	6.55	122.83	118.90
54	BA	2874	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	1404	C	O4'-C1'-N1	6.55	113.44	108.20
54	BA	2880	C	N3-C2-O2	-6.55	117.31	121.90
25	BC	86	ARG	NE-CZ-NH1	6.55	123.57	120.30
54	BA	1221	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	1451	C	P-O3'-C3'	6.55	127.56	119.70
54	BA	1655	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	2207	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	2800	A	N1-C6-N6	-6.55	114.67	118.60
54	BA	804	A	C5-C6-N1	6.55	120.97	117.70
54	BA	815	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	893	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	2212	A	C4-C5-C6	-6.55	113.73	117.00
31	BI	126	ARG	NE-CZ-NH1	6.55	123.57	120.30
54	BA	1577	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	2013	A	C5-C6-N1	6.55	120.97	117.70
54	BA	2835	A	C4-C5-C6	-6.54	113.73	117.00
24	A3	58	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	430	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	669	G	C5-C6-N1	6.54	114.77	111.50
54	BA	2287	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	2362	C	O4'-C1'-N1	6.54	113.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	71	C	O4'-C1'-N1	6.54	113.44	108.20
21	AA	496	A	N1-C6-N6	-6.54	114.67	118.60
21	AA	530	G	N3-C4-C5	-6.54	125.33	128.60
54	BA	103	A	C5-C6-N1	6.54	120.97	117.70
54	BA	2731	G	N1-C6-O6	-6.54	115.98	119.90
21	AA	26	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1475	G	N1-C6-O6	-6.54	115.98	119.90
54	BA	2576	G	N3-C4-C5	-6.54	125.33	128.60
21	AA	607	A	C5-C6-N1	6.54	120.97	117.70
21	AA	864	A	N1-C6-N6	-6.54	114.68	118.60
54	BA	1744	A	N1-C6-N6	-6.54	114.68	118.60
21	AA	171	A	C5-C6-N1	6.53	120.97	117.70
21	AA	1492	A	C5-C6-N1	6.53	120.97	117.70
54	BA	1420	A	C4-C5-C6	-6.53	113.73	117.00
21	AA	1367	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1678	A	C5-C6-N1	6.53	120.97	117.70
1	AB	212	TYR	CB-CG-CD1	6.53	124.92	121.00
21	AA	642	A	C5-C6-N1	6.53	120.97	117.70
21	AA	1288	A	N1-C6-N6	-6.53	114.68	118.60
54	BA	2183	A	C5-C6-N1	6.53	120.97	117.70
21	AA	490	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1566	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	2469	A	C4-C5-C6	-6.53	113.73	117.00
24	A3	38	A	C5-C6-N1	6.53	120.96	117.70
54	BA	972	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1347	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1609	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1864	U	O4'-C1'-N1	6.53	113.42	108.20
54	BA	677	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	814	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	965	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	948	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	1598	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	507	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1726	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	2333	A	C5-C6-N1	6.52	120.96	117.70
21	AA	65	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	1044	A	C5-C6-N1	6.52	120.96	117.70
21	AA	814	A	C5-C6-N1	6.52	120.96	117.70
21	AA	895	G	N1-C6-O6	-6.52	115.99	119.90
34	BL	18	ARG	NE-CZ-NH1	6.52	123.56	120.30
54	BA	348	A	C4-C5-C6	-6.52	113.74	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	353	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	1270	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	1692	U	N3-C2-O2	-6.52	117.64	122.20
54	BA	1978	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	2790	U	N3-C2-O2	-6.52	117.64	122.20
55	BB	34	A	C5-C6-N6	6.52	128.91	123.70
54	BA	1722	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	694	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1755	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1272	A	C5-C6-N1	6.51	120.96	117.70
55	BB	23	G	N1-C6-O6	-6.51	115.99	119.90
21	AA	993	G	N3-C4-C5	-6.51	125.34	128.60
54	BA	743	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1153	C	O4'-C1'-N1	6.51	113.41	108.20
54	BA	1505	A	C5-C6-N1	6.51	120.96	117.70
54	BA	2042	A	N1-C6-N6	-6.51	114.69	118.60
21	AA	797	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	300	A	C5-C6-N1	6.51	120.95	117.70
54	BA	706	A	O4'-C1'-N9	6.51	113.41	108.20
54	BA	1637	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1866	A	C4-C5-C6	-6.51	113.75	117.00
21	AA	108	G	O4'-C1'-N9	6.51	113.41	108.20
54	BA	433	C	N1-C2-O2	6.51	122.81	118.90
21	AA	66	A	N1-C6-N6	-6.51	114.70	118.60
54	BA	1499	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	25	C	N3-C2-O2	-6.50	117.35	121.90
46	BX	2	ARG	NE-CZ-NH1	6.50	123.55	120.30
54	BA	191	A	C5-C6-N1	6.50	120.95	117.70
21	AA	320	A	C3'-C2'-C1'	6.50	106.70	101.50
54	BA	2282	G	O4'-C1'-N9	6.50	113.40	108.20
54	BA	2541	A	C4-C5-C6	-6.50	113.75	117.00
55	BB	15	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	55	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	353	A	N1-C6-N6	-6.50	114.70	118.60
37	BO	111	ARG	NE-CZ-NH1	6.50	123.55	120.30
54	BA	1555	G	C5-C6-N1	6.50	114.75	111.50
21	AA	195	A	C1'-O4'-C4'	-6.50	104.70	109.90
26	BD	59	ARG	NE-CZ-NH1	6.50	123.55	120.30
54	BA	251	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	905	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1451	C	C6-N1-C2	-6.50	117.70	120.30
54	BA	2539	C	N3-C2-O2	-6.50	117.35	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	223	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	550	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1446	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2179	C	N3-C2-O2	-6.49	117.35	121.90
21	AA	65	A	C5-C6-N1	6.49	120.94	117.70
21	AA	195	A	N1-C6-N6	-6.49	114.71	118.60
21	AA	1410	A	C5-C6-N1	6.49	120.95	117.70
54	BA	678	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1853	A	C5-C6-N1	6.49	120.94	117.70
54	BA	2420	C	N1-C2-O2	6.49	122.79	118.90
21	AA	599	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	1531	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	207	A	C5-C6-N1	6.49	120.94	117.70
54	BA	366	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	436	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	722	A	N1-C6-N6	-6.49	114.71	118.60
54	BA	2196	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1342	A	N1-C6-N6	-6.49	114.71	118.60
54	BA	2748	A	C5-C6-N1	6.49	120.94	117.70
21	AA	908	A	N1-C6-N6	-6.48	114.71	118.60
54	BA	402	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1030	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1553	A	C5-C6-N1	6.48	120.94	117.70
54	BA	2142	A	C5-C6-N1	6.48	120.94	117.70
54	BA	590	A	C5-C6-N1	6.48	120.94	117.70
54	BA	927	A	C5-C6-N1	6.48	120.94	117.70
54	BA	2461	A	N1-C6-N6	-6.48	114.71	118.60
21	AA	563	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	1609	A	C1'-O4'-C4'	-6.48	104.72	109.90
21	AA	412	A	C5-C6-N1	6.48	120.94	117.70
21	AA	779	C	N1-C2-O2	6.48	122.79	118.90
23	A2	79	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	2374	C	N1-C2-O2	6.48	122.79	118.90
54	BA	2547	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	565	U	O4'-C1'-N1	6.48	113.38	108.20
54	BA	1247	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	948	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1157	A	C5-C6-N1	6.47	120.94	117.70
54	BA	829	A	N1-C6-N6	-6.47	114.72	118.60
54	BA	1321	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	1999	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	415	A	O4'-C1'-N9	6.47	113.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	621	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	1705	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	1071	C	O4'-C1'-N1	6.47	113.38	108.20
54	BA	2103	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	630	G	N1-C6-O6	-6.47	116.02	119.90
54	BA	825	A	C5-C6-N1	6.47	120.94	117.70
54	BA	1367	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	2000	C	N3-C2-O2	-6.47	117.37	121.90
22	A1	6	A	C5-C6-N1	6.47	120.93	117.70
54	BA	2373	G	O4'-C1'-N9	6.47	113.37	108.20
21	AA	1257	A	C5-C6-N1	6.47	120.93	117.70
22	A1	60	C	N1-C2-O2	6.47	122.78	118.90
41	BS	92	ARG	NE-CZ-NH1	6.47	123.53	120.30
54	BA	412	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1502	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	2462	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2872	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	1080	A	N1-C6-N6	-6.46	114.72	118.60
28	BF	70	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	1230	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1950	G	N9-C4-C5	6.46	107.99	105.40
15	AP	25	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	231	A	C5-C6-N1	6.46	120.93	117.70
54	BA	592	A	C5-C6-N1	6.46	120.93	117.70
54	BA	621	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1894	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	656	G	N1-C6-O6	-6.46	116.02	119.90
21	AA	1480	A	C5-C6-N1	6.46	120.93	117.70
54	BA	753	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	1800	C	N3-C2-O2	-6.46	117.38	121.90
15	AP	56	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	251	G	P-O3'-C3'	6.46	127.45	119.70
21	AA	253	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	906	A	C4-C5-C6	-6.46	113.77	117.00
22	A1	21	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1597	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1779	U	C5-C6-N1	-6.46	119.47	122.70
54	BA	1895	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2006	C	N1-C2-O2	6.46	122.78	118.90
21	AA	1246	A	C5-C6-N1	6.46	120.93	117.70
24	A3	7	G	O4'-C1'-N9	6.46	113.36	108.20
54	BA	2287	A	C2-N3-C4	6.46	113.83	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2601	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	716	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	176	C	N3-C2-O2	-6.45	117.38	121.90
21	AA	825	A	C5-C6-N1	6.45	120.93	117.70
54	BA	2652	C	N3-C2-O2	-6.45	117.38	121.90
6	AG	101	ARG	NE-CZ-NH1	6.45	123.53	120.30
54	BA	184	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	684	G	N3-C2-N2	-6.45	115.38	119.90
54	BA	915	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1150	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1322	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	2295	C	O4'-C1'-N1	6.45	113.36	108.20
54	BA	2412	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	979	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	1218	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	1480	A	N1-C6-N6	-6.45	114.73	118.60
24	A3	35	C	N3-C2-O2	-6.45	117.39	121.90
29	BG	2	ARG	NE-CZ-NH1	6.45	123.52	120.30
54	BA	671	C	N3-C4-C5	6.45	124.48	121.90
54	BA	829	A	C5-C6-N1	6.45	120.92	117.70
54	BA	945	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1156	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1544	A	C5-C6-N1	6.44	120.92	117.70
21	AA	461	A	N1-C6-N6	-6.44	114.73	118.60
21	AA	705	G	N1-C6-O6	-6.44	116.03	119.90
54	BA	2191	A	O4'-C1'-N9	6.44	113.35	108.20
12	AM	86	ARG	NE-CZ-NH1	6.44	123.52	120.30
3	AD	80	ARG	NE-CZ-NH1	6.44	123.52	120.30
21	AA	1287	A	C4-C5-C6	-6.44	113.78	117.00
24	A3	16	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	342	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	1461	G	N1-C6-O6	-6.44	116.04	119.90
54	BA	233	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1340	U	P-O3'-C3'	6.44	127.42	119.70
54	BA	2274	A	C5-C6-N1	6.44	120.92	117.70
21	AA	635	A	C5-C6-N1	6.44	120.92	117.70
54	BA	996	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2517	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	391	G	O4'-C1'-N9	6.43	113.35	108.20
54	BA	401	A	C5-C6-N1	6.43	120.92	117.70
54	BA	631	A	C5-C6-N1	6.43	120.92	117.70
21	AA	90	C	N3-C2-O2	-6.43	117.40	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	724	U	O4'-C1'-N1	6.43	113.35	108.20
54	BA	1428	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2534	A	C5-C6-N1	6.43	120.92	117.70
54	BA	558	U	O4'-C1'-N1	6.43	113.34	108.20
54	BA	1311	G	O4'-C1'-N9	6.43	113.34	108.20
21	AA	1219	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	661	A	C4-C5-C6	-6.43	113.78	117.00
21	AA	81	A	N1-C6-N6	-6.43	114.74	118.60
22	A1	57	G	C1'-O4'-C4'	-6.43	104.76	109.90
54	BA	574	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	271	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	1446	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	2442	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2497	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	2860	A	C5-C6-N1	6.43	120.91	117.70
21	AA	403	C	N3-C2-O2	-6.42	117.40	121.90
54	BA	943	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1020	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2468	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2614	A	N1-C6-N6	-6.42	114.75	118.60
54	BA	1151	A	C4-C5-C6	-6.42	113.79	117.00
22	A1	36	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	457	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2013	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	264	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1590	A	C5-C6-N1	6.42	120.91	117.70
21	AA	1028	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	1151	A	P-O3'-C3'	6.42	127.40	119.70
21	AA	1465	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1384	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2636	C	N3-C2-O2	-6.42	117.41	121.90
55	BB	19	C	N1-C2-O2	6.42	122.75	118.90
21	AA	78	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	193	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	1430	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	845	A	C5-C6-N1	6.42	120.91	117.70
54	BA	2200	C	O4'-C1'-N1	6.42	113.33	108.20
46	BX	36	ARG	NE-CZ-NH1	6.42	123.51	120.30
54	BA	384	A	C5-C6-N1	6.42	120.91	117.70
21	AA	183	C	N3-C4-N4	-6.41	113.51	118.00
21	AA	1298	U	N3-C2-O2	-6.41	117.71	122.20
24	A3	66	C	N3-C2-O2	-6.41	117.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	195	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	1639	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	2270	A	C5-C6-N1	6.41	120.91	117.70
21	AA	194	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	374	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2606	C	N1-C2-O2	6.41	122.75	118.90
54	BA	557	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	220	G	N3-C2-N2	-6.41	115.42	119.90
21	AA	1314	C	N3-C2-O2	-6.41	117.42	121.90
23	A2	82	A	N1-C6-N6	-6.41	114.76	118.60
54	BA	1349	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	998	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2512	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	94	A	C5-C6-N1	6.40	120.90	117.70
54	BA	95	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	355	U	O4'-C1'-N1	6.40	113.32	108.20
21	AA	1147	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2145	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2205	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	696	A	C4-C5-C6	-6.40	113.80	117.00
25	BC	176	ARG	NE-CZ-NH1	6.40	123.50	120.30
54	BA	6	A	N1-C6-N6	-6.40	114.76	118.60
54	BA	510	C	N1-C2-O2	6.40	122.74	118.90
54	BA	637	A	C5-C6-N1	6.40	120.90	117.70
54	BA	1494	A	C5-C6-N1	6.40	120.90	117.70
54	BA	2646	C	N1-C2-O2	6.40	122.74	118.90
54	BA	238	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	788	A	N1-C6-N6	-6.40	114.76	118.60
21	AA	618	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	198	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	20	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	252	G	N1-C6-O6	-6.39	116.06	119.90
54	BA	1317	G	N1-C6-O6	-6.39	116.06	119.90
54	BA	1536	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1646	C	N1-C2-O2	6.39	122.73	118.90
21	AA	807	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	1735	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	1767	G	O4'-C1'-N9	6.39	113.31	108.20
21	AA	44	A	C5-C6-N1	6.39	120.89	117.70
54	BA	513	A	C5-C6-N1	6.39	120.89	117.70
54	BA	1204	A	C2-N3-C4	6.39	113.80	110.60
54	BA	2173	A	N1-C6-N6	-6.39	114.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2498	C	O4'-C1'-N1	6.39	113.31	108.20
54	BA	275	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	727	A	C5-C6-N1	6.39	120.89	117.70
54	BA	2061	G	N3-C2-N2	-6.39	115.43	119.90
21	AA	34	C	N3-C2-O2	-6.39	117.43	121.90
21	AA	124	C	N3-C2-O2	-6.38	117.43	121.90
21	AA	1453	G	O4'-C1'-N9	6.38	113.31	108.20
54	BA	2037	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2590	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2793	C	O4'-C1'-N1	6.38	113.31	108.20
54	BA	1503	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2824	C	N3-C4-N4	-6.38	113.53	118.00
21	AA	413	G	O4'-C1'-N9	6.38	113.30	108.20
21	AA	669	G	N1-C6-O6	-6.38	116.07	119.90
21	AA	974	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2321	U	N3-C2-O2	-6.38	117.74	122.20
54	BA	2771	C	N1-C2-O2	6.38	122.73	118.90
21	AA	912	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	616	A	C5-C6-N1	6.38	120.89	117.70
54	BA	835	C	O4'-C1'-N1	6.38	113.30	108.20
54	BA	946	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	1475	G	C5-C6-N1	6.38	114.69	111.50
54	BA	1900	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2392	A	C5-C6-N1	6.38	120.89	117.70
9	AJ	16	ARG	NE-CZ-NH2	-6.38	117.11	120.30
54	BA	1697	G	C8-N9-C4	-6.38	103.85	106.40
54	BA	2273	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	490	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1048	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	1749	A	N1-C6-N6	-6.37	114.78	118.60
54	BA	2747	G	N3-C4-C5	-6.37	125.41	128.60
53	B4	24	ARG	NE-CZ-NH2	-6.37	117.11	120.30
54	BA	610	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1253	A	C5-C6-N1	6.37	120.89	117.70
54	BA	1668	A	C5-C6-N1	6.37	120.89	117.70
4	AE	53	ARG	NE-CZ-NH1	6.37	123.48	120.30
22	A1	27	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1385	G	N1-C6-O6	-6.37	116.08	119.90
54	BA	14	A	C5-C6-N1	6.37	120.88	117.70
54	BA	643	A	N1-C6-N6	-6.37	114.78	118.60
54	BA	1644	C	O4'-C1'-N1	6.37	113.30	108.20
54	BA	1786	A	C5-C6-N1	6.37	120.88	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2846	G	N3-C2-N2	-6.37	115.44	119.90
21	AA	1080	A	C5-C6-N1	6.37	120.88	117.70
21	AA	1397	C	N1-C2-O2	6.37	122.72	118.90
21	AA	1513	A	C4-C5-C6	-6.36	113.82	117.00
22	A1	72	C	N1-C2-O2	6.36	122.72	118.90
54	BA	185	G	N7-C8-N9	6.36	116.28	113.10
54	BA	2226	C	O4'-C1'-N1	6.36	113.29	108.20
54	BA	2683	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	44	A	N1-C6-N6	-6.36	114.78	118.60
54	BA	346	A	C2-N3-C4	6.36	113.78	110.60
54	BA	670	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1876	A	C5-C6-N1	6.36	120.88	117.70
54	BA	109	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2283	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	13	U	C5'-C4'-C3'	-6.36	105.83	116.00
21	AA	1456	A	C5-C6-N1	6.36	120.88	117.70
54	BA	640	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	630	A	C5-C6-N1	6.36	120.88	117.70
21	AA	1263	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1745	A	N1-C6-N6	-6.36	114.79	118.60
54	BA	2752	C	N1-C2-O2	6.36	122.71	118.90
54	BA	2753	A	N1-C6-N6	-6.36	114.79	118.60
54	BA	2805	C	O4'-C1'-N1	6.36	113.28	108.20
54	BA	1165	A	C5-C6-N1	6.35	120.88	117.70
21	AA	269	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	1284	A	C5-C6-N1	6.35	120.88	117.70
21	AA	1496	C	N1-C2-O2	6.35	122.71	118.90
54	BA	462	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	2199	A	C5-C6-N1	6.35	120.88	117.70
55	BB	65	U	C5-C6-N1	-6.35	119.53	122.70
21	AA	339	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	420	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	432	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	1241	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	1768	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	2454	G	O4'-C1'-N9	6.35	113.28	108.20
54	BA	2822	G	C1'-O4'-C4'	-6.35	104.82	109.90
21	AA	348	G	C1'-O4'-C4'	-6.35	104.82	109.90
21	AA	1365	G	N3-C2-N2	-6.35	115.46	119.90
54	BA	181	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	515	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	532	A	C4-C5-C6	-6.35	113.83	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1593	A	C5-C6-N1	6.35	120.87	117.70
54	BA	2486	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	315	A	C5-C6-N1	6.34	120.87	117.70
21	AA	608	A	C5-C6-N1	6.34	120.87	117.70
54	BA	1858	A	C5-C6-N1	6.34	120.87	117.70
54	BA	2284	A	C6-C5-N7	6.34	136.74	132.30
21	AA	161	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	964	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	788	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1610	A	C1'-O4'-C4'	-6.34	104.83	109.90
54	BA	338	G	N3-C4-C5	-6.34	125.43	128.60
54	BA	633	A	C5-C6-N1	6.34	120.87	117.70
54	BA	903	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1515	A	C5-C6-N1	6.34	120.87	117.70
54	BA	1871	A	O4'-C1'-N9	6.34	113.27	108.20
54	BA	2143	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2425	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	355	C	N1-C2-O2	6.34	122.70	118.90
21	AA	602	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	574	A	C5-C6-N1	6.34	120.87	117.70
21	AA	963	G	N1-C6-O6	-6.34	116.10	119.90
54	BA	705	A	N1-C6-N6	-6.33	114.80	118.60
54	BA	1099	G	C8-N9-C4	-6.33	103.87	106.40
21	AA	77	A	C5-C6-N1	6.33	120.87	117.70
21	AA	1104	G	N1-C6-O6	-6.33	116.10	119.90
54	BA	147	C	O4'-C1'-N1	6.33	113.27	108.20
54	BA	705	A	C5-C6-N1	6.33	120.87	117.70
21	AA	6	G	N3-C4-C5	-6.33	125.44	128.60
21	AA	624	C	N3-C2-O2	-6.33	117.47	121.90
39	BQ	69	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	717	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2163	A	C5-C6-N1	6.33	120.86	117.70
21	AA	60	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	181	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	1324	A	C5-C6-N1	6.33	120.86	117.70
54	BA	542	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	814	C	O4'-C1'-N1	6.33	113.26	108.20
54	BA	1328	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	1889	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	2273	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	130	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	478	A	C5-C6-N1	6.33	120.86	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	612	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	686	U	N1-C2-N3	6.33	118.70	114.90
54	BA	97	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	389	G	N9-C4-C5	6.32	107.93	105.40
54	BA	415	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1625	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	2516	A	C5-C6-N1	6.32	120.86	117.70
54	BA	2001	C	N3-C2-O2	-6.32	117.47	121.90
22	A1	35	A	C4-C5-C6	-6.32	113.84	117.00
27	BE	88	ARG	NE-CZ-NH1	6.32	123.46	120.30
21	AA	610	U	N3-C2-O2	-6.32	117.78	122.20
21	AA	1112	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	413	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	414	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2862	G	O4'-C1'-N9	6.32	113.25	108.20
21	AA	117	G	N1-C6-O6	-6.32	116.11	119.90
21	AA	578	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	719	C	N1-C2-O2	6.32	122.69	118.90
54	BA	1032	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	2078	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2756	U	C5-C6-N1	-6.32	119.54	122.70
21	AA	1256	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	1579	A	C4-C5-C6	-6.31	113.84	117.00
21	AA	572	A	C5-C6-N1	6.31	120.86	117.70
54	BA	647	G	C5-C6-N1	6.31	114.66	111.50
54	BA	2483	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	1395	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	316	C	O4'-C1'-N1	6.31	113.25	108.20
54	BA	711	G	C8-N9-C4	-6.31	103.88	106.40
54	BA	749	A	C4-C5-C6	-6.31	113.84	117.00
21	AA	866	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	1342	C	N1-C2-O2	6.31	122.68	118.90
54	BA	1123	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1650	A	C5-C6-N1	6.31	120.85	117.70
22	A1	74	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	31	C	N1-C2-O2	6.31	122.68	118.90
21	AA	181	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1249	U	O4'-C1'-N1	6.30	113.24	108.20
54	BA	1671	U	C5-C6-N1	-6.30	119.55	122.70
54	BA	2471	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2657	A	C5-C6-N1	6.30	120.85	117.70
21	AA	961	U	O4'-C1'-N1	6.30	113.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1319	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	191	A	N1-C6-N6	-6.30	114.82	118.60
54	BA	402	A	N1-C6-N6	-6.30	114.82	118.60
21	AA	1000	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1836	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2461	A	C5-C6-N1	6.30	120.85	117.70
21	AA	149	A	N1-C6-N6	-6.30	114.82	118.60
54	BA	1403	A	C6-C5-N7	6.29	136.71	132.30
39	BQ	54	ARG	NE-CZ-NH1	6.29	123.45	120.30
54	BA	2236	U	O4'-C1'-N1	6.29	113.23	108.20
21	AA	101	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	1112	C	O4'-C1'-N1	6.29	113.23	108.20
54	BA	758	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1640	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1745	A	C5-C6-N1	6.29	120.84	117.70
54	BA	1754	A	C5-C6-N1	6.29	120.84	117.70
54	BA	1991	U	C5-C6-N1	-6.29	119.56	122.70
21	AA	327	A	C5-C6-N1	6.29	120.84	117.70
21	AA	349	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	803	G	N1-C6-O6	-6.29	116.13	119.90
21	AA	1311	A	C5-C6-N1	6.29	120.84	117.70
21	AA	1366	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	316	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2254	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2600	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1300	G	P-O3'-C3'	6.29	127.25	119.70
55	BB	110	C	O4'-C1'-N1	6.29	113.23	108.20
21	AA	67	C	O4'-C1'-N1	6.29	113.23	108.20
21	AA	73	C	N1-C2-O2	6.29	122.67	118.90
21	AA	712	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1293	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1960	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	910	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	1303	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	460	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1670	C	O4'-C1'-N1	6.28	113.23	108.20
54	BA	2235	G	O4'-C1'-N9	6.28	113.23	108.20
54	BA	2355	G	N1-C6-O6	-6.28	116.13	119.90
21	AA	1369	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2899	A	C4-C5-C6	-6.28	113.86	117.00
13	AN	90	ARG	NE-CZ-NH1	6.28	123.44	120.30
46	BX	10	ARG	NE-CZ-NH1	6.28	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	573	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1681	G	O4'-C1'-N9	6.28	113.22	108.20
54	BA	1771	C	N3-C2-O2	-6.28	117.50	121.90
55	BB	2	G	N3-C4-C5	-6.28	125.46	128.60
21	AA	907	A	N1-C6-N6	-6.28	114.83	118.60
54	BA	163	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	203	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1158	C	N3-C2-O2	-6.28	117.51	121.90
2	AC	155	ARG	NE-CZ-NH1	6.27	123.44	120.30
54	BA	38	A	C5-C6-N1	6.27	120.84	117.70
21	AA	234	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	634	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	301	G	N3-C4-C5	-6.27	125.46	128.60
54	BA	937	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	862	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1151	A	C5-C6-N1	6.27	120.83	117.70
54	BA	435	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1057	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	311	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	461	A	C5-C6-N1	6.27	120.83	117.70
39	BQ	52	ARG	NE-CZ-NH1	6.27	123.44	120.30
54	BA	191	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	944	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2095	A	C5-C6-N1	6.27	120.83	117.70
54	BA	538	A	C5-C6-N1	6.27	120.83	117.70
54	BA	1233	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1334	G	N1-C6-O6	-6.27	116.14	119.90
54	BA	1368	G	O4'-C1'-N9	6.27	113.21	108.20
8	AI	10	ARG	NE-CZ-NH1	6.27	123.43	120.30
54	BA	1749	A	C5-C6-N1	6.27	120.83	117.70
21	AA	487	A	C5-C6-N1	6.26	120.83	117.70
54	BA	13	A	C5-C6-N1	6.26	120.83	117.70
54	BA	483	A	C5-C6-N1	6.26	120.83	117.70
54	BA	2052	A	N1-C6-N6	-6.26	114.84	118.60
54	BA	2358	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	1333	A	C5-C6-N1	6.26	120.83	117.70
21	AA	1473	G	N1-C6-O6	-6.26	116.14	119.90
54	BA	1901	A	C5-C6-N1	6.26	120.83	117.70
54	BA	2035	G	O4'-C1'-N9	6.26	113.21	108.20
54	BA	2589	A	C5-C6-N1	6.26	120.83	117.70
54	BA	479	A	C6-C5-N7	6.26	136.68	132.30
54	BA	1169	A	C4-C5-C6	-6.26	113.87	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1936	A	P-O3'-C3'	6.26	127.21	119.70
54	BA	2446	G	O4'-C4'-C3'	6.26	111.11	106.10
24	A3	1	C	N1-C2-O2	6.26	122.66	118.90
54	BA	718	A	O4'-C1'-N9	6.26	113.21	108.20
54	BA	1504	A	C4-C5-C6	-6.26	113.87	117.00
8	AI	11	ARG	NE-CZ-NH1	6.26	123.43	120.30
54	BA	1046	A	C5-C6-N1	6.26	120.83	117.70
54	BA	1998	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	125	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	221	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	1113	U	C5-C6-N1	-6.25	119.57	122.70
54	BA	1505	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	2515	C	N3-C2-O2	-6.25	117.52	121.90
24	A3	76	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	314	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	331	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	328	C	N1-C2-O2	6.25	122.65	118.90
54	BA	251	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2773	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	814	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	522	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	666	A	N1-C6-N6	-6.25	114.85	118.60
54	BA	943	A	O4'-C1'-N9	6.25	113.20	108.20
54	BA	1319	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1658	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	900	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	327	G	N3-C2-N2	-6.25	115.53	119.90
54	BA	753	A	N1-C6-N6	-6.25	114.85	118.60
54	BA	788	A	C5-C6-N1	6.25	120.82	117.70
54	BA	1033	U	O4'-C1'-N1	6.25	113.20	108.20
54	BA	2736	A	O4'-C1'-N9	6.25	113.20	108.20
54	BA	28	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	237	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1614	A	C4-C5-C6	-6.25	113.88	117.00
6	AG	2	ARG	NE-CZ-NH1	6.24	123.42	120.30
21	AA	1497	G	N1-C6-O6	-6.24	116.15	119.90
22	A1	69	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	820	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1507	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2459	A	N1-C6-N6	-6.24	114.85	118.60
54	BA	2815	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1144	A	C5-C6-N1	6.24	120.82	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1343	G	C8-N9-C4	-6.24	103.90	106.40
21	AA	1176	A	N1-C6-N6	-6.24	114.86	118.60
54	BA	957	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	736	C	N3-C4-N4	-6.24	113.63	118.00
31	BI	133	ARG	NE-CZ-NH1	6.24	123.42	120.30
55	BB	30	C	N3-C2-O2	-6.24	117.53	121.90
55	BB	35	C	N3-C2-O2	-6.24	117.53	121.90
55	BB	41	G	O4'-C1'-N9	6.24	113.19	108.20
2	AC	39	ARG	NE-CZ-NH1	6.24	123.42	120.30
21	AA	791	G	N3-C2-N2	-6.24	115.53	119.90
21	AA	990	C	N1-C2-O2	6.24	122.64	118.90
21	AA	1533	C	C2-N1-C1'	6.24	125.66	118.80
54	BA	8	C	O4'-C1'-N1	6.24	113.19	108.20
54	BA	364	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	415	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1441	G	N1-C6-O6	-6.24	116.16	119.90
54	BA	2158	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1001	A	N1-C6-N6	-6.23	114.86	118.60
54	BA	2016	U	C5-C6-N1	-6.23	119.58	122.70
21	AA	501	C	N1-C2-O2	6.23	122.64	118.90
21	AA	549	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	580	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1029	U	O4'-C1'-N1	6.23	113.19	108.20
54	BA	1001	A	C5-C6-N1	6.23	120.82	117.70
54	BA	2286	G	C1'-O4'-C4'	-6.23	104.91	109.90
21	AA	935	A	C5-C6-N1	6.23	120.81	117.70
21	AA	1157	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	1438	U	O4'-C1'-N1	6.23	113.19	108.20
54	BA	2276	G	C5'-C4'-C3'	-6.23	106.03	116.00
22	A1	14	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	243	A	C5-C6-N1	6.23	120.81	117.70
21	AA	1012	A	C5-C6-N1	6.23	120.81	117.70
54	BA	19	A	C5-C6-N1	6.23	120.81	117.70
54	BA	178	G	N7-C8-N9	6.23	116.21	113.10
54	BA	1286	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	2736	A	C5-C6-N1	6.23	120.81	117.70
21	AA	379	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	658	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	834	G	N7-C8-N9	6.23	116.21	113.10
54	BA	9	G	N3-C2-N2	-6.22	115.54	119.90
54	BA	68	G	N1-C6-O6	-6.22	116.17	119.90
21	AA	221	C	N3-C2-O2	-6.22	117.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	341	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1419	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1973	G	N1-C6-O6	-6.22	116.17	119.90
21	AA	186	C	N1-C2-O2	6.22	122.63	118.90
21	AA	1331	G	N3-C2-N2	-6.22	115.55	119.90
54	BA	183	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	253	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	324	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	565	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1746	A	C5-C6-N1	6.22	120.81	117.70
54	BA	2675	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	605	U	C5-C6-N1	-6.22	119.59	122.70
21	AA	1384	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	1418	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	262	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	787	C	N1-C2-O2	6.22	122.63	118.90
21	AA	459	A	C5-C6-N1	6.21	120.81	117.70
21	AA	1133	G	N1-C6-O6	-6.21	116.17	119.90
54	BA	1211	C	N1-C2-O2	6.21	122.63	118.90
54	BA	1617	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2417	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1307	A	N1-C6-N6	-6.21	114.87	118.60
54	BA	2783	U	C5-C6-N1	-6.21	119.59	122.70
21	AA	1509	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1246	A	C5-C6-N1	6.21	120.81	117.70
54	BA	2176	A	C6-C5-N7	6.21	136.65	132.30
55	BB	91	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	306	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1588	G	N1-C6-O6	-6.21	116.17	119.90
54	BA	2238	G	N3-C4-C5	-6.21	125.50	128.60
21	AA	1229	A	C5-C6-N1	6.21	120.80	117.70
54	BA	51	G	N1-C6-O6	-6.21	116.18	119.90
54	BA	1434	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1434	A	C2-N3-C4	6.21	113.70	110.60
54	BA	1498	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	1603	A	C4-C5-C6	-6.21	113.90	117.00
21	AA	893	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	1022	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	870	U	O4'-C1'-N1	6.21	113.16	108.20
54	BA	1597	A	C4-C5-C6	-6.21	113.90	117.00
1	AB	19	THR	C-N-CA	6.20	137.21	121.70
21	AA	1223	C	N3-C4-C5	6.20	124.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1263	U	O4'-C1'-N1	6.20	113.16	108.20
54	BA	1480	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	923	A	N1-C6-N6	-6.20	114.88	118.60
54	BA	247	G	C5'-C4'-O4'	6.20	116.54	109.10
54	BA	1175	A	C5-C6-N1	6.20	120.80	117.70
54	BA	1290	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1934	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1492	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	466	A	C5-C6-N1	6.20	120.80	117.70
54	BA	502	A	O4'-C1'-N9	6.20	113.16	108.20
21	AA	873	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1111	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	145	C	N1-C2-O2	6.20	122.62	118.90
54	BA	2503	A	C5-C6-N1	6.19	120.80	117.70
36	BN	30	ARG	NE-CZ-NH1	6.19	123.40	120.30
54	BA	1313	U	N3-C2-O2	-6.19	117.86	122.20
54	BA	2103	C	O4'-C1'-N1	6.19	113.15	108.20
21	AA	1066	C	N3-C4-C5	6.19	124.38	121.90
54	BA	574	A	C5-C6-N1	6.19	120.80	117.70
54	BA	626	A	C5-C6-N1	6.19	120.80	117.70
21	AA	532	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	1302	C	N1-C2-O2	6.19	122.61	118.90
4	AE	92	ARG	NE-CZ-NH2	-6.19	117.21	120.30
21	AA	647	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	708	C	N3-C2-O2	-6.19	117.57	121.90
22	A1	38	A	C6-C5-N7	6.19	136.63	132.30
55	BB	81	G	N1-C6-O6	-6.19	116.19	119.90
21	AA	817	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	983	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	1236	A	N1-C6-N6	-6.18	114.89	118.60
54	BA	877	A	C5-C6-N1	6.18	120.79	117.70
54	BA	959	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2048	G	N9-C4-C5	6.18	107.87	105.40
24	A3	11	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	276	U	O4'-C1'-N1	6.18	113.15	108.20
54	BA	1237	A	N1-C6-N6	-6.18	114.89	118.60
54	BA	2088	A	C5-C6-N1	6.18	120.79	117.70
54	BA	2760	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	560	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	1641	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1715	G	C5-C6-N1	6.18	114.59	111.50
54	BA	2518	A	C4-C5-C6	-6.18	113.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	113	C	N3-C4-C5	6.18	124.37	121.90
54	BA	362	A	C5-C6-N1	6.18	120.79	117.70
54	BA	1344	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	2851	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2227	A	C5-C6-N1	6.18	120.79	117.70
54	BA	2427	C	O4'-C1'-N1	6.18	113.14	108.20
21	AA	169	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	182	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	1295	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1435	G	N3-C2-N2	-6.17	115.58	119.90
54	BA	2476	A	C5-C6-N1	6.17	120.79	117.70
21	AA	586	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1837	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1196	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1451	C	N1-C2-O2	6.17	122.60	118.90
54	BA	2436	G	N1-C6-O6	-6.17	116.20	119.90
54	BA	2513	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	712	A	C5-C6-N1	6.17	120.78	117.70
54	BA	349	U	C5-C6-N1	-6.17	119.62	122.70
54	BA	540	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	823	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2560	A	C5-C6-N1	6.17	120.78	117.70
21	AA	846	G	N3-C4-C5	-6.17	125.52	128.60
21	AA	1101	A	C5-C6-N1	6.17	120.78	117.70
21	AA	1225	A	C5-C6-N1	6.17	120.78	117.70
54	BA	718	A	C2-N3-C4	6.17	113.68	110.60
54	BA	1082	U	C5-C6-N1	-6.17	119.62	122.70
54	BA	1744	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	1886	U	O4'-C1'-N1	6.17	113.13	108.20
54	BA	1909	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2309	A	C5-C6-N1	6.17	120.78	117.70
21	AA	648	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	272	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	1061	G	N1-C6-O6	-6.16	116.20	119.90
21	AA	1465	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	177	G	N3-C2-N2	-6.16	115.59	119.90
54	BA	1217	U	O4'-C1'-N1	6.16	113.13	108.20
54	BA	1759	A	C5-C6-N1	6.16	120.78	117.70
54	BA	2603	G	C5-C6-N1	6.16	114.58	111.50
54	BA	1306	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1431	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	795	C	N1-C2-O2	6.16	122.60	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	847	U	C3'-C2'-C1'	6.16	106.43	101.50
54	BA	2525	G	N1-C6-O6	-6.16	116.20	119.90
21	AA	967	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	61	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1495	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1849	G	N1-C6-O6	-6.16	116.20	119.90
54	BA	1583	A	C5-C6-N1	6.16	120.78	117.70
38	BP	50	ARG	NE-CZ-NH1	6.16	123.38	120.30
54	BA	311	A	C5-C6-N1	6.16	120.78	117.70
54	BA	354	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1438	U	C5-C6-N1	-6.16	119.62	122.70
54	BA	1699	G	N3-C2-N2	-6.16	115.59	119.90
54	BA	1798	U	C5-C6-N1	-6.16	119.62	122.70
1	AB	112	ARG	NE-CZ-NH1	6.15	123.38	120.30
21	AA	1399	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2067	G	N1-C6-O6	-6.15	116.21	119.90
54	BA	397	U	N3-C2-O2	-6.15	117.89	122.20
54	BA	620	G	N7-C8-N9	6.15	116.18	113.10
54	BA	1001	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	1918	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	1918	A	C5-C6-N1	6.15	120.78	117.70
54	BA	1417	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	1860	G	N1-C6-O6	-6.15	116.21	119.90
54	BA	2268	A	C5'-C4'-O4'	6.15	116.48	109.10
54	BA	2350	C	O4'-C1'-N1	6.15	113.12	108.20
21	AA	1413	A	N1-C6-N6	-6.15	114.91	118.60
54	BA	1862	G	N3-C2-N2	-6.15	115.59	119.90
54	BA	2289	G	N3-C4-C5	-6.15	125.53	128.60
21	AA	1289	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	192	C	O4'-C1'-N1	6.15	113.12	108.20
54	BA	1305	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	1834	U	O4'-C4'-C3'	6.15	111.02	106.10
54	BA	64	A	C4-C5-C6	-6.15	113.93	117.00
45	BW	38	ARG	NE-CZ-NH1	6.14	123.37	120.30
55	BB	27	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	497	G	C5-C6-N1	6.14	114.57	111.50
54	BA	320	A	C5-C6-N1	6.14	120.77	117.70
54	BA	541	A	O4'-C1'-N9	6.14	113.11	108.20
54	BA	1385	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	2356	U	C5-C6-N1	-6.14	119.63	122.70
54	BA	1929	G	N1-C6-O6	-6.14	116.22	119.90
21	AA	286	C	N3-C2-O2	-6.14	117.60	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	457	G	N1-C6-O6	-6.14	116.22	119.90
21	AA	1396	A	C5-C6-N1	6.14	120.77	117.70
54	BA	609	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1669	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1098	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	865	C	N3-C2-O2	-6.14	117.60	121.90
42	BT	3	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	229	C	N1-C2-O2	6.14	122.58	118.90
54	BA	812	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1036	G	N3-C4-C5	-6.14	125.53	128.60
54	BA	2717	C	N1-C2-O2	6.14	122.58	118.90
55	BB	106	G	C5-C6-N1	6.14	114.57	111.50
7	AH	76	ARG	NE-CZ-NH1	6.13	123.37	120.30
21	AA	795	C	O4'-C1'-N1	6.13	113.11	108.20
21	AA	892	A	C5-C6-N1	6.13	120.77	117.70
24	A3	73	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	278	A	N1-C6-N6	-6.13	114.92	118.60
21	AA	859	G	N1-C6-O6	-6.13	116.22	119.90
54	BA	581	C	O4'-C1'-N1	6.13	113.11	108.20
54	BA	1768	C	N3-C4-C5	6.13	124.35	121.90
54	BA	1265	A	C5-C6-N1	6.13	120.77	117.70
54	BA	1768	C	N1-C2-O2	6.13	122.58	118.90
54	BA	2184	A	C5-C6-N1	6.13	120.77	117.70
21	AA	1113	C	N1-C2-O2	6.13	122.58	118.90
27	BE	40	ARG	NE-CZ-NH1	6.13	123.36	120.30
29	BG	148	ARG	NE-CZ-NH1	6.13	123.36	120.30
21	AA	909	A	C5-C6-N1	6.13	120.77	117.70
21	AA	1403	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	925	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	1706	C	N3-C2-O2	-6.13	117.61	121.90
56	B5	71	ARG	NE-CZ-NH1	6.13	123.36	120.30
24	A3	66	C	O4'-C1'-N1	6.13	113.10	108.20
28	BF	111	ARG	NE-CZ-NH1	6.13	123.36	120.30
54	BA	1661	G	C5'-C4'-O4'	6.13	116.45	109.10
21	AA	15	G	C5-C6-N1	6.12	114.56	111.50
21	AA	1030	U	N3-C2-O2	-6.12	117.91	122.20
54	BA	801	G	N3-C2-N2	-6.12	115.61	119.90
54	BA	2602	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2863	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	669	G	N1-C6-O6	-6.12	116.23	119.90
54	BA	2576	G	N1-C6-O6	-6.12	116.23	119.90
54	BA	153	U	O4'-C1'-N1	6.12	113.10	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	951	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	1021	A	C4-C5-C6	-6.12	113.94	117.00
34	BL	33	ARG	NE-CZ-NH1	6.12	123.36	120.30
54	BA	227	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	284	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	2837	A	C5-C6-N1	6.12	120.76	117.70
55	BB	91	C	N1-C2-O2	6.12	122.57	118.90
21	AA	874	G	C5-C6-N1	6.12	114.56	111.50
54	BA	2627	G	N3-C2-N2	-6.12	115.62	119.90
54	BA	305	C	O4'-C1'-N1	6.12	113.09	108.20
54	BA	488	G	C5-C6-N1	6.12	114.56	111.50
54	BA	501	A	C5-C6-N1	6.12	120.76	117.70
21	AA	304	U	O4'-C1'-N1	6.12	113.09	108.20
21	AA	306	A	N1-C6-N6	-6.12	114.93	118.60
21	AA	663	A	N1-C6-N6	-6.12	114.93	118.60
21	AA	958	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	1306	A	C5-C6-N1	6.12	120.76	117.70
54	BA	1307	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2082	A	N1-C6-N6	-6.12	114.93	118.60
21	AA	1306	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	256	A	C5-C6-N1	6.11	120.76	117.70
54	BA	2055	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	692	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2071	A	C4-C5-C6	-6.11	113.94	117.00
55	BB	63	C	O4'-C1'-N1	6.11	113.09	108.20
21	AA	670	G	O4'-C1'-N9	6.11	113.09	108.20
54	BA	1064	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1135	C	N1-C2-O2	6.11	122.57	118.90
54	BA	1167	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2045	C	N1-C2-O2	6.11	122.57	118.90
18	AS	40	PHE	CB-CG-CD2	-6.11	116.52	120.80
54	BA	1294	U	O4'-C1'-N1	6.11	113.09	108.20
54	BA	1516	G	N1-C6-O6	-6.11	116.23	119.90
21	AA	372	C	N1-C2-O2	6.11	122.56	118.90
54	BA	442	G	N9-C4-C5	6.11	107.84	105.40
54	BA	2551	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2597	G	N1-C6-O6	-6.11	116.24	119.90
54	BA	2893	A	C5-C6-N1	6.11	120.75	117.70
55	BB	50	A	C4-C5-C6	-6.11	113.95	117.00
21	AA	334	C	O4'-C1'-N1	6.11	113.08	108.20
21	AA	1234	C	N1-C2-O2	6.11	122.56	118.90
25	BC	181	ARG	NE-CZ-NH2	-6.11	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	32	C	N3-C4-C5	6.11	124.34	121.90
54	BA	257	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	1928	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	2339	C	N1-C2-O2	6.11	122.56	118.90
21	AA	777	A	C5-C6-N1	6.10	120.75	117.70
54	BA	809	G	C8-N9-C4	-6.10	103.96	106.40
21	AA	964	A	N1-C6-N6	-6.10	114.94	118.60
21	AA	1390	U	N1-C2-N3	6.10	118.56	114.90
54	BA	97	C	O4'-C1'-N1	6.10	113.08	108.20
54	BA	2901	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	974	A	N1-C6-N6	-6.10	114.94	118.60
54	BA	1015	U	O4'-C1'-N1	6.10	113.08	108.20
54	BA	1340	U	N3-C2-O2	-6.10	117.93	122.20
54	BA	2226	C	N3-C4-N4	-6.10	113.73	118.00
54	BA	2669	G	O4'-C1'-N9	6.10	113.08	108.20
55	BB	97	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1150	A	C4-C5-C6	-6.10	113.95	117.00
44	BV	18	ARG	NE-CZ-NH1	6.10	123.35	120.30
54	BA	222	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	442	G	O4'-C1'-N9	6.10	113.08	108.20
54	BA	594	U	O4'-C1'-N1	6.10	113.08	108.20
54	BA	1010	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2424	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	946	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	1279	G	O4'-C1'-N9	6.09	113.08	108.20
54	BA	2432	A	N1-C6-N6	-6.09	114.94	118.60
54	BA	290	U	O4'-C1'-N1	6.09	113.08	108.20
54	BA	2805	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	560	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	1275	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	2330	G	O4'-C1'-N9	6.09	113.07	108.20
54	BA	2473	U	O4'-C1'-N1	6.09	113.07	108.20
54	BA	2645	G	C5-C6-N1	6.09	114.55	111.50
21	AA	117	G	C5-C6-N1	6.09	114.54	111.50
21	AA	408	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	702	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	1274	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	921	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	1526	C	N3-C2-O2	-6.09	117.64	121.90
6	AG	94	ARG	NE-CZ-NH1	6.09	123.34	120.30
54	BA	794	A	C5-C6-N1	6.09	120.74	117.70
54	BA	2505	G	N1-C6-O6	-6.09	116.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	432	A	C4-C5-C6	-6.09	113.96	117.00
21	AA	1325	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	74	A	N1-C6-N6	-6.09	114.95	118.60
54	BA	203	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	69	C	N1-C2-O2	6.08	122.55	118.90
54	BA	1100	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	78	A	C6-C5-N7	6.08	136.56	132.30
21	AA	648	A	N1-C6-N6	-6.08	114.95	118.60
22	A1	26	A	C4-C5-C6	-6.08	113.96	117.00
24	A3	69	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	752	A	C5-C6-N1	6.08	120.74	117.70
55	BB	58	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	71	A	C5-C6-N1	6.08	120.74	117.70
21	AA	726	C	N1-C2-O2	6.08	122.55	118.90
21	AA	896	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	1502	A	C5-C6-N1	6.08	120.74	117.70
54	BA	592	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2020	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2238	G	N1-C6-O6	-6.08	116.25	119.90
54	BA	1127	A	C5-C6-N1	6.08	120.74	117.70
21	AA	872	A	O4'-C1'-N9	6.08	113.06	108.20
54	BA	1130	U	O4'-C1'-N1	6.08	113.06	108.20
54	BA	1557	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	782	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1345	C	N1-C2-O2	6.08	122.55	118.90
21	AA	274	A	C5-C6-N1	6.08	120.74	117.70
21	AA	1341	U	N3-C2-O2	-6.08	117.95	122.20
54	BA	1382	G	C8-N9-C4	-6.08	103.97	106.40
54	BA	1569	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2778	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	9	G	N9-C4-C5	6.07	107.83	105.40
54	BA	37	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2129	C	O4'-C1'-N1	6.07	113.06	108.20
36	BN	17	ARG	NE-CZ-NH1	6.07	123.34	120.30
54	BA	267	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1942	C	O4'-C1'-N1	6.07	113.06	108.20
54	BA	2699	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2885	G	N1-C6-O6	-6.07	116.26	119.90
54	BA	246	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	426	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1028	A	C5-C6-N1	6.07	120.73	117.70
22	A1	25	C	N3-C2-O2	-6.07	117.65	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	109	C	O4'-C1'-N1	6.07	113.06	108.20
21	AA	206	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	596	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	897	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	1531	A	C5-C6-N1	6.07	120.73	117.70
33	BK	98	ARG	NE-CZ-NH1	6.07	123.33	120.30
54	BA	890	C	N1-C2-O2	6.07	122.54	118.90
24	A3	22	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	358	U	C3'-C2'-C1'	6.06	106.35	101.50
54	BA	787	C	C5'-C4'-O4'	6.06	116.37	109.10
54	BA	1287	A	C4-C5-C6	-6.06	113.97	117.00
55	BB	34	A	C5-C6-N1	6.06	120.73	117.70
21	AA	1084	G	N9-C4-C5	6.06	107.83	105.40
21	AA	68	G	C5-C6-N1	6.06	114.53	111.50
54	BA	119	A	O4'-C1'-N9	6.06	113.05	108.20
54	BA	1542	U	O4'-C1'-N1	6.06	113.05	108.20
54	BA	1857	G	O4'-C1'-N9	6.06	113.05	108.20
54	BA	2201	G	O4'-C1'-N9	6.06	113.05	108.20
54	BA	2222	C	N1-C2-O2	6.06	122.54	118.90
54	BA	2473	U	N3-C2-O2	-6.06	117.96	122.20
54	BA	2565	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	136	C	N1-C2-O2	6.06	122.53	118.90
21	AA	806	C	N3-C2-O2	-6.06	117.66	121.90
33	BK	70	ARG	NE-CZ-NH1	6.06	123.33	120.30
54	BA	1155	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1612	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1892	C	N3-C2-O2	-6.06	117.66	121.90
1	AB	138	ARG	NE-CZ-NH1	6.06	123.33	120.30
54	BA	1126	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2466	C	N3-C2-O2	-6.06	117.66	121.90
55	BB	47	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	1280	A	C1'-O4'-C4'	-6.05	105.06	109.90
54	BA	344	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	1902	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	2559	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	23	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	701	U	C5-C6-N1	-6.05	119.67	122.70
21	AA	1250	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	2313	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	2535	G	N3-C2-N2	-6.05	115.66	119.90
23	A2	82	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	979	A	C4-C5-C6	-6.05	113.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1531	C	N3-C2-O2	-6.05	117.67	121.90
21	AA	810	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	74	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	1241	A	C2-N3-C4	6.05	113.62	110.60
54	BA	1626	A	C4-C5-C6	-6.05	113.98	117.00
55	BB	51	G	N1-C6-O6	-6.05	116.27	119.90
54	BA	1275	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1386	C	N3-C2-O2	-6.04	117.67	121.90
55	BB	87	U	N3-C2-O2	-6.04	117.97	122.20
21	AA	1520	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	93	G	O4'-C1'-N9	6.04	113.04	108.20
54	BA	2508	G	C5-C6-N1	6.04	114.52	111.50
21	AA	452	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	572	A	N1-C6-N6	-6.04	114.97	118.60
27	BE	49	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	165	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2505	G	C8-N9-C4	-6.04	103.98	106.40
21	AA	750	C	N1-C2-O2	6.04	122.52	118.90
54	BA	1914	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2309	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	412	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	595	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	608	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	1462	C	O4'-C1'-N1	6.04	113.03	108.20
54	BA	727	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	360	G	C5-C6-N1	6.04	114.52	111.50
54	BA	2430	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	52	C	N1-C2-O2	6.04	122.52	118.90
22	A1	65	C	N3-C2-O2	-6.04	117.68	121.90
54	BA	671	C	N1-C2-O2	6.04	122.52	118.90
54	BA	973	A	C4-C5-C6	-6.04	113.98	117.00
55	BB	27	C	N1-C2-O2	6.04	122.52	118.90
21	AA	487	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	746	A	C5-C6-N1	6.03	120.72	117.70
54	BA	546	U	O4'-C1'-N1	6.03	113.03	108.20
54	BA	791	C	O4'-C1'-N1	6.03	113.03	108.20
54	BA	1080	A	C5-C6-N1	6.03	120.72	117.70
54	BA	1800	C	C2-N3-C4	-6.03	116.88	119.90
54	BA	1871	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	307	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	584	G	N3-C4-C5	-6.03	125.58	128.60
21	AA	1021	A	C5-C6-N1	6.03	120.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1184	G	C5-C6-N1	6.03	114.52	111.50
21	AA	1500	A	C5-C6-N1	6.03	120.72	117.70
32	BJ	27	ARG	NE-CZ-NH1	6.03	123.32	120.30
54	BA	922	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1821	A	C6-C5-N7	6.03	136.52	132.30
55	BB	11	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	205	A	C5-C6-N1	6.03	120.72	117.70
21	AA	736	C	O4'-C1'-N1	6.03	113.02	108.20
54	BA	389	G	C8-N9-C4	-6.03	103.99	106.40
54	BA	1207	C	O4'-C1'-N1	6.03	113.02	108.20
21	AA	417	G	N1-C6-O6	-6.03	116.28	119.90
21	AA	635	A	N1-C6-N6	-6.03	114.98	118.60
21	AA	884	U	C3'-C2'-C1'	6.03	106.32	101.50
21	AA	1228	C	N3-C4-C5	6.03	124.31	121.90
47	BY	52	ARG	NE-CZ-NH1	6.03	123.31	120.30
54	BA	472	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	650	C	C6-N1-C2	-6.03	117.89	120.30
54	BA	1428	C	N1-C2-O2	6.03	122.52	118.90
21	AA	770	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	972	C	N3-C2-O2	-6.03	117.68	121.90
37	BO	10	ARG	NH1-CZ-NH2	-6.03	112.77	119.40
54	BA	832	U	O4'-C1'-N1	6.03	113.02	108.20
54	BA	1765	U	O4'-C1'-N1	6.03	113.02	108.20
54	BA	1929	G	N3-C4-C5	-6.03	125.59	128.60
54	BA	372	G	N3-C4-C5	-6.02	125.59	128.60
54	BA	402	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	355	U	C5-C6-N1	-6.02	119.69	122.70
54	BA	1674	G	O4'-C1'-N9	6.02	113.02	108.20
21	AA	1081	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	575	A	C5-C6-N1	6.02	120.71	117.70
54	BA	735	A	O4'-C1'-N9	6.02	113.02	108.20
54	BA	2520	C	N1-C2-O2	6.02	122.51	118.90
54	BA	2691	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	812	G	N3-C4-C5	-6.02	125.59	128.60
21	AA	1437	A	C5-C6-N1	6.02	120.71	117.70
54	BA	812	C	O4'-C1'-N1	6.02	113.01	108.20
54	BA	1395	A	N1-C6-N6	-6.02	114.99	118.60
54	BA	2069	G	C5-C6-N1	6.02	114.51	111.50
54	BA	2679	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2711	A	C5-C6-N1	6.02	120.71	117.70
21	AA	208	U	C5-C6-N1	-6.01	119.69	122.70
21	AA	1059	C	N3-C2-O2	-6.01	117.69	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1150	A	C5-C6-N1	6.01	120.71	117.70
21	AA	1254	A	N1-C6-N6	-6.01	114.99	118.60
21	AA	1378	C	O4'-C1'-N1	6.01	113.01	108.20
33	BK	64	ARG	NE-CZ-NH1	6.01	123.31	120.30
54	BA	355	U	N3-C2-O2	-6.01	117.99	122.20
54	BA	1420	A	O4'-C1'-N9	6.01	113.01	108.20
17	AR	52	ARG	NE-CZ-NH2	-6.01	117.29	120.30
54	BA	2282	G	N1-C6-O6	-6.01	116.29	119.90
21	AA	303	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	1339	A	C5-C6-N1	6.01	120.71	117.70
54	BA	210	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1514	G	N1-C6-O6	-6.01	116.29	119.90
54	BA	1604	C	O4'-C1'-N1	6.01	113.01	108.20
54	BA	1961	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1978	A	C5-C6-N1	6.01	120.71	117.70
21	AA	740	U	O4'-C1'-N1	6.01	113.01	108.20
21	AA	1383	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	160	A	C5-C6-N1	6.01	120.70	117.70
21	AA	857	C	N3-C2-O2	-6.01	117.70	121.90
21	AA	1262	C	N3-C2-O2	-6.01	117.70	121.90
21	AA	1293	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	1415	G	C5'-C4'-C3'	-6.01	106.39	116.00
21	AA	1529	G	N3-C2-N2	-6.01	115.70	119.90
54	BA	723	C	N3-C2-O2	-6.01	117.70	121.90
54	BA	2135	A	N1-C6-N6	-6.01	115.00	118.60
54	BA	2699	C	N3-C4-C5	6.01	124.30	121.90
54	BA	231	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	244	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	564	C	N1-C2-O2	6.00	122.50	118.90
55	BB	4	C	N3-C2-O2	-6.00	117.70	121.90
55	BB	57	A	N1-C6-N6	-6.00	115.00	118.60
21	AA	673	A	C5-C6-N1	6.00	120.70	117.70
21	AA	732	C	N3-C4-C5	6.00	124.30	121.90
21	AA	749	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	989	U	C5-C6-N1	-6.00	119.70	122.70
21	AA	1216	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1437	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2093	G	C5-C6-N1	6.00	114.50	111.50
54	BA	685	A	C5-C6-N1	6.00	120.70	117.70
54	BA	2134	A	C5-C6-N1	6.00	120.70	117.70
54	BA	2241	A	C6-C5-N7	6.00	136.50	132.30
54	BA	2202	U	N3-C2-O2	-6.00	118.00	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	615	G	C5-C6-N1	6.00	114.50	111.50
54	BA	652	U	C5'-C4'-O4'	6.00	116.30	109.10
54	BA	1799	G	N1-C6-O6	-6.00	116.30	119.90
54	BA	2136	G	N3-C2-N2	-6.00	115.70	119.90
21	AA	637	C	N3-C2-O2	-6.00	117.70	121.90
38	BP	87	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	87	U	O4'-C1'-N1	6.00	113.00	108.20
54	BA	1752	C	N3-C2-O2	-6.00	117.70	121.90
24	A3	23	G	N3-C2-N2	-6.00	115.70	119.90
54	BA	1650	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1342	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1741	C	N1-C2-O2	5.99	122.50	118.90
55	BB	8	C	O4'-C1'-N1	5.99	113.00	108.20
54	BA	342	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1790	C	N1-C2-O2	5.99	122.50	118.90
54	BA	1930	G	O4'-C1'-N9	5.99	112.99	108.20
21	AA	626	G	N1-C6-O6	-5.99	116.31	119.90
21	AA	1078	U	C5-C6-N1	-5.99	119.70	122.70
21	AA	1155	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	1390	U	O4'-C1'-N1	5.99	112.99	108.20
54	BA	2097	A	C5-C6-N1	5.99	120.69	117.70
21	AA	347	G	O4'-C1'-N9	5.99	112.99	108.20
24	A3	13	C	N3-C2-O2	-5.99	117.71	121.90
34	BL	47	ARG	NE-CZ-NH1	5.99	123.29	120.30
54	BA	1006	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	1178	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	2198	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	1035	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	99	U	N3-C2-O2	-5.99	118.01	122.20
54	BA	2089	C	N3-C2-O2	-5.99	117.71	121.90
13	AN	41	ARG	NE-CZ-NH1	5.99	123.29	120.30
21	AA	385	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	465	A	C4-C5-C6	-5.99	114.01	117.00
29	BG	54	ARG	NE-CZ-NH1	5.99	123.29	120.30
54	BA	225	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	378	C	N1-C2-O2	5.99	122.49	118.90
54	BA	1095	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1937	A	O4'-C1'-N9	5.99	112.99	108.20
54	BA	2630	G	C5-C6-N1	5.99	114.49	111.50
54	BA	2766	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	1086	U	N3-C2-O2	-5.98	118.01	122.20
24	A3	57	C	N1-C2-O2	5.98	122.49	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	969	G	O4'-C1'-N9	5.98	112.99	108.20
54	BA	1230	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1632	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2119	A	N1-C6-N6	-5.98	115.01	118.60
54	BA	2211	A	C5-C6-N1	5.98	120.69	117.70
4	AE	92	ARG	NE-CZ-NH1	5.98	123.29	120.30
21	AA	615	G	N3-C2-N2	-5.98	115.71	119.90
54	BA	19	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	231	A	N1-C6-N6	-5.98	115.01	118.60
54	BA	2746	U	O4'-C1'-N1	5.98	112.98	108.20
54	BA	2810	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	58	G	C8-N9-C4	-5.98	104.01	106.40
54	BA	2420	C	N3-C4-C5	5.98	124.29	121.90
54	BA	1476	U	O4'-C1'-N1	5.98	112.98	108.20
54	BA	1802	A	C5-C6-N1	5.98	120.69	117.70
54	BA	2191	A	C6-C5-N7	5.98	136.49	132.30
54	BA	2661	G	N1-C6-O6	-5.98	116.31	119.90
21	AA	169	C	O4'-C1'-N1	5.97	112.98	108.20
54	BA	449	A	C5-C6-N1	5.97	120.69	117.70
54	BA	1773	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	2407	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	36	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	533	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	1048	A	N1-C6-N6	-5.97	115.02	118.60
54	BA	1278	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	290	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1782	U	N1-C2-N3	5.97	118.48	114.90
21	AA	98	A	N1-C6-N6	-5.97	115.02	118.60
21	AA	499	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	1317	C	N1-C2-O2	5.97	122.48	118.90
54	BA	565	C	N3-C4-C5	5.97	124.29	121.90
54	BA	633	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	2154	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	1077	G	C5-C6-N1	5.97	114.48	111.50
21	AA	1239	A	O4'-C1'-N9	5.97	112.97	108.20
54	BA	256	A	N1-C6-N6	-5.97	115.02	118.60
54	BA	717	C	N1-C2-O2	5.97	122.48	118.90
54	BA	1102	C	N1-C2-O2	5.97	122.48	118.90
54	BA	1433	A	N1-C6-N6	-5.97	115.02	118.60
21	AA	314	C	N3-C4-C5	5.97	124.29	121.90
21	AA	1328	C	N1-C2-O2	5.97	122.48	118.90
54	BA	60	G	N3-C4-C5	-5.97	125.62	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1946	U	O4'-C1'-N1	5.97	112.97	108.20
8	AI	94	ARG	NE-CZ-NH2	-5.96	117.32	120.30
21	AA	211	G	N1-C6-O6	-5.96	116.32	119.90
54	BA	22	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	51	G	N9-C4-C5	5.96	107.79	105.40
54	BA	485	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	2394	C	N3-C2-O2	-5.96	117.72	121.90
21	AA	490	C	N1-C2-O2	5.96	122.48	118.90
54	BA	1258	U	O4'-C1'-N1	5.96	112.97	108.20
54	BA	1427	A	C6-C5-N7	5.96	136.47	132.30
54	BA	1586	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1609	A	C5-C6-N1	5.96	120.68	117.70
54	BA	2800	A	C5-C6-N1	5.96	120.68	117.70
21	AA	930	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	994	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1164	C	O4'-C1'-N1	5.96	112.97	108.20
21	AA	236	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	653	U	O4'-C1'-N1	5.96	112.97	108.20
21	AA	1136	C	N3-C2-O2	-5.96	117.73	121.90
24	A3	63	C	N1-C2-O2	5.96	122.47	118.90
28	BF	166	ARG	NE-CZ-NH1	5.96	123.28	120.30
54	BA	1045	C	N1-C2-O2	5.96	122.47	118.90
54	BA	8	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	53	A	C5-C6-N1	5.96	120.68	117.70
54	BA	487	C	N1-C2-O2	5.96	122.47	118.90
54	BA	2499	C	N3-C4-C5	5.96	124.28	121.90
54	BA	2722	G	N1-C6-O6	-5.96	116.33	119.90
21	AA	114	U	O4'-C1'-N1	5.95	112.96	108.20
21	AA	418	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	848	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	1224	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	1857	G	C8-N9-C4	-5.95	104.02	106.40
54	BA	2533	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	2682	A	C5-C6-N1	5.95	120.68	117.70
54	BA	2741	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	547	A	C1'-O4'-C4'	-5.95	105.14	109.90
21	AA	51	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	132	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	1327	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	1508	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	666	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	1285	A	C6-C5-N7	5.95	136.47	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1298	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	1602	U	C5-C6-N1	-5.95	119.72	122.70
54	BA	1770	G	N3-C2-N2	-5.95	115.73	119.90
54	BA	2273	A	C5-C6-N1	5.95	120.67	117.70
54	BA	2540	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	2667	C	N3-C2-O2	-5.95	117.73	121.90
55	BB	108	A	C5-C6-N1	5.95	120.67	117.70
54	BA	340	A	N1-C6-N6	-5.95	115.03	118.60
54	BA	571	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	2538	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	2658	C	N3-C2-O2	-5.95	117.74	121.90
21	AA	493	A	O4'-C1'-N9	5.95	112.96	108.20
24	A3	63	C	N3-C4-C5	5.95	124.28	121.90
54	BA	2732	G	C1'-O4'-C4'	-5.95	105.14	109.90
55	BB	111	U	C5-C6-N1	-5.95	119.73	122.70
54	BA	968	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	2519	U	O4'-C1'-N1	5.95	112.96	108.20
55	BB	106	G	N1-C6-O6	-5.95	116.33	119.90
22	A1	72	C	N3-C4-C5	5.94	124.28	121.90
54	BA	182	A	N1-C6-N6	-5.94	115.03	118.60
54	BA	822	G	N1-C6-O6	-5.94	116.33	119.90
54	BA	1128	G	C1'-O4'-C4'	-5.94	105.14	109.90
21	AA	611	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	818	G	O4'-C1'-N9	5.94	112.95	108.20
21	AA	926	G	N1-C6-O6	-5.94	116.33	119.90
51	B2	41	ARG	NE-CZ-NH1	5.94	123.27	120.30
54	BA	209	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	305	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	650	C	C4'-C3'-C2'	-5.94	96.66	102.60
54	BA	873	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1550	C	N1-C2-O2	5.94	122.47	118.90
54	BA	1665	A	C6-C5-N7	5.94	136.46	132.30
54	BA	2200	C	N3-C2-O2	-5.94	117.74	121.90
22	A1	69	A	C5-C6-N1	5.94	120.67	117.70
54	BA	212	G	O4'-C1'-N9	5.94	112.95	108.20
54	BA	1092	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1165	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	2757	A	C4-C5-C6	-5.94	114.03	117.00
55	BB	12	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	920	U	N3-C2-O2	-5.94	118.04	122.20
27	BE	170	ARG	NE-CZ-NH1	5.94	123.27	120.30
54	BA	719	C	N1-C2-O2	5.94	122.46	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1562	U	C5-C6-N1	-5.94	119.73	122.70
54	BA	1874	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2426	A	C5-C6-N1	5.94	120.67	117.70
21	AA	941	G	N1-C6-O6	-5.94	116.34	119.90
22	A1	70	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	613	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	2092	U	N1-C2-N3	5.94	118.46	114.90
54	BA	2190	G	C8-N9-C4	-5.94	104.03	106.40
21	AA	1005	A	C6-C5-N7	5.93	136.45	132.30
42	BT	77	ARG	NE-CZ-NH1	5.93	123.27	120.30
54	BA	43	G	C5-C6-N1	5.93	114.47	111.50
54	BA	246	C	O4'-C1'-N1	5.93	112.95	108.20
54	BA	1081	U	C5-C6-N1	-5.93	119.73	122.70
54	BA	1981	A	O4'-C1'-N9	5.93	112.95	108.20
54	BA	2299	U	O4'-C1'-N1	5.93	112.95	108.20
54	BA	2799	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	38	G	N9-C1'-C2'	-5.93	105.47	112.00
21	AA	57	G	N1-C6-O6	-5.93	116.34	119.90
21	AA	658	C	N3-C4-C5	5.93	124.27	121.90
21	AA	821	G	C5-C6-N1	5.93	114.47	111.50
21	AA	1228	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1271	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	541	A	C5-C6-N1	5.93	120.67	117.70
54	BA	1481	U	C5-C6-N1	-5.93	119.73	122.70
54	BA	2336	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	99	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	334	C	N3-C2-O2	-5.93	117.75	121.90
24	A3	3	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	727	G	C5-C6-N1	5.93	114.47	111.50
54	BA	967	U	O4'-C1'-N1	5.93	112.94	108.20
21	AA	680	C	O4'-C1'-N1	5.93	112.94	108.20
54	BA	1241	A	O4'-C1'-N9	5.93	112.94	108.20
54	BA	1705	A	C5-C6-N1	5.93	120.66	117.70
54	BA	2806	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	8	A	C4-C5-C6	-5.93	114.04	117.00
22	A1	28	C	O4'-C1'-N1	5.93	112.94	108.20
25	BC	174	ARG	NE-CZ-NH1	5.93	123.26	120.30
54	BA	677	A	C5-C6-N1	5.93	120.66	117.70
54	BA	817	C	O4'-C1'-N1	5.93	112.94	108.20
54	BA	1347	A	C5-C6-N1	5.93	120.66	117.70
21	AA	913	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	1509	C	N1-C2-O2	5.92	122.45	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	48	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1680	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2174	C	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2516	A	C4-C5-C6	-5.92	114.04	117.00
55	BB	37	C	O4'-C1'-N1	5.92	112.94	108.20
55	BB	102	G	C5-C6-N1	5.92	114.46	111.50
21	AA	197	A	C5-C6-N1	5.92	120.66	117.70
21	AA	210	C	N3-C2-O2	-5.92	117.75	121.90
21	AA	619	U	N3-C2-O2	-5.92	118.05	122.20
54	BA	42	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1515	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1699	G	C5-C6-N1	5.92	114.46	111.50
54	BA	1804	C	N1-C2-O2	5.92	122.45	118.90
21	AA	344	A	C2-N3-C4	5.92	113.56	110.60
54	BA	732	C	O4'-C1'-N1	5.92	112.94	108.20
54	BA	1351	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1513	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	1980	G	C5-C6-N1	5.92	114.46	111.50
54	BA	2802	G	N1-C6-O6	-5.92	116.35	119.90
21	AA	702	A	C3'-C2'-C1'	5.92	106.24	101.50
21	AA	1408	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	1499	A	N1-C6-N6	-5.92	115.05	118.60
21	AA	642	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	79	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	526	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2762	C	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2764	A	N1-C6-N6	-5.92	115.05	118.60
54	BA	2862	G	C5-C6-N1	5.92	114.46	111.50
21	AA	1391	U	C5-C6-N1	-5.92	119.74	122.70
54	BA	577	G	N3-C4-C5	-5.92	125.64	128.60
21	AA	1284	C	O4'-C1'-N1	5.91	112.93	108.20
54	BA	1255	U	C1'-O4'-C4'	-5.91	105.17	109.90
54	BA	1442	U	N3-C2-O2	-5.91	118.06	122.20
54	BA	1646	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	1735	A	O4'-C1'-N9	5.91	112.93	108.20
43	BU	85	ARG	NE-CZ-NH1	5.91	123.26	120.30
54	BA	578	G	C5-C6-N1	5.91	114.46	111.50
54	BA	1502	A	C5-C6-N1	5.91	120.66	117.70
21	AA	199	A	C5-C6-N1	5.91	120.66	117.70
21	AA	582	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	794	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1123	C	C6-N1-C2	-5.91	117.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2050	C	N1-C2-O2	5.91	122.45	118.90
55	BB	111	U	O4'-C1'-N1	5.91	112.93	108.20
21	AA	309	A	C5-C6-N1	5.91	120.66	117.70
54	BA	740	C	N1-C2-O2	5.91	122.44	118.90
54	BA	1435	G	C8-N9-C4	-5.91	104.04	106.40
54	BA	1512	C	O4'-C1'-N1	5.91	112.93	108.20
21	AA	518	C	N1-C2-O2	5.91	122.44	118.90
3	AD	72	ARG	NE-CZ-NH1	5.91	123.25	120.30
21	AA	315	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	796	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	2077	A	C5-C6-N1	5.91	120.65	117.70
54	BA	2575	C	N3-C4-C5	5.91	124.26	121.90
21	AA	353	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	1232	U	C5-C6-N1	-5.90	119.75	122.70
54	BA	2170	A	C6-C5-N7	5.90	136.43	132.30
54	BA	2475	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1067	A	C4-C5-C6	-5.90	114.05	117.00
34	BL	123	ARG	NE-CZ-NH1	5.90	123.25	120.30
54	BA	601	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	833	A	C5-C6-N1	5.90	120.65	117.70
54	BA	908	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	2267	A	O4'-C4'-C3'	5.90	110.82	106.10
21	AA	839	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1279	G	N1-C6-O6	-5.90	116.36	119.90
54	BA	897	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	2346	A	C6-C5-N7	5.90	136.43	132.30
54	BA	2505	G	N3-C4-C5	-5.90	125.65	128.60
54	BA	2858	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1432	G	N1-C6-O6	-5.90	116.36	119.90
35	BM	114	ARG	NE-CZ-NH1	5.90	123.25	120.30
54	BA	262	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	2692	G	N3-C4-C5	-5.90	125.65	128.60
21	AA	96	U	O4'-C1'-N1	5.90	112.92	108.20
21	AA	1019	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	1282	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	346	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1940	U	N3-C2-O2	-5.90	118.07	122.20
54	BA	2394	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	1535	A	C5-C6-N1	5.90	120.65	117.70
21	AA	1109	C	N1-C2-O2	5.89	122.44	118.90
24	A3	20	G	C5-C6-N1	5.89	114.45	111.50
55	BB	43	C	N3-C2-O2	-5.89	117.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	60	A	P-O3'-C3'	5.89	126.77	119.70
21	AA	1252	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	199	A	O4'-C1'-N9	5.89	112.91	108.20
54	BA	1113	U	N1-C2-N3	5.89	118.44	114.90
54	BA	1713	A	C5-C6-N1	5.89	120.65	117.70
54	BA	176	A	C5-C6-N1	5.89	120.65	117.70
54	BA	2199	A	N1-C6-N6	-5.89	115.07	118.60
21	AA	695	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	1045	C	N1-C2-O2	5.89	122.43	118.90
53	B4	24	ARG	NE-CZ-NH1	5.89	123.25	120.30
54	BA	481	G	C1'-O4'-C4'	-5.89	105.19	109.90
54	BA	1072	C	N1-C2-O2	5.89	122.43	118.90
21	AA	48	C	N1-C2-O2	5.89	122.43	118.90
21	AA	1412	C	N1-C2-O2	5.89	122.43	118.90
54	BA	552	U	C5'-C4'-O4'	5.89	116.17	109.10
54	BA	1584	U	C5-C6-N1	-5.89	119.76	122.70
54	BA	1919	A	C5-C6-N1	5.89	120.64	117.70
21	AA	575	G	P-O3'-C3'	5.89	126.76	119.70
21	AA	705	G	C5-C6-N1	5.89	114.44	111.50
54	BA	34	U	O4'-C1'-N1	5.89	112.91	108.20
54	BA	1039	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	1052	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	968	A	C4-C5-C6	-5.88	114.06	117.00
22	A1	49	G	C5-C6-N1	5.88	114.44	111.50
54	BA	1208	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	1708	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	2459	A	C4-C5-C6	-5.88	114.06	117.00
24	A3	36	A	C5-C6-N1	5.88	120.64	117.70
33	BK	71	ARG	NE-CZ-NH1	5.88	123.24	120.30
21	AA	556	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	1113	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	1152	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	126	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	59	A	N1-C6-N6	-5.88	115.07	118.60
21	AA	163	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	209	U	N3-C2-O2	-5.88	118.08	122.20
21	AA	744	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	914	A	C5-C6-N1	5.88	120.64	117.70
21	AA	1049	U	P-O3'-C3'	5.88	126.75	119.70
21	AA	1096	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	1102	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	24	G	C8-N9-C4	-5.88	104.05	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	188	C	N1-C2-O2	5.88	122.43	118.90
21	AA	1523	G	C5-C6-N1	5.88	114.44	111.50
54	BA	508	A	C5-C6-N1	5.88	120.64	117.70
54	BA	1384	A	C5-C6-N1	5.88	120.64	117.70
55	BB	115	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	945	G	C5-C6-N1	5.87	114.44	111.50
21	AA	1046	A	N1-C6-N6	-5.87	115.08	118.60
21	AA	1082	A	C6-C5-N7	5.87	136.41	132.30
21	AA	1120	C	O4'-C1'-N1	5.87	112.90	108.20
54	BA	1826	G	C8-N9-C4	-5.87	104.05	106.40
21	AA	1061	G	N9-C4-C5	5.87	107.75	105.40
21	AA	1238	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	1522	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2074	U	C5-C6-N1	-5.87	119.77	122.70
54	BA	2123	G	N1-C6-O6	-5.87	116.38	119.90
54	BA	2340	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2511	U	O4'-C1'-N1	5.87	112.90	108.20
21	AA	1273	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2298	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2320	U	C1'-O4'-C4'	-5.87	105.20	109.90
21	AA	1495	U	O4'-C1'-N1	5.87	112.89	108.20
54	BA	240	C	N1-C2-O2	5.87	122.42	118.90
54	BA	1382	G	N3-C4-C5	-5.87	125.67	128.60
54	BA	1945	G	C3'-C2'-C1'	5.87	106.19	101.50
54	BA	2160	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1830	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2847	U	O4'-C1'-N1	5.87	112.89	108.20
55	BB	3	C	O4'-C1'-N1	5.87	112.89	108.20
54	BA	159	G	C5-C6-N1	5.87	114.43	111.50
54	BA	443	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	544	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1575	C	O4'-C1'-N1	5.87	112.89	108.20
54	BA	2662	A	C5-C6-N1	5.87	120.63	117.70
54	BA	2832	U	O4'-C1'-N1	5.87	112.89	108.20
54	BA	987	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1977	A	N1-C6-N6	-5.86	115.08	118.60
55	BB	34	A	C4-C5-C6	-5.86	114.07	117.00
12	AM	2	ARG	NE-CZ-NH1	5.86	123.23	120.30
21	AA	620	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	704	A	C5-C6-N1	5.86	120.63	117.70
21	AA	980	C	N3-C4-C5	5.86	124.25	121.90
54	BA	1780	A	C5-C6-N1	5.86	120.63	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2500	U	C1'-O4'-C4'	-5.86	105.21	109.90
54	BA	2824	C	N1-C2-O2	5.86	122.42	118.90
21	AA	831	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	786	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1145	C	O4'-C1'-N1	5.86	112.89	108.20
54	BA	1379	U	N3-C2-O2	-5.86	118.10	122.20
54	BA	1582	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2039	U	O4'-C1'-N1	5.86	112.89	108.20
54	BA	2900	A	C6-C5-N7	5.86	136.40	132.30
3	AD	153	ARG	NE-CZ-NH2	-5.86	117.37	120.30
21	AA	451	A	O4'-C1'-N9	5.86	112.89	108.20
21	AA	1430	A	C5-C6-N1	5.86	120.63	117.70
54	BA	4	U	C5-C6-N1	-5.86	119.77	122.70
54	BA	1893	C	O4'-C1'-N1	5.86	112.89	108.20
55	BB	95	U	N3-C2-O2	-5.86	118.10	122.20
23	A2	91	A	C5-C6-N1	5.86	120.63	117.70
24	A3	44	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	52	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	795	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	915	C	O4'-C1'-N1	5.86	112.88	108.20
54	BA	986	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1947	C	N1-C2-O2	5.86	122.41	118.90
54	BA	2391	G	N1-C6-O6	-5.86	116.39	119.90
21	AA	216	U	C5-C6-N1	-5.85	119.77	122.70
54	BA	130	C	N1-C2-O2	5.85	122.41	118.90
54	BA	1585	C	N1-C2-O2	5.85	122.41	118.90
55	BB	51	G	C8-N9-C4	-5.85	104.06	106.40
21	AA	465	A	N1-C6-N6	-5.85	115.09	118.60
21	AA	842	U	N3-C2-O2	-5.85	118.10	122.20
22	A1	75	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	806	C	N3-C4-C5	5.85	124.24	121.90
54	BA	1786	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	1879	C	N1-C2-O2	5.85	122.41	118.90
21	AA	1055	A	C5'-C4'-C3'	-5.85	106.64	116.00
31	BI	64	ARG	NE-CZ-NH2	-5.85	117.38	120.30
54	BA	1327	A	C4-C5-C6	-5.85	114.08	117.00
21	AA	34	C	C3'-C2'-C1'	-5.85	96.82	101.50
21	AA	164	G	C8-N9-C4	-5.85	104.06	106.40
21	AA	344	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	21	A	C5-C6-N1	5.85	120.62	117.70
54	BA	382	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	654	A	O4'-C1'-N9	5.85	112.88	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1455	G	N1-C6-O6	-5.85	116.39	119.90
54	BA	1607	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	2091	C	N3-C4-C5	5.85	124.24	121.90
54	BA	2285	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	735	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	878	A	C4-C5-C6	-5.85	114.08	117.00
21	AA	1120	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	833	A	O4'-C1'-N9	5.84	112.88	108.20
54	BA	1248	G	C5-C6-N1	5.84	114.42	111.50
54	BA	1363	C	N1-C2-O2	5.84	122.41	118.90
21	AA	340	U	O4'-C1'-N1	5.84	112.88	108.20
21	AA	521	G	N1-C6-O6	-5.84	116.39	119.90
54	BA	2742	G	N1-C6-O6	-5.84	116.39	119.90
21	AA	802	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1791	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1810	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1942	C	N3-C2-O2	-5.84	117.81	121.90
55	BB	15	A	C1'-O4'-C4'	-5.84	105.23	109.90
21	AA	728	A	C2-N3-C4	5.84	113.52	110.60
21	AA	1024	G	N1-C6-O6	-5.84	116.40	119.90
28	BF	94	ARG	NE-CZ-NH1	5.84	123.22	120.30
54	BA	564	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	1974	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	2083	G	C8-N9-C4	-5.84	104.06	106.40
54	BA	2202	U	C5-C6-N1	-5.84	119.78	122.70
54	BA	2226	C	N1-C2-O2	5.84	122.40	118.90
22	A1	53	G	N1-C6-O6	-5.84	116.40	119.90
21	AA	658	C	N1-C2-O2	5.84	122.40	118.90
54	BA	55	G	N1-C6-O6	-5.84	116.40	119.90
54	BA	1692	U	N1-C2-N3	5.84	118.40	114.90
54	BA	1774	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2496	C	N3-C2-O2	-5.84	117.81	121.90
55	BB	49	C	O4'-C1'-N1	5.84	112.87	108.20
21	AA	653	U	N3-C2-O2	-5.83	118.12	122.20
54	BA	2067	G	O4'-C1'-N9	5.83	112.87	108.20
21	AA	1110	A	C5-C6-N1	5.83	120.62	117.70
54	BA	557	C	O4'-C1'-N1	5.83	112.87	108.20
54	BA	2330	G	N1-C6-O6	-5.83	116.40	119.90
21	AA	212	G	C5-C6-N1	5.83	114.42	111.50
21	AA	440	C	O4'-C1'-N1	5.83	112.86	108.20
21	AA	728	A	C6-C5-N7	5.83	136.38	132.30
54	BA	73	A	C5-C6-N1	5.83	120.62	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	732	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2815	C	O4'-C1'-N1	5.83	112.87	108.20
55	BB	116	G	C8-N9-C4	-5.83	104.07	106.40
21	AA	346	G	N3-C4-C5	-5.83	125.69	128.60
21	AA	687	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	868	C	N1-C2-O2	5.83	122.40	118.90
54	BA	397	U	C5-C6-N1	-5.83	119.79	122.70
21	AA	108	G	N3-C4-C5	-5.83	125.69	128.60
21	AA	531	U	N3-C2-O2	-5.83	118.12	122.20
21	AA	1404	C	C6-N1-C2	-5.83	117.97	120.30
54	BA	1453	A	C5-C6-N1	5.83	120.61	117.70
54	BA	2838	G	O4'-C1'-N9	5.83	112.86	108.20
21	AA	174	A	C5-C6-N1	5.83	120.61	117.70
21	AA	718	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	819	A	C4-C5-C6	-5.83	114.09	117.00
22	A1	30	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	340	A	C5-C6-N1	5.83	120.61	117.70
54	BA	353	C	O4'-C1'-N1	5.83	112.86	108.20
54	BA	2358	A	C6-C5-N7	5.83	136.38	132.30
12	AM	106	ARG	NE-CZ-NH1	5.82	123.21	120.30
24	A3	17	C	N1-C2-O2	5.82	122.39	118.90
54	BA	1076	C	N3-C2-O2	-5.82	117.82	121.90
54	BA	1213	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1679	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	1121	U	C5-C6-N1	-5.82	119.79	122.70
21	AA	368	U	C1'-O4'-C4'	-5.82	105.24	109.90
21	AA	685	G	N3-C4-C5	-5.82	125.69	128.60
54	BA	624	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1594	U	C5-C6-N1	-5.82	119.79	122.70
54	BA	2611	C	C6-N1-C2	-5.82	117.97	120.30
16	AQ	63	CYS	CA-C-N	5.82	130.00	117.20
21	AA	287	U	O4'-C1'-N1	5.82	112.86	108.20
21	AA	452	A	C5-C6-N1	5.82	120.61	117.70
54	BA	2038	G	N3-C4-C5	-5.82	125.69	128.60
54	BA	2687	U	N3-C2-O2	-5.82	118.13	122.20
22	A1	19	G	N1-C6-O6	-5.82	116.41	119.90
54	BA	55	G	C5-C6-N1	5.82	114.41	111.50
54	BA	847	U	N3-C2-O2	-5.82	118.13	122.20
54	BA	1133	A	C5-C6-N1	5.82	120.61	117.70
54	BA	1262	A	C5-C6-N1	5.82	120.61	117.70
54	BA	1293	C	O4'-C1'-N1	5.82	112.85	108.20
54	BA	2285	C	N1-C2-O2	5.82	122.39	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2840	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	37	U	N3-C2-O2	-5.82	118.13	122.20
21	AA	405	U	O4'-C1'-N1	5.82	112.85	108.20
21	AA	1076	U	C5-C6-N1	-5.82	119.79	122.70
54	BA	144	A	O4'-C1'-N9	5.82	112.85	108.20
54	BA	486	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1786	A	N1-C6-N6	-5.82	115.11	118.60
54	BA	2084	C	O4'-C1'-N1	5.82	112.85	108.20
54	BA	2213	U	O4'-C1'-N1	5.82	112.85	108.20
21	AA	6	G	C1'-O4'-C4'	-5.81	105.25	109.90
21	AA	90	C	O4'-C1'-N1	5.81	112.85	108.20
54	BA	1408	G	N3-C4-C5	-5.81	125.69	128.60
54	BA	1726	C	N1-C2-O2	5.81	122.39	118.90
54	BA	1819	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2534	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	50	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	119	A	C5-C6-N1	5.81	120.61	117.70
54	BA	239	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	396	G	N9-C4-C5	5.81	107.72	105.40
54	BA	804	A	C3'-C2'-C1'	5.81	106.15	101.50
54	BA	1572	A	N1-C6-N6	-5.81	115.11	118.60
54	BA	2792	A	C5-C6-N1	5.81	120.61	117.70
54	BA	928	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1442	U	O4'-C1'-N1	5.81	112.85	108.20
54	BA	2427	C	N1-C2-O2	5.81	122.39	118.90
21	AA	13	U	O4'-C1'-N1	5.81	112.85	108.20
21	AA	978	A	C4-C5-C6	-5.81	114.10	117.00
21	AA	998	C	N3-C2-O2	-5.81	117.83	121.90
31	BI	102	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
54	BA	357	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	508	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	680	C	O4'-C1'-N1	5.81	112.85	108.20
6	AG	3	ARG	NE-CZ-NH1	5.81	123.20	120.30
7	AH	79	ARG	NE-CZ-NH1	5.81	123.20	120.30
21	AA	460	A	C5-C6-N1	5.81	120.60	117.70
21	AA	918	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	2403	C	N1-C2-O2	5.81	122.39	118.90
54	BA	2670	A	N1-C6-N6	-5.81	115.11	118.60
55	BB	118	C	N3-C4-C5	5.81	124.22	121.90
54	BA	1783	A	C6-C5-N7	5.81	136.36	132.30
21	AA	512	U	C5-C6-N1	-5.80	119.80	122.70
21	AA	1521	C	N3-C2-O2	-5.80	117.84	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	493	G	C5-C6-N1	5.80	114.40	111.50
54	BA	681	G	C5-C6-N1	5.80	114.40	111.50
54	BA	1855	U	O4'-C1'-N1	5.80	112.84	108.20
55	BB	95	U	C5-C6-N1	-5.80	119.80	122.70
24	A3	68	C	N1-C2-O2	5.80	122.38	118.90
54	BA	2079	U	C5-C6-N1	-5.80	119.80	122.70
55	BB	13	G	N3-C2-N2	-5.80	115.84	119.90
21	AA	437	U	O4'-C1'-N1	5.80	112.84	108.20
21	AA	557	G	N1-C6-O6	-5.80	116.42	119.90
21	AA	1239	A	C6-C5-N7	5.80	136.36	132.30
21	AA	1299	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	1053	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1174	U	O4'-C1'-N1	5.80	112.84	108.20
54	BA	1214	A	C5-C6-N1	5.80	120.60	117.70
54	BA	2215	C	O4'-C1'-N1	5.80	112.84	108.20
54	BA	59	U	C5-C6-N1	-5.80	119.80	122.70
54	BA	105	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	2217	G	C5-C6-N1	5.80	114.40	111.50
54	BA	2826	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	758	C	N1-C2-O2	5.80	122.38	118.90
54	BA	1561	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	318	G	C5-C6-N1	5.80	114.40	111.50
21	AA	579	A	C5-C6-N1	5.80	120.60	117.70
54	BA	53	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	139	U	O4'-C1'-N1	5.80	112.84	108.20
54	BA	2608	G	N3-C4-C5	-5.80	125.70	128.60
21	AA	454	G	N3-C4-C5	-5.79	125.70	128.60
21	AA	660	C	N3-C2-O2	-5.79	117.84	121.90
54	BA	1888	G	O4'-C1'-N9	5.79	112.84	108.20
54	BA	1895	C	N1-C2-O2	5.79	122.38	118.90
54	BA	2723	C	N1-C2-O2	5.79	122.38	118.90
21	AA	83	C	N3-C2-O2	-5.79	117.84	121.90
21	AA	183	C	N3-C4-C5	5.79	124.22	121.90
21	AA	1094	G	O4'-C1'-N9	5.79	112.83	108.20
21	AA	1100	C	C2-N3-C4	-5.79	117.00	119.90
21	AA	1523	G	N1-C6-O6	-5.79	116.42	119.90
54	BA	706	A	C5-C6-N1	5.79	120.60	117.70
54	BA	914	G	N1-C6-O6	-5.79	116.42	119.90
54	BA	1877	A	C5-C6-N1	5.79	120.60	117.70
54	BA	2043	C	N3-C2-O2	-5.79	117.84	121.90
54	BA	2166	U	C5-C6-N1	-5.79	119.80	122.70
54	BA	2369	A	N1-C6-N6	-5.79	115.12	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2427	C	N3-C4-C5	5.79	124.22	121.90
21	AA	95	C	N3-C2-O2	-5.79	117.84	121.90
21	AA	330	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	171	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	1103	A	C5-C6-N1	5.79	120.60	117.70
54	BA	1229	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	416	U	O4'-C1'-N1	5.79	112.83	108.20
21	AA	1352	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1264	A	O4'-C1'-N9	5.79	112.83	108.20
54	BA	1754	A	N1-C6-N6	-5.79	115.13	118.60
54	BA	2725	A	C5-C6-N1	5.79	120.59	117.70
54	BA	193	U	N1-C2-N3	5.79	118.37	114.90
54	BA	1929	G	O4'-C1'-N9	5.79	112.83	108.20
54	BA	2730	C	N3-C2-O2	-5.79	117.85	121.90
47	BY	7	ARG	NE-CZ-NH1	5.79	123.19	120.30
54	BA	394	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	885	C	O4'-C1'-N1	5.79	112.83	108.20
54	BA	2725	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	906	A	N1-C6-N6	-5.78	115.13	118.60
21	AA	1509	C	N3-C4-C5	5.78	124.21	121.90
54	BA	78	U	O4'-C1'-N1	5.78	112.83	108.20
54	BA	2210	U	O4'-C1'-N1	5.78	112.83	108.20
54	BA	2480	C	N3-C2-O2	-5.78	117.85	121.90
10	AK	36	ARG	NE-CZ-NH1	5.78	123.19	120.30
21	AA	97	G	C5-C6-N1	5.78	114.39	111.50
54	BA	480	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	975	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	335	C	O4'-C1'-N1	5.78	112.82	108.20
21	AA	653	U	C3'-C2'-C1'	5.78	106.12	101.50
21	AA	1400	C	N3-C2-O2	-5.78	117.85	121.90
21	AA	1412	C	N3-C4-C5	5.78	124.21	121.90
54	BA	1121	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	1402	U	C5-C6-N1	-5.78	119.81	122.70
54	BA	1952	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2018	G	N1-C6-O6	-5.78	116.43	119.90
2	AC	10	ARG	NE-CZ-NH2	-5.78	117.41	120.30
21	AA	1064	G	C8-N9-C4	-5.78	104.09	106.40
54	BA	1099	G	N7-C8-N9	5.78	115.99	113.10
54	BA	2128	G	C8-N9-C4	-5.78	104.09	106.40
21	AA	1161	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	811	U	O4'-C1'-N1	5.78	112.82	108.20
54	BA	1960	A	C6-C5-N7	5.78	136.34	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2651	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	2760	C	O4'-C1'-N1	5.78	112.82	108.20
15	AP	8	ARG	NE-CZ-NH1	5.78	123.19	120.30
21	AA	715	A	O4'-C1'-N9	5.78	112.82	108.20
21	AA	1063	C	N3-C4-C5	5.78	124.21	121.90
35	BM	114	ARG	NE-CZ-NH2	-5.78	117.41	120.30
51	B2	28	ARG	NE-CZ-NH1	5.78	123.19	120.30
54	BA	1149	G	C5'-C4'-O4'	5.78	116.03	109.10
54	BA	1589	U	C5-C6-N1	-5.78	119.81	122.70
54	BA	1797	G	O4'-C1'-N9	5.78	112.82	108.20
54	BA	2111	U	O4'-C1'-N1	5.78	112.82	108.20
55	BB	118	C	N1-C2-O2	5.78	122.36	118.90
21	AA	833	G	N1-C6-O6	-5.77	116.44	119.90
24	A3	63	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	485	C	N1-C2-O2	5.77	122.36	118.90
54	BA	2029	G	O4'-C1'-N9	5.77	112.82	108.20
2	AC	71	ARG	NE-CZ-NH1	5.77	123.19	120.30
21	AA	508	U	C5-C6-N1	-5.77	119.81	122.70
21	AA	917	G	N7-C8-N9	5.77	115.99	113.10
21	AA	1371	G	N3-C2-N2	-5.77	115.86	119.90
21	AA	1465	A	N1-C6-N6	-5.77	115.14	118.60
22	A1	73	A	N1-C6-N6	-5.77	115.14	118.60
54	BA	698	C	N1-C2-O2	5.77	122.36	118.90
54	BA	1697	G	N7-C8-N9	5.77	115.99	113.10
54	BA	2616	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	1477	U	C5-C6-N1	-5.77	119.81	122.70
54	BA	1772	A	O4'-C1'-N9	5.77	112.82	108.20
54	BA	2428	G	N9-C4-C5	5.77	107.71	105.40
4	AE	28	ARG	NE-CZ-NH1	5.77	123.19	120.30
23	A2	88	U	C5-C6-N1	-5.77	119.81	122.70
54	BA	587	C	N3-C4-C5	5.77	124.21	121.90
54	BA	1456	G	N1-C6-O6	-5.77	116.44	119.90
54	BA	2446	G	C8-N9-C4	-5.77	104.09	106.40
21	AA	926	G	N3-C4-C5	-5.77	125.72	128.60
54	BA	10	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	1767	G	C5-C6-N1	5.77	114.38	111.50
21	AA	19	A	C5-C6-N1	5.77	120.58	117.70
21	AA	1349	A	C5-C6-N1	5.77	120.58	117.70
54	BA	1029	A	O4'-C1'-N9	5.77	112.81	108.20
21	AA	86	G	N3-C2-N2	-5.76	115.86	119.90
21	AA	483	C	N3-C2-O2	-5.76	117.86	121.90
23	A2	87	U	N1-C2-N3	5.76	118.36	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	272	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	863	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	961	C	O4'-C1'-N1	5.76	112.81	108.20
54	BA	1324	G	N1-C6-O6	-5.76	116.44	119.90
21	AA	1308	U	N3-C2-O2	-5.76	118.17	122.20
21	AA	1519	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1153	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2197	U	C5-C6-N1	-5.76	119.82	122.70
54	BA	2376	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	997	U	O4'-C1'-N1	5.76	112.81	108.20
21	AA	1476	A	C4-C5-C6	-5.76	114.12	117.00
24	A3	2	G	C5-C6-N1	5.76	114.38	111.50
54	BA	360	U	C5-C6-N1	-5.76	119.82	122.70
54	BA	501	A	N1-C6-N6	-5.76	115.14	118.60
54	BA	385	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2250	G	O4'-C1'-C2'	-5.76	100.04	105.80
21	AA	1181	G	O4'-C1'-N9	5.76	112.81	108.20
54	BA	593	U	O4'-C1'-N1	5.76	112.81	108.20
54	BA	1204	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1332	G	C5-C6-N1	5.76	114.38	111.50
54	BA	2354	C	O4'-C1'-N1	5.76	112.81	108.20
21	AA	282	A	C5-C6-N1	5.76	120.58	117.70
21	AA	422	C	N3-C4-C5	5.76	124.20	121.90
54	BA	309	A	C5-C6-N1	5.76	120.58	117.70
54	BA	2356	U	O4'-C1'-N1	5.76	112.81	108.20
54	BA	2425	A	C5-C6-N1	5.76	120.58	117.70
55	BB	24	G	C3'-C2'-C1'	5.76	106.11	101.50
21	AA	20	U	C5-C6-N1	-5.75	119.82	122.70
21	AA	848	C	N3-C2-O2	-5.75	117.87	121.90
21	AA	883	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	2378	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	164	G	C1'-O4'-C4'	-5.75	105.30	109.90
21	AA	1426	G	C8-N9-C4	-5.75	104.10	106.40
33	BK	17	ARG	NE-CZ-NH1	5.75	123.18	120.30
54	BA	439	A	N1-C6-N6	-5.75	115.15	118.60
54	BA	1314	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	1814	G	N1-C6-O6	-5.75	116.45	119.90
54	BA	2821	A	C5-C6-N1	5.75	120.58	117.70
1	AB	207	ARG	NE-CZ-NH1	5.75	123.18	120.30
54	BA	1089	A	C2-N3-C4	5.75	113.47	110.60
21	AA	1128	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	1261	C	O4'-C1'-N1	5.75	112.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1887	C	C6-N1-C2	-5.75	118.00	120.30
21	AA	421	U	C2-N1-C1'	5.75	124.60	117.70
54	BA	2234	G	C8-N9-C4	-5.75	104.10	106.40
25	BC	101	ARG	NE-CZ-NH2	-5.75	117.43	120.30
54	BA	1216	G	C5-C6-N1	5.75	114.37	111.50
54	BA	1260	A	C5-C6-N1	5.75	120.57	117.70
54	BA	1585	C	N3-C4-C5	5.75	124.20	121.90
21	AA	427	U	N3-C2-O2	-5.75	118.18	122.20
21	AA	1296	C	N3-C2-O2	-5.75	117.88	121.90
3	AD	72	ARG	NE-CZ-NH2	-5.74	117.43	120.30
10	AK	68	ARG	NE-CZ-NH1	5.74	123.17	120.30
21	AA	148	G	C5-C6-N1	5.74	114.37	111.50
21	AA	209	U	C1'-O4'-C4'	-5.74	105.31	109.90
21	AA	274	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2530	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	55	A	C5-C6-N1	5.74	120.57	117.70
54	BA	420	C	C6-N1-C2	-5.74	118.00	120.30
54	BA	1319	C	N1-C2-O2	5.74	122.34	118.90
54	BA	2496	C	O4'-C1'-N1	5.74	112.79	108.20
21	AA	1067	A	C5-C6-N1	5.74	120.57	117.70
54	BA	527	C	N1-C1'-C2'	5.74	121.46	114.00
54	BA	1334	G	O4'-C1'-N9	5.74	112.79	108.20
21	AA	122	G	N1-C6-O6	-5.74	116.46	119.90
21	AA	865	A	C5-C6-N1	5.74	120.57	117.70
21	AA	1320	C	N3-C4-N4	-5.74	113.98	118.00
54	BA	310	A	C5-C6-N1	5.74	120.57	117.70
54	BA	324	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2060	A	P-O3'-C3'	5.74	126.58	119.70
21	AA	1280	A	C5-C6-N1	5.74	120.57	117.70
21	AA	1288	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2051	A	C3'-C2'-C1'	5.74	106.09	101.50
21	AA	113	G	C8-N9-C4	-5.74	104.11	106.40
21	AA	199	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	775	G	N3-C2-N2	-5.74	115.89	119.90
54	BA	270	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	679	C	N3-C2-O2	-5.74	117.89	121.90
54	BA	1531	C	C3'-C2'-C1'	5.74	106.09	101.50
54	BA	1533	C	N3-C4-C5	5.74	124.19	121.90
54	BA	2301	C	N3-C2-O2	-5.74	117.89	121.90
21	AA	227	G	N3-C4-C5	-5.73	125.73	128.60
21	AA	336	A	C6-C5-N7	5.73	136.31	132.30
54	BA	1600	C	O4'-C1'-N1	5.73	112.79	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2837	A	N1-C6-N6	-5.73	115.16	118.60
21	AA	285	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	575	G	N1-C6-O6	-5.73	116.46	119.90
54	BA	201	C	N3-C4-C5	5.73	124.19	121.90
54	BA	2306	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2465	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2521	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2755	C	C6-N1-C2	-5.73	118.01	120.30
21	AA	138	G	C1'-O4'-C4'	-5.73	105.32	109.90
44	BV	21	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	1009	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	1152	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1587	G	O4'-C1'-N9	5.73	112.78	108.20
54	BA	1801	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	1477	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	1511	G	O4'-C1'-N9	5.73	112.78	108.20
55	BB	62	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1913	A	C5-C6-N1	5.73	120.56	117.70
54	BA	2101	A	N1-C6-N6	-5.73	115.16	118.60
22	A1	66	A	C4-C5-C6	-5.72	114.14	117.00
51	B2	35	ARG	NE-CZ-NH1	5.72	123.16	120.30
54	BA	650	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	274	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	902	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	960	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1881	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	2042	A	C5-C6-N1	5.72	120.56	117.70
21	AA	34	C	C5'-C4'-C3'	-5.72	106.85	116.00
21	AA	755	G	C3'-C2'-C1'	5.72	106.08	101.50
21	AA	977	A	C2-N3-C4	5.72	113.46	110.60
21	AA	1492	A	N1-C6-N6	-5.72	115.17	118.60
54	BA	2274	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	209	U	O4'-C1'-N1	5.72	112.78	108.20
21	AA	379	C	N1-C2-O2	5.72	122.33	118.90
21	AA	735	C	N3-C2-O2	-5.72	117.90	121.90
21	AA	1437	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	782	A	O4'-C1'-N9	5.72	112.78	108.20
54	BA	1499	C	O4'-C1'-N1	5.72	112.78	108.20
54	BA	1556	C	N3-C4-C5	5.72	124.19	121.90
21	AA	1006	G	N3-C2-N2	-5.72	115.90	119.90
54	BA	748	G	N9-C4-C5	5.72	107.69	105.40
54	BA	1144	A	C4-C5-C6	-5.72	114.14	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	781	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	1501	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	32	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	2020	A	C5'-C4'-C3'	-5.72	106.86	116.00
54	BA	2639	A	C5-C6-N1	5.72	120.56	117.70
21	AA	233	C	N1-C2-O2	5.71	122.33	118.90
21	AA	666	G	N3-C2-N2	-5.71	115.90	119.90
21	AA	969	A	C6-C5-N7	5.71	136.30	132.30
54	BA	586	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1042	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	1262	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1508	A	O4'-C1'-N9	5.71	112.77	108.20
55	BB	36	C	N1-C2-O2	5.71	122.33	118.90
55	BB	57	A	C4-C5-C6	-5.71	114.14	117.00
21	AA	732	C	N1-C2-O2	5.71	122.33	118.90
21	AA	859	G	C5-C6-N1	5.71	114.36	111.50
50	B1	27	ARG	NE-CZ-NH1	5.71	123.16	120.30
54	BA	309	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	748	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	1271	G	C5-C6-N1	5.71	114.36	111.50
54	BA	1342	A	C5-C6-N1	5.71	120.56	117.70
54	BA	1343	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	1541	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	2119	A	C5-C6-N1	5.71	120.56	117.70
54	BA	2425	A	O4'-C1'-N9	5.71	112.77	108.20
54	BA	2575	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	488	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	2055	C	C3'-C2'-C1'	-5.71	96.93	101.50
3	AD	114	ARG	NE-CZ-NH1	5.71	123.15	120.30
21	AA	179	A	C5-C6-N1	5.71	120.55	117.70
21	AA	1063	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1463	U	C5-C6-N1	-5.71	119.85	122.70
22	A1	58	A	C4-C5-C6	-5.71	114.14	117.00
39	BQ	2	ARG	NE-CZ-NH1	5.71	123.15	120.30
54	BA	623	C	N1-C2-O2	5.71	122.33	118.90
54	BA	810	U	C5-C6-N1	-5.71	119.85	122.70
14	AO	71	ARG	NE-CZ-NH1	5.71	123.15	120.30
21	AA	372	C	N3-C4-C5	5.71	124.18	121.90
23	A2	79	A	C2-N3-C4	5.71	113.45	110.60
21	AA	865	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	948	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1164	C	N3-C2-O2	-5.70	117.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2127	G	O4'-C1'-N9	5.70	112.76	108.20
6	AG	137	ARG	NE-CZ-NH2	-5.70	117.45	120.30
21	AA	528	C	N1-C2-O2	5.70	122.32	118.90
21	AA	1078	U	O4'-C1'-N1	5.70	112.76	108.20
21	AA	1528	U	C5-C6-N1	-5.70	119.85	122.70
7	AH	116	ARG	NE-CZ-NH1	5.70	123.15	120.30
21	AA	749	A	C6-C5-N7	5.70	136.29	132.30
21	AA	1285	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	331	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1378	A	N1-C6-N6	-5.70	115.18	118.60
54	BA	1979	U	C5-C6-N1	-5.70	119.85	122.70
54	BA	2427	C	C1'-O4'-C4'	-5.70	105.34	109.90
21	AA	1020	G	N1-C6-O6	-5.70	116.48	119.90
54	BA	168	G	C5-C6-N1	5.70	114.35	111.50
54	BA	437	U	N3-C2-O2	-5.70	118.21	122.20
54	BA	776	G	C8-N9-C4	-5.70	104.12	106.40
21	AA	466	A	C2-N3-C4	5.70	113.45	110.60
21	AA	1063	C	N1-C2-O2	5.70	122.32	118.90
54	BA	435	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1122	G	N3-C2-N2	-5.70	115.91	119.90
54	BA	1830	C	C6-N1-C2	-5.70	118.02	120.30
21	AA	189	A	N1-C6-N6	-5.70	115.18	118.60
54	BA	265	A	C5-C6-N1	5.70	120.55	117.70
54	BA	825	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1207	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	1454	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1761	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	124	C	N1-C2-O2	5.69	122.32	118.90
21	AA	167	A	C5-C6-N1	5.69	120.55	117.70
39	BQ	32	ARG	NE-CZ-NH2	5.69	123.15	120.30
54	BA	359	G	O4'-C1'-N9	5.69	112.75	108.20
54	BA	478	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2710	C	N1-C2-O2	5.69	122.32	118.90
21	AA	151	A	C5-C6-N1	5.69	120.55	117.70
21	AA	844	G	N7-C8-N9	5.69	115.95	113.10
21	AA	1428	A	C6-C5-N7	5.69	136.28	132.30
54	BA	148	U	C3'-C2'-C1'	5.69	106.06	101.50
54	BA	180	G	N1-C6-O6	-5.69	116.48	119.90
54	BA	1539	U	N3-C2-O2	-5.69	118.22	122.20
54	BA	2807	U	O4'-C1'-N1	5.69	112.75	108.20
21	AA	618	C	N1-C2-O2	5.69	122.31	118.90
24	A3	47	G	C3'-C2'-C1'	5.69	106.05	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	730	A	C5'-C4'-O4'	5.69	115.93	109.10
54	BA	859	G	C4'-C3'-C2'	-5.69	96.91	102.60
54	BA	2794	C	N1-C2-O2	5.69	122.31	118.90
21	AA	129	A	C6-C5-N7	5.69	136.28	132.30
21	AA	720	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1409	U	O4'-C1'-N1	5.69	112.75	108.20
54	BA	1727	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1963	U	N3-C2-O2	-5.69	118.22	122.20
54	BA	2277	G	N1-C6-O6	-5.69	116.49	119.90
54	BA	2442	C	N1-C2-O2	5.69	122.31	118.90
21	AA	892	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	1833	C	N1-C2-O2	5.69	122.31	118.90
54	BA	1969	A	C6-C5-N7	5.69	136.28	132.30
13	AN	69	ARG	NE-CZ-NH1	5.68	123.14	120.30
21	AA	165	G	N1-C6-O6	-5.68	116.49	119.90
21	AA	309	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	558	G	C5-C6-N1	5.68	114.34	111.50
54	BA	431	U	N3-C2-O2	-5.68	118.22	122.20
54	BA	1359	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	246	A	C1'-O4'-C4'	-5.68	105.35	109.90
21	AA	985	C	N1-C2-O2	5.68	122.31	118.90
21	AA	1153	G	C5-C6-N1	5.68	114.34	111.50
54	BA	64	A	C2-N3-C4	5.68	113.44	110.60
54	BA	348	A	C6-C5-N7	5.68	136.28	132.30
54	BA	1775	U	O4'-C1'-N1	5.68	112.75	108.20
55	BB	2	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	1732	C	N1-C2-O2	5.68	122.31	118.90
54	BA	2290	G	C5-C6-N1	5.68	114.34	111.50
54	BA	2476	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	9	G	C5-C6-N1	5.68	114.34	111.50
21	AA	827	U	C5-C6-N1	-5.68	119.86	122.70
21	AA	844	G	C8-N9-C4	-5.68	104.13	106.40
54	BA	184	C	O4'-C1'-N1	5.68	112.74	108.20
54	BA	564	C	N3-C4-C5	5.68	124.17	121.90
54	BA	797	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	1209	U	C5-C6-N1	-5.68	119.86	122.70
54	BA	1597	A	O4'-C4'-C3'	5.68	110.64	106.10
21	AA	874	G	N3-C4-C5	-5.68	125.76	128.60
21	AA	1092	A	C5-C6-N1	5.68	120.54	117.70
24	A3	52	C	N3-C2-O2	-5.68	117.93	121.90
26	BD	179	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	851	C	N3-C2-O2	-5.68	117.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	90	C	N3-C2-O2	-5.68	117.92	121.90
21	AA	509	A	O4'-C1'-N9	5.68	112.74	108.20
21	AA	1225	A	N1-C6-N6	-5.68	115.19	118.60
21	AA	1297	G	O4'-C1'-N9	5.68	112.74	108.20
21	AA	1497	G	C5-C6-N1	5.68	114.34	111.50
54	BA	161	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	300	A	N1-C6-N6	-5.68	115.19	118.60
54	BA	359	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	438	G	C5-C6-N1	5.68	114.34	111.50
21	AA	177	G	O4'-C1'-N9	5.67	112.74	108.20
21	AA	192	A	C6-C5-N7	5.67	136.27	132.30
21	AA	204	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	803	G	C5-C6-N1	5.67	114.34	111.50
21	AA	933	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	1217	C	N1-C2-O2	5.67	122.31	118.90
21	AA	1468	A	C4-C5-C6	-5.67	114.16	117.00
35	BM	10	ARG	NE-CZ-NH1	5.67	123.14	120.30
54	BA	1728	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	1872	A	C5-C6-N1	5.67	120.54	117.70
54	BA	2636	C	N1-C2-O2	5.67	122.31	118.90
54	BA	2823	A	C5-C6-N1	5.67	120.54	117.70
55	BB	24	G	C4-C5-N7	-5.67	108.53	110.80
55	BB	99	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1472	C	N3-C4-C5	5.67	124.17	121.90
54	BA	1527	G	N3-C4-C5	-5.67	125.76	128.60
54	BA	2022	U	C5-C6-N1	-5.67	119.86	122.70
54	BA	2353	G	C4'-C3'-C2'	-5.67	96.93	102.60
21	AA	919	A	C4-C5-C6	-5.67	114.16	117.00
21	AA	1458	G	N3-C4-C5	-5.67	125.76	128.60
40	BR	21	ARG	NE-CZ-NH2	-5.67	117.47	120.30
54	BA	392	U	N3-C2-O2	-5.67	118.23	122.20
54	BA	1657	U	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2090	A	C6-C5-N7	5.67	136.27	132.30
54	BA	2625	G	C5-C6-N1	5.67	114.34	111.50
21	AA	1450	U	N3-C2-O2	-5.67	118.23	122.20
54	BA	41	C	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2378	A	C5-C6-N1	5.67	120.53	117.70
8	AI	79	ARG	NE-CZ-NH1	5.67	123.13	120.30
54	BA	396	G	N1-C6-O6	-5.67	116.50	119.90
54	BA	471	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	2844	G	C5-C6-N1	5.67	114.33	111.50
21	AA	398	U	C5-C6-N1	-5.67	119.87	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	525	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	776	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	1408	A	C5-C6-N1	5.67	120.53	117.70
54	BA	793	A	C6-C5-N7	5.67	136.27	132.30
54	BA	1162	G	N1-C6-O6	-5.67	116.50	119.90
54	BA	1790	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2246	G	C5-C6-N1	5.67	114.33	111.50
54	BA	2314	A	C5-C6-N1	5.67	120.53	117.70
54	BA	787	C	O4'-C1'-N1	5.67	112.73	108.20
54	BA	885	C	N1-C2-O2	5.67	122.30	118.90
54	BA	1121	C	N1-C2-O2	5.67	122.30	118.90
54	BA	1302	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	1798	U	O4'-C1'-N1	5.67	112.73	108.20
54	BA	2102	G	C8-N9-C4	-5.67	104.13	106.40
54	BA	1259	G	C5-C6-N1	5.66	114.33	111.50
54	BA	2336	A	C5-C6-N1	5.66	120.53	117.70
54	BA	2620	C	N3-C4-C5	5.66	124.17	121.90
54	BA	783	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	893	C	N1-C2-O2	5.66	122.30	118.90
21	AA	1430	A	N1-C6-N6	-5.66	115.20	118.60
54	BA	60	G	C5-C6-N1	5.66	114.33	111.50
54	BA	343	C	N3-C4-C5	5.66	124.16	121.90
54	BA	1211	C	N3-C4-C5	5.66	124.16	121.90
54	BA	1730	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	953	G	C8-N9-C4	-5.66	104.14	106.40
21	AA	1093	A	C1'-O4'-C4'	-5.66	105.37	109.90
54	BA	1369	G	N1-C6-O6	-5.66	116.51	119.90
54	BA	2267	A	C3'-C2'-C1'	5.66	106.03	101.50
8	AI	121	ARG	NE-CZ-NH2	-5.66	117.47	120.30
21	AA	646	G	N1-C6-O6	-5.66	116.51	119.90
54	BA	128	C	O4'-C1'-N1	5.66	112.72	108.20
54	BA	839	U	N1-C2-N3	5.66	118.29	114.90
54	BA	2209	G	C5-C6-N1	5.66	114.33	111.50
54	BA	2576	G	C2-N3-C4	5.66	114.73	111.90
54	BA	522	A	C5-C6-N1	5.65	120.53	117.70
21	AA	729	A	N1-C6-N6	-5.65	115.21	118.60
21	AA	863	U	N1-C2-N3	5.65	118.29	114.90
54	BA	49	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	101	A	O4'-C1'-N9	5.65	112.72	108.20
54	BA	542	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	1180	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	2029	G	C5-C6-N1	5.65	114.33	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2230	G	N1-C6-O6	-5.65	116.51	119.90
54	BA	2707	U	O4'-C1'-N1	5.65	112.72	108.20
21	AA	234	C	N1-C2-O2	5.65	122.29	118.90
21	AA	759	A	C4-C5-C6	-5.65	114.17	117.00
49	B0	39	ARG	NE-CZ-NH1	5.65	123.12	120.30
54	BA	274	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	401	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	1436	G	N1-C6-O6	-5.65	116.51	119.90
54	BA	2268	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	82	U	N1-C2-N3	5.65	118.29	114.90
21	AA	1201	A	C4-C5-C6	-5.65	114.18	117.00
21	AA	1373	G	C5-C6-N1	5.65	114.32	111.50
31	BI	126	ARG	NE-CZ-NH2	-5.65	117.48	120.30
54	BA	340	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	2730	C	O4'-C1'-N1	5.65	112.72	108.20
55	BB	70	C	N1-C2-O2	5.65	122.29	118.90
54	BA	27	G	N3-C4-C5	-5.65	125.78	128.60
54	BA	152	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	393	C	N3-C2-O2	-5.65	117.95	121.90
54	BA	884	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	1590	A	C4-C5-C6	-5.65	114.18	117.00
21	AA	66	A	C5-C6-N1	5.64	120.52	117.70
21	AA	84	U	N3-C2-O2	-5.64	118.25	122.20
21	AA	204	G	N3-C4-C5	-5.64	125.78	128.60
21	AA	429	U	C5-C6-N1	-5.64	119.88	122.70
21	AA	522	C	N1-C2-O2	5.64	122.29	118.90
54	BA	738	G	N3-C4-C5	-5.64	125.78	128.60
54	BA	1199	U	O4'-C1'-N1	5.64	112.72	108.20
54	BA	1574	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1956	U	O4'-C1'-N1	5.64	112.72	108.20
54	BA	2540	C	N1-C2-O2	5.64	122.29	118.90
21	AA	734	G	C8-N9-C4	-5.64	104.14	106.40
54	BA	1994	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	2863	C	N3-C4-C5	5.64	124.16	121.90
21	AA	639	G	C5-C6-N1	5.64	114.32	111.50
21	AA	970	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	1341	U	N1-C2-N3	5.64	118.28	114.90
54	BA	207	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1210	G	N1-C6-O6	-5.64	116.52	119.90
54	BA	1314	C	N1-C2-O2	5.64	122.28	118.90
54	BA	1353	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1882	U	N1-C2-N3	5.64	118.28	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2054	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	2083	G	N9-C4-C5	5.64	107.66	105.40
21	AA	1050	G	C5-C6-N1	5.64	114.32	111.50
52	B3	41	ARG	NE-CZ-NH1	5.64	123.12	120.30
54	BA	44	A	C5-C6-N1	5.64	120.52	117.70
54	BA	160	A	C5'-C4'-O4'	5.64	115.86	109.10
54	BA	816	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	1189	U	N3-C2-O2	-5.64	118.25	122.20
21	AA	1396	A	O4'-C1'-N9	5.64	112.71	108.20
54	BA	1869	G	N3-C4-C5	-5.64	125.78	128.60
54	BA	2250	G	N3-C2-N2	-5.64	115.95	119.90
21	AA	1184	G	N1-C6-O6	-5.63	116.52	119.90
21	AA	1401	G	C5-C6-N1	5.63	114.32	111.50
25	BC	166	ARG	NE-CZ-NH1	5.63	123.12	120.30
54	BA	855	G	N3-C2-N2	-5.63	115.96	119.90
54	BA	1225	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	1594	U	O4'-C1'-N1	5.63	112.71	108.20
54	BA	2562	U	O4'-C1'-N1	5.63	112.71	108.20
54	BA	2661	G	C5-C6-N1	5.63	114.32	111.50
21	AA	20	U	N1-C2-N3	5.63	118.28	114.90
21	AA	1337	G	C5-C6-N1	5.63	114.32	111.50
54	BA	1964	G	C5-C6-N1	5.63	114.32	111.50
21	AA	794	A	C5-C6-N1	5.63	120.52	117.70
21	AA	1016	A	C4-C5-C6	-5.63	114.18	117.00
22	A1	75	C	N3-C4-C5	5.63	124.15	121.90
54	BA	100	U	O4'-C1'-N1	5.63	112.71	108.20
54	BA	620	G	O4'-C1'-N9	5.63	112.70	108.20
54	BA	1029	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	1253	A	O4'-C1'-N9	5.63	112.70	108.20
54	BA	2439	A	C4-C5-C6	-5.63	114.18	117.00
5	AF	38	ARG	NE-CZ-NH1	5.63	123.11	120.30
54	BA	806	C	N1-C2-O2	5.63	122.28	118.90
21	AA	342	C	N3-C4-C5	5.63	124.15	121.90
21	AA	1182	G	N9-C4-C5	5.63	107.65	105.40
54	BA	358	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	620	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	2417	C	O4'-C1'-N1	5.63	112.70	108.20
3	AD	12	ARG	NH1-CZ-NH2	-5.63	113.21	119.40
21	AA	767	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	847	G	N1-C6-O6	-5.63	116.52	119.90
24	A3	49	C	O4'-C1'-N1	5.63	112.70	108.20
54	BA	823	C	N1-C2-O2	5.63	122.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1457	U	O4'-C1'-N1	5.63	112.70	108.20
21	AA	272	C	N1-C2-O2	5.62	122.28	118.90
54	BA	1508	A	C4-C5-C6	-5.62	114.19	117.00
55	BB	68	C	N3-C2-O2	-5.62	117.96	121.90
3	AD	45	PRO	C-N-CA	5.62	135.76	121.70
21	AA	155	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	202	G	C5-C6-N1	5.62	114.31	111.50
21	AA	328	C	P-O3'-C3'	5.62	126.45	119.70
21	AA	1085	U	N3-C2-O2	-5.62	118.26	122.20
54	BA	743	A	C5-C6-N1	5.62	120.51	117.70
54	BA	992	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	1351	C	O4'-C1'-N1	5.62	112.70	108.20
54	BA	1381	G	N3-C2-N2	-5.62	115.96	119.90
21	AA	602	A	C5-C6-N1	5.62	120.51	117.70
22	A1	17	U	N1-C2-N3	5.62	118.27	114.90
54	BA	3	U	O4'-C1'-N1	5.62	112.70	108.20
54	BA	111	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	695	G	N3-C2-N2	-5.62	115.97	119.90
54	BA	1161	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	1432	G	C5-C6-N1	5.62	114.31	111.50
54	BA	2028	U	C4-C5-C6	5.62	123.07	119.70
54	BA	2854	G	O4'-C1'-N9	5.62	112.70	108.20
21	AA	96	U	C5-C6-N1	-5.62	119.89	122.70
21	AA	1450	U	C5-C6-N1	-5.62	119.89	122.70
22	A1	40	G	N3-C2-N2	-5.62	115.97	119.90
54	BA	170	U	O4'-C1'-N1	5.62	112.69	108.20
54	BA	565	C	N1-C2-O2	5.62	122.27	118.90
54	BA	608	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2112	G	N3-C2-N2	-5.62	115.97	119.90
54	BA	2482	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	109	A	O4'-C1'-N9	5.62	112.69	108.20
21	AA	1036	A	O4'-C1'-N9	5.62	112.69	108.20
54	BA	2545	G	N1-C6-O6	-5.62	116.53	119.90
54	BA	2772	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	2846	G	N9-C4-C5	5.62	107.65	105.40
21	AA	890	G	O4'-C1'-N9	5.62	112.69	108.20
21	AA	1089	G	N3-C2-N2	-5.62	115.97	119.90
21	AA	1472	U	O4'-C1'-N1	5.62	112.69	108.20
33	BK	108	ARG	NE-CZ-NH1	5.62	123.11	120.30
36	BN	22	ARG	NE-CZ-NH1	5.62	123.11	120.30
49	B0	51	ARG	NE-CZ-NH1	5.62	123.11	120.30
54	BA	1345	C	N3-C4-C5	5.62	124.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1796	U	O4'-C1'-N1	5.62	112.69	108.20
54	BA	2080	A	C6-C5-N7	5.62	136.23	132.30
21	AA	289	G	C5-C6-N1	5.61	114.31	111.50
21	AA	843	U	N3-C2-O2	-5.61	118.27	122.20
54	BA	33	C	N3-C4-C5	5.61	124.14	121.90
54	BA	211	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	475	C	N3-C4-C5	5.61	124.15	121.90
54	BA	1537	G	C5-C6-N1	5.61	114.31	111.50
54	BA	1873	G	O4'-C1'-N9	5.61	112.69	108.20
54	BA	2869	G	O4'-C1'-N9	5.61	112.69	108.20
21	AA	989	U	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1711	A	C6-C5-N7	5.61	136.23	132.30
54	BA	2208	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	2531	A	C4-C5-C6	-5.61	114.19	117.00
8	AI	94	ARG	NE-CZ-NH1	5.61	123.11	120.30
21	AA	638	U	O4'-C1'-N1	5.61	112.69	108.20
21	AA	993	G	O4'-C1'-N9	5.61	112.69	108.20
34	BL	126	ARG	NE-CZ-NH1	5.61	123.11	120.30
54	BA	341	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1090	A	C4-C5-C6	-5.61	114.19	117.00
24	A3	50	G	N1-C6-O6	-5.61	116.53	119.90
54	BA	332	A	C5-C6-N1	5.61	120.50	117.70
54	BA	1200	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	2602	A	O4'-C1'-C2'	-5.61	100.19	105.80
21	AA	87	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	1004	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	1068	G	C5-C6-N1	5.61	114.30	111.50
21	AA	277	C	N1-C2-O2	5.61	122.26	118.90
21	AA	942	G	C5-C6-N1	5.61	114.30	111.50
21	AA	1105	A	C6-C5-N7	5.61	136.22	132.30
24	A3	45	A	C6-C5-N7	5.61	136.22	132.30
54	BA	1378	A	C5-C6-N1	5.61	120.50	117.70
54	BA	2201	G	N3-C4-C5	-5.61	125.80	128.60
54	BA	2225	A	N1-C6-N6	-5.61	115.24	118.60
55	BB	63	C	P-O3'-C3'	5.61	126.43	119.70
21	AA	1190	G	P-O3'-C3'	5.60	126.42	119.70
54	BA	2757	A	C5'-C4'-C3'	-5.60	107.03	116.00
21	AA	271	C	N1-C2-O2	5.60	122.26	118.90
21	AA	283	U	N3-C2-O2	-5.60	118.28	122.20
21	AA	647	C	N1-C2-O2	5.60	122.26	118.90
32	BJ	96	ARG	NE-CZ-NH1	5.60	123.10	120.30
54	BA	188	G	N1-C6-O6	-5.60	116.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	648	G	C5-C6-N1	5.60	114.30	111.50
54	BA	2205	A	C5-C6-N1	5.60	120.50	117.70
54	BA	679	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	2336	A	O4'-C1'-N9	5.60	112.68	108.20
21	AA	1275	A	C5-C6-N1	5.60	120.50	117.70
54	BA	451	U	O4'-C1'-N1	5.60	112.68	108.20
54	BA	789	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	970	U	C5'-C4'-O4'	5.60	115.82	109.10
54	BA	1947	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	2128	G	O4'-C1'-N9	5.60	112.68	108.20
21	AA	415	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	856	C	O4'-C1'-N1	5.60	112.68	108.20
21	AA	1447	A	C5-C6-N1	5.60	120.50	117.70
54	BA	601	C	N1-C2-O2	5.60	122.26	118.90
54	BA	1050	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1382	G	N1-C6-O6	-5.60	116.54	119.90
54	BA	2628	C	N1-C2-O2	5.60	122.26	118.90
54	BA	450	G	N3-C4-C5	-5.60	125.80	128.60
54	BA	678	C	N1-C2-O2	5.60	122.26	118.90
54	BA	2332	C	N1-C2-O2	5.60	122.26	118.90
54	BA	2406	A	O4'-C1'-N9	5.60	112.68	108.20
36	BN	118	ARG	NE-CZ-NH1	5.59	123.10	120.30
54	BA	233	A	C6-C5-N7	5.59	136.22	132.30
54	BA	614	A	O4'-C1'-N9	5.59	112.67	108.20
54	BA	762	U	P-O3'-C3'	5.59	126.41	119.70
54	BA	1104	C	O4'-C1'-N1	5.59	112.68	108.20
54	BA	1815	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	2337	G	N1-C6-O6	-5.59	116.54	119.90
54	BA	2354	C	N3-C2-O2	-5.59	117.98	121.90
54	BA	2498	C	C3'-C2'-C1'	5.59	105.98	101.50
54	BA	2502	G	N7-C8-N9	5.59	115.90	113.10
54	BA	91	A	C5-C6-N1	5.59	120.50	117.70
54	BA	1591	A	C5-C6-N1	5.59	120.50	117.70
13	AN	24	ARG	NE-CZ-NH1	5.59	123.10	120.30
21	AA	305	G	N1-C6-O6	-5.59	116.55	119.90
21	AA	316	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1338	G	C5-C6-N1	5.59	114.30	111.50
54	BA	1864	U	C5-C6-N1	-5.59	119.90	122.70
54	BA	2071	A	C5-C6-N1	5.59	120.50	117.70
21	AA	546	A	C6-C5-N7	5.59	136.21	132.30
21	AA	1370	G	N3-C2-N2	-5.59	115.99	119.90
22	A1	8	U	N3-C2-O2	-5.59	118.29	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	41	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	382	A	C6-C5-N7	5.59	136.21	132.30
54	BA	410	G	C8-N9-C4	-5.59	104.16	106.40
54	BA	593	U	N1-C2-N3	5.59	118.25	114.90
54	BA	1274	A	N1-C6-N6	-5.59	115.25	118.60
54	BA	2085	U	O4'-C1'-N1	5.59	112.67	108.20
55	BB	34	A	C6-C5-N7	5.59	136.21	132.30
55	BB	58	A	N1-C6-N6	-5.59	115.25	118.60
21	AA	48	C	C2-N3-C4	-5.59	117.11	119.90
54	BA	2478	A	C4-C5-C6	-5.59	114.21	117.00
21	AA	456	A	C5-C6-N1	5.59	120.49	117.70
21	AA	940	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1245	C	N3-C2-O2	-5.59	117.99	121.90
22	A1	52	G	N3-C4-C5	-5.59	125.81	128.60
54	BA	278	A	C5-C6-N1	5.59	120.49	117.70
54	BA	1667	G	C8-N9-C4	-5.59	104.17	106.40
54	BA	2721	A	C5-C6-N1	5.59	120.49	117.70
54	BA	2899	A	C6-C5-N7	5.59	136.21	132.30
54	BA	1289	C	O4'-C1'-N1	5.58	112.67	108.20
54	BA	1999	C	O4'-C1'-N1	5.58	112.67	108.20
54	BA	2623	G	N3-C4-C5	-5.58	125.81	128.60
21	AA	450	G	O4'-C1'-N9	5.58	112.67	108.20
21	AA	617	G	C1'-O4'-C4'	-5.58	105.43	109.90
54	BA	634	C	O4'-C1'-N1	5.58	112.67	108.20
21	AA	731	G	C5-C6-N1	5.58	114.29	111.50
21	AA	1103	C	O4'-C1'-N1	5.58	112.67	108.20
50	B1	43	ARG	NE-CZ-NH1	5.58	123.09	120.30
54	BA	279	A	C5-C6-N1	5.58	120.49	117.70
54	BA	585	G	C8-N9-C4	-5.58	104.17	106.40
54	BA	938	G	N1-C6-O6	-5.58	116.55	119.90
54	BA	1048	A	C5-C6-N1	5.58	120.49	117.70
54	BA	1101	U	O4'-C1'-N1	5.58	112.67	108.20
54	BA	2048	G	C8-N9-C4	-5.58	104.17	106.40
54	BA	2145	C	N1-C2-O2	5.58	122.25	118.90
54	BA	1248	G	N3-C4-C5	-5.58	125.81	128.60
54	BA	1386	C	N3-C4-C5	5.58	124.13	121.90
54	BA	1460	U	O4'-C1'-N1	5.58	112.66	108.20
54	BA	2250	G	N7-C8-N9	5.58	115.89	113.10
54	BA	2729	G	C8-N9-C4	-5.58	104.17	106.40
21	AA	493	A	C8-N9-C4	-5.58	103.57	105.80
21	AA	737	C	N1-C2-O2	5.58	122.25	118.90
54	BA	658	U	C5-C6-N1	-5.58	119.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1044	C	C4'-C3'-C2'	-5.58	97.02	102.60
54	BA	1055	G	C5-C6-N1	5.58	114.29	111.50
54	BA	2786	U	O4'-C1'-N1	5.58	112.66	108.20
55	BB	9	G	C5-C6-N1	5.58	114.29	111.50
9	AJ	7	ARG	NE-CZ-NH1	5.58	123.09	120.30
21	AA	682	G	C5-C6-N1	5.58	114.29	111.50
21	AA	1069	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	982	C	N1-C1'-C2'	5.58	121.25	114.00
54	BA	1793	C	N3-C4-C5	5.58	124.13	121.90
54	BA	2756	U	N3-C2-O2	-5.58	118.30	122.20
54	BA	2770	G	N1-C6-O6	-5.58	116.55	119.90
21	AA	238	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	838	C	N1-C2-O2	5.58	122.25	118.90
54	BA	1607	C	N1-C2-O2	5.58	122.25	118.90
21	AA	52	C	N3-C4-C5	5.57	124.13	121.90
21	AA	999	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1021	A	C6-C5-N7	5.57	136.20	132.30
54	BA	2515	C	C4'-C3'-C2'	-5.57	97.03	102.60
54	BA	2870	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	572	A	C5-C6-N1	5.57	120.49	117.70
54	BA	2284	A	O4'-C1'-N9	5.57	112.66	108.20
9	AJ	45	ARG	NE-CZ-NH1	5.57	123.08	120.30
21	AA	244	U	N3-C2-O2	-5.57	118.30	122.20
54	BA	826	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	1566	A	C6-C5-N7	5.57	136.20	132.30
54	BA	2353	G	N9-C4-C5	5.57	107.63	105.40
54	BA	2429	G	C5-C6-N1	5.57	114.28	111.50
54	BA	2023	C	O4'-C1'-N1	5.57	112.66	108.20
21	AA	874	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	419	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	549	G	C5-C6-N1	5.57	114.28	111.50
54	BA	1359	A	C6-C5-N7	5.57	136.20	132.30
54	BA	1446	C	O4'-C1'-N1	5.57	112.65	108.20
54	BA	1577	C	N1-C2-O2	5.57	122.24	118.90
54	BA	1757	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	1364	U	N3-C2-O2	-5.57	118.31	122.20
22	A1	62	C	C5-C4-N4	-5.57	116.30	120.20
54	BA	297	G	C5-C6-N1	5.57	114.28	111.50
54	BA	556	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	976	G	N9-C4-C5	5.56	107.63	105.40
54	BA	2883	A	C5-C6-N1	5.56	120.48	117.70
54	BA	285	G	N9-C4-C5	5.56	107.62	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1114	C	N1-C2-O2	5.56	122.24	118.90
54	BA	1118	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	1263	U	C3'-C2'-C1'	5.56	105.95	101.50
54	BA	2739	U	C5-C6-N1	-5.56	119.92	122.70
54	BA	914	G	N3-C4-C5	-5.56	125.82	128.60
54	BA	1519	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	1779	U	N3-C2-O2	-5.56	118.31	122.20
54	BA	2331	G	O4'-C1'-N9	5.56	112.65	108.20
55	BB	60	C	C2-N3-C4	-5.56	117.12	119.90
21	AA	500	G	N3-C4-C5	-5.56	125.82	128.60
21	AA	564	C	N1-C2-O2	5.56	122.24	118.90
21	AA	586	C	N1-C2-O2	5.56	122.23	118.90
21	AA	1091	U	N1-C2-N3	5.56	118.23	114.90
21	AA	1317	C	N3-C4-N4	-5.56	114.11	118.00
21	AA	1407	C	N3-C2-O2	-5.56	118.01	121.90
24	A3	68	C	N3-C4-C5	5.56	124.12	121.90
38	BP	20	ARG	NE-CZ-NH1	5.56	123.08	120.30
55	BB	40	U	O4'-C4'-C3'	5.56	110.55	106.10
21	AA	681	A	C6-C5-N7	5.56	136.19	132.30
54	BA	594	U	C5-C6-N1	-5.56	119.92	122.70
54	BA	1170	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1648	U	C5-C6-N1	-5.56	119.92	122.70
54	BA	1370	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	2474	U	C5-C6-N1	-5.56	119.92	122.70
35	BM	38	ARG	NE-CZ-NH2	-5.55	117.52	120.30
54	BA	54	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	1119	U	C5-C6-N1	-5.55	119.92	122.70
54	BA	1595	C	N1-C2-O2	5.55	122.23	118.90
54	BA	2787	C	C5'-C4'-O4'	5.55	115.77	109.10
10	AK	127	ARG	NE-CZ-NH2	-5.55	117.52	120.30
21	AA	1083	U	C1'-O4'-C4'	-5.55	105.46	109.90
24	A3	39	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	179	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	476	G	C5'-C4'-O4'	5.55	115.76	109.10
54	BA	1276	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1674	G	C5-C6-N1	5.55	114.28	111.50
21	AA	670	G	N1-C6-O6	-5.55	116.57	119.90
21	AA	860	A	N1-C6-N6	-5.55	115.27	118.60
21	AA	1448	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	163	C	O4'-C1'-N1	5.55	112.64	108.20
21	AA	585	G	C5-C6-N1	5.55	114.28	111.50
21	AA	747	A	C5-C6-N1	5.55	120.47	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	768	A	C6-C5-N7	5.55	136.19	132.30
54	BA	129	C	N1-C2-O2	5.55	122.23	118.90
54	BA	800	A	N1-C6-N6	-5.55	115.27	118.60
54	BA	1257	C	C6-N1-C2	-5.55	118.08	120.30
54	BA	1670	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	1851	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	2294	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	383	C	N3-C2-O2	-5.55	118.02	121.90
21	AA	453	G	N3-C4-C5	-5.55	125.83	128.60
21	AA	755	G	C8-N9-C4	-5.55	104.18	106.40
21	AA	1478	U	C5-C6-N1	-5.55	119.93	122.70
54	BA	123	G	O4'-C1'-N9	5.55	112.64	108.20
54	BA	147	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	824	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	854	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	1402	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1950	G	C8-N9-C4	-5.55	104.18	106.40
54	BA	2229	U	P-O3'-C3'	5.55	126.36	119.70
54	BA	518	G	N7-C8-N9	5.54	115.87	113.10
54	BA	2572	A	N1-C6-N6	-5.54	115.27	118.60
54	BA	2733	A	C6-C5-N7	5.54	136.18	132.30
9	AJ	62	ARG	NE-CZ-NH1	5.54	123.07	120.30
21	AA	191	G	N1-C6-O6	-5.54	116.57	119.90
21	AA	488	C	O4'-C1'-N1	5.54	112.64	108.20
24	A3	70	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	220	G	C8-N9-C4	-5.54	104.18	106.40
54	BA	1618	A	C5-C6-N1	5.54	120.47	117.70
54	BA	1751	U	O4'-C1'-N1	5.54	112.64	108.20
54	BA	1817	G	N3-C4-C5	-5.54	125.83	128.60
22	A1	61	C	N1-C2-O2	5.54	122.22	118.90
54	BA	1065	U	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1161	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1772	A	C6-C5-N7	5.54	136.18	132.30
54	BA	2790	U	C5-C6-N1	-5.54	119.93	122.70
21	AA	613	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	1109	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	2384	U	O4'-C1'-N1	5.54	112.63	108.20
22	A1	44	G	C5-C6-N1	5.54	114.27	111.50
54	BA	2349	G	N1-C6-O6	-5.54	116.58	119.90
21	AA	43	C	N3-C2-O2	-5.54	118.03	121.90
21	AA	648	A	C5-C6-N1	5.54	120.47	117.70
21	AA	1037	C	N1-C2-O2	5.54	122.22	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1228	C	N1-C2-O2	5.54	122.22	118.90
54	BA	404	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	701	G	N1-C6-O6	-5.54	116.58	119.90
54	BA	1339	G	N3-C4-C5	-5.54	125.83	128.60
54	BA	2020	A	N1-C6-N6	-5.54	115.28	118.60
22	A1	47	U	C1'-O4'-C4'	-5.53	105.47	109.90
54	BA	123	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	727	A	N1-C6-N6	-5.53	115.28	118.60
54	BA	1552	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1781	U	N3-C2-O2	-5.53	118.33	122.20
54	BA	1921	G	C3'-C2'-C1'	5.53	105.93	101.50
54	BA	2285	C	N3-C4-C5	5.53	124.11	121.90
21	AA	313	A	C6-C5-N7	5.53	136.17	132.30
21	AA	816	A	C5-C6-N1	5.53	120.47	117.70
21	AA	1385	G	C5-C6-N1	5.53	114.27	111.50
36	BN	86	ARG	NE-CZ-NH1	5.53	123.07	120.30
54	BA	44	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1028	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1368	G	N1-C6-O6	-5.53	116.58	119.90
21	AA	308	C	N3-C4-C5	5.53	124.11	121.90
21	AA	941	G	C5'-C4'-C3'	-5.53	107.15	116.00
21	AA	1218	C	N1-C2-O2	5.53	122.22	118.90
54	BA	420	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	1814	G	C5-C6-N1	5.53	114.27	111.50
54	BA	2716	C	N1-C2-O2	5.53	122.22	118.90
54	BA	222	A	O4'-C1'-N9	5.53	112.62	108.20
21	AA	330	C	N3-C4-C5	5.53	124.11	121.90
21	AA	793	U	C3'-C2'-C1'	5.53	105.92	101.50
35	BM	38	ARG	NE-CZ-NH1	5.53	123.06	120.30
54	BA	365	U	O4'-C1'-N1	5.53	112.62	108.20
54	BA	586	A	C5-C6-N1	5.53	120.46	117.70
54	BA	672	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	1316	U	N3-C2-O2	-5.53	118.33	122.20
54	BA	1397	U	O4'-C1'-N1	5.53	112.62	108.20
54	BA	2395	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	2783	U	O4'-C1'-N1	5.53	112.62	108.20
54	BA	2361	G	N3-C2-N2	-5.53	116.03	119.90
21	AA	1164	G	C5-C6-N1	5.52	114.26	111.50
21	AA	1389	C	C6-N1-C2	-5.52	118.09	120.30
21	AA	978	A	C3'-C2'-C1'	5.52	105.92	101.50
21	AA	1371	G	C8-N9-C4	-5.52	104.19	106.40
54	BA	1035	U	N1-C2-N3	5.52	118.21	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1828	G	C3'-C2'-C1'	-5.52	97.08	101.50
54	BA	2301	C	O4'-C1'-N1	5.52	112.62	108.20
54	BA	2361	G	N9-C4-C5	5.52	107.61	105.40
54	BA	2391	G	N3-C4-C5	-5.52	125.84	128.60
21	AA	143	A	C6-C5-N7	5.52	136.16	132.30
21	AA	289	G	C1'-O4'-C4'	-5.52	105.48	109.90
54	BA	845	A	O4'-C1'-N9	5.52	112.62	108.20
54	BA	2250	G	C8-N9-C4	-5.52	104.19	106.40
55	BB	86	G	N9-C4-C5	5.52	107.61	105.40
11	AL	85	ARG	NE-CZ-NH1	5.52	123.06	120.30
21	AA	125	U	O4'-C1'-N1	5.52	112.61	108.20
21	AA	217	C	N1-C2-O2	5.52	122.21	118.90
24	A3	19	G	C8-N9-C4	-5.52	104.19	106.40
54	BA	267	C	N1-C2-O2	5.52	122.21	118.90
54	BA	530	G	C5-C6-N1	5.52	114.26	111.50
54	BA	2450	A	C6-C5-N7	5.52	136.16	132.30
54	BA	2662	A	N1-C6-N6	-5.52	115.29	118.60
21	AA	211	G	N3-C4-C5	-5.52	125.84	128.60
21	AA	288	A	C6-C5-N7	5.52	136.16	132.30
21	AA	357	G	C3'-C2'-C1'	5.52	105.91	101.50
21	AA	1226	C	N1-C2-O2	5.52	122.21	118.90
54	BA	33	C	N1-C2-O2	5.52	122.21	118.90
54	BA	423	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1109	C	C3'-C2'-C1'	5.52	105.91	101.50
54	BA	1369	G	C5-C6-N1	5.52	114.26	111.50
54	BA	1806	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	2245	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	2573	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	2752	C	O4'-C1'-N1	5.52	112.61	108.20
55	BB	115	A	C5-C6-N1	5.52	120.46	117.70
54	BA	1677	A	C5-C6-N1	5.52	120.46	117.70
54	BA	2338	C	N1-C2-O2	5.52	122.21	118.90
14	AO	63	ARG	NE-CZ-NH1	5.51	123.06	120.30
21	AA	290	C	N1-C2-O2	5.51	122.21	118.90
21	AA	665	A	C6-C5-N7	5.51	136.16	132.30
21	AA	1398	A	N1-C2-N3	-5.51	126.54	129.30
54	BA	2601	C	O4'-C1'-N1	5.51	112.61	108.20
21	AA	237	G	C8-N9-C4	-5.51	104.19	106.40
54	BA	257	C	O4'-C1'-N1	5.51	112.61	108.20
54	BA	520	G	N1-C6-O6	-5.51	116.59	119.90
54	BA	1442	U	C5-C6-N1	-5.51	119.94	122.70
21	AA	714	G	O4'-C1'-N9	5.51	112.61	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	720	C	N1-C2-O2	5.51	122.21	118.90
21	AA	811	C	C3'-C2'-C1'	5.51	105.91	101.50
21	AA	1129	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	1140	C	O4'-C1'-N1	5.51	112.61	108.20
21	AA	1174	G	C5-C6-N1	5.51	114.26	111.50
21	AA	1227	A	O4'-C1'-N9	5.51	112.61	108.20
21	AA	1389	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	431	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	1550	C	N3-C4-C5	5.51	124.10	121.90
54	BA	2624	G	C5-C6-N1	5.51	114.26	111.50
21	AA	101	A	O4'-C1'-N9	5.51	112.61	108.20
21	AA	785	G	C5-C6-N1	5.51	114.25	111.50
54	BA	971	G	C3'-C2'-C1'	-5.51	97.09	101.50
54	BA	1464	G	N1-C6-O6	-5.51	116.59	119.90
54	BA	1582	C	N1-C2-O2	5.51	122.21	118.90
54	BA	2189	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	2211	A	O4'-C1'-N9	5.51	112.61	108.20
54	BA	2850	A	C5-C6-N1	5.51	120.45	117.70
54	BA	386	G	P-O3'-C3'	5.51	126.31	119.70
54	BA	1176	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	1538	G	N9-C4-C5	5.51	107.60	105.40
54	BA	2599	G	N7-C8-N9	5.51	115.85	113.10
55	BB	54	G	N1-C6-O6	-5.51	116.59	119.90
21	AA	877	G	N7-C8-N9	5.51	115.85	113.10
39	BQ	63	ARG	NE-CZ-NH1	5.51	123.05	120.30
54	BA	1441	G	N9-C4-C5	5.51	107.60	105.40
54	BA	1916	A	C6-C5-N7	5.51	136.16	132.30
54	BA	2486	C	N1-C2-O2	5.51	122.20	118.90
55	BB	67	G	C5-C6-N1	5.51	114.25	111.50
54	BA	183	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	377	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	1318	U	C5-C6-N1	-5.50	119.95	122.70
54	BA	2039	U	N3-C2-O2	-5.50	118.35	122.20
21	AA	115	G	C5-C6-N1	5.50	114.25	111.50
21	AA	1490	U	C5-C6-N1	-5.50	119.95	122.70
54	BA	79	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1033	U	C5-C6-N1	-5.50	119.95	122.70
54	BA	1638	C	N1-C2-O2	5.50	122.20	118.90
21	AA	139	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	802	A	C5-C6-N1	5.50	120.45	117.70
21	AA	1443	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	1476	A	C5-C6-N1	5.50	120.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	60	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	797	G	C5-C6-N1	5.50	114.25	111.50
54	BA	1583	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1588	G	C5-C6-N1	5.50	114.25	111.50
54	BA	1844	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	2803	G	N3-C4-C5	-5.50	125.85	128.60
54	BA	1133	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1533	C	N1-C2-O2	5.50	122.20	118.90
54	BA	1645	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	2418	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	2443	C	N3-C4-C5	5.50	124.10	121.90
54	BA	2665	A	C4-C5-C6	-5.50	114.25	117.00
55	BB	109	A	C1'-O4'-C4'	-5.50	105.50	109.90
21	AA	69	G	C5-C6-N1	5.50	114.25	111.50
54	BA	481	G	N3-C4-C5	-5.50	125.85	128.60
54	BA	1563	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	2676	C	N1-C2-O2	5.50	122.20	118.90
54	BA	1202	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	1523	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1764	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1931	U	O4'-C1'-N1	5.50	112.60	108.20
21	AA	1398	A	C6-C5-N7	5.49	136.15	132.30
27	BE	102	ARG	NE-CZ-NH1	5.49	123.05	120.30
54	BA	606	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	830	G	N3-C2-N2	-5.49	116.06	119.90
54	BA	2150	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	2655	G	C8-N9-C4	-5.49	104.20	106.40
21	AA	369	G	N3-C4-C5	-5.49	125.85	128.60
21	AA	1469	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1041	G	C5'-C4'-O4'	5.49	115.69	109.10
54	BA	1077	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	1459	G	N3-C4-C5	-5.49	125.85	128.60
54	BA	730	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	958	U	C5-C6-N1	-5.49	119.95	122.70
54	BA	1079	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	2779	U	O4'-C1'-N1	5.49	112.59	108.20
21	AA	246	A	C6-C5-N7	5.49	136.14	132.30
21	AA	511	C	O4'-C1'-N1	5.49	112.59	108.20
54	BA	337	C	N1-C2-O2	5.49	122.19	118.90
54	BA	435	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1092	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1876	A	C4-C5-C6	-5.49	114.25	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2441	U	O4'-C1'-N1	5.49	112.59	108.20
21	AA	91	U	C5-C6-N1	-5.49	119.96	122.70
54	BA	393	C	N1-C2-O2	5.49	122.19	118.90
21	AA	197	A	C5'-C4'-C3'	-5.49	107.22	116.00
21	AA	1070	U	N1-C2-N3	5.49	118.19	114.90
54	BA	228	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1266	G	N3-C4-N9	5.49	129.29	126.00
54	BA	1288	G	N3-C4-C5	-5.49	125.86	128.60
54	BA	2712	C	N1-C2-O2	5.49	122.19	118.90
54	BA	2549	G	C8-N9-C4	-5.48	104.21	106.40
54	BA	2657	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2832	U	C3'-C2'-C1'	5.48	105.89	101.50
21	AA	634	C	N1-C2-O2	5.48	122.19	118.90
21	AA	901	A	C4-C5-C6	-5.48	114.26	117.00
22	A1	52	G	C8-N9-C4	-5.48	104.21	106.40
45	BW	10	ARG	NE-CZ-NH2	5.48	123.04	120.30
54	BA	595	C	N1-C2-O2	5.48	122.19	118.90
54	BA	774	G	C8-N9-C4	-5.48	104.21	106.40
54	BA	1494	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2556	C	C5'-C4'-O4'	5.48	115.68	109.10
21	AA	566	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	1919	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2443	C	N1-C2-O2	5.48	122.19	118.90
54	BA	2645	G	N3-C4-C5	-5.48	125.86	128.60
54	BA	2825	G	N3-C4-C5	-5.48	125.86	128.60
21	AA	559	A	O4'-C1'-N9	5.48	112.58	108.20
21	AA	634	C	N3-C4-C5	5.48	124.09	121.90
54	BA	2847	U	C5-C6-N1	-5.48	119.96	122.70
21	AA	212	G	N3-C4-C5	-5.48	125.86	128.60
22	A1	42	G	N3-C4-C5	-5.48	125.86	128.60
54	BA	293	U	C5-C6-N1	-5.48	119.96	122.70
54	BA	453	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	507	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1007	C	N3-C2-O2	-5.48	118.07	121.90
54	BA	1244	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2467	C	O4'-C1'-N1	5.48	112.58	108.20
54	BA	2902	C	N3-C2-O2	-5.48	118.06	121.90
16	AQ	39	ARG	NE-CZ-NH1	5.48	123.04	120.30
21	AA	495	A	C5-C6-N1	5.48	120.44	117.70
21	AA	514	C	N3-C2-O2	-5.48	118.07	121.90
26	BD	33	ARG	CD-NE-CZ	5.48	131.27	123.60
54	BA	712	G	C5-C6-N1	5.48	114.24	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2456	C	N3-C2-O2	-5.48	118.07	121.90
54	BA	2863	C	N1-C2-O2	5.48	122.19	118.90
21	AA	146	G	N3-C4-C5	-5.47	125.86	128.60
21	AA	265	G	N1-C6-O6	-5.47	116.61	119.90
21	AA	920	U	C5-C6-N1	-5.47	119.96	122.70
21	AA	1031	C	C6-N1-C2	-5.47	118.11	120.30
21	AA	1268	G	N3-C4-C5	-5.47	125.86	128.60
54	BA	776	G	N9-C4-C5	5.47	107.59	105.40
54	BA	1961	C	N1-C2-O2	5.47	122.18	118.90
54	BA	2795	C	N3-C2-O2	-5.47	118.07	121.90
24	A3	19	G	N9-C4-C5	5.47	107.59	105.40
54	BA	1430	G	N9-C4-C5	5.47	107.59	105.40
54	BA	1710	G	C8-N9-C4	-5.47	104.21	106.40
54	BA	2031	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	2068	U	O4'-C1'-N1	5.47	112.58	108.20
55	BB	46	A	C5-C6-N1	5.47	120.44	117.70
21	AA	564	C	C3'-C2'-C1'	5.47	105.88	101.50
22	A1	20	G	O4'-C1'-N9	5.47	112.58	108.20
54	BA	1077	A	C5-C6-N1	5.47	120.44	117.70
54	BA	2571	U	C5-C6-N1	-5.47	119.96	122.70
15	AP	5	ARG	NE-CZ-NH2	-5.47	117.56	120.30
21	AA	22	G	C5-C6-N1	5.47	114.23	111.50
21	AA	1521	C	O4'-C1'-N1	5.47	112.58	108.20
54	BA	663	G	N3-C4-C5	-5.47	125.86	128.60
54	BA	741	U	N3-C2-O2	-5.47	118.37	122.20
54	BA	1095	A	C5-N7-C8	-5.47	101.17	103.90
54	BA	1120	G	C5-C6-N1	5.47	114.23	111.50
54	BA	1679	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	2028	U	O4'-C1'-N1	5.47	112.58	108.20
55	BB	82	U	C3'-C2'-C1'	5.47	105.88	101.50
19	AT	17	ARG	NE-CZ-NH1	5.47	123.03	120.30
21	AA	606	G	C5-C6-N1	5.47	114.23	111.50
21	AA	1076	U	O4'-C1'-N1	5.47	112.57	108.20
54	BA	1281	G	N1-C6-O6	-5.47	116.62	119.90
54	BA	2235	G	C5-C6-N1	5.47	114.23	111.50
54	BA	2719	G	C8-N9-C4	-5.47	104.21	106.40
21	AA	177	G	N3-C4-C5	-5.47	125.87	128.60
21	AA	686	U	C4-C5-C6	5.47	122.98	119.70
21	AA	1458	G	C5-C6-N1	5.47	114.23	111.50
54	BA	1370	C	N1-C2-O2	5.47	122.18	118.90
54	BA	2708	G	N3-C4-C5	-5.47	125.87	128.60
21	AA	540	G	C5-C6-N1	5.46	114.23	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1221	G	N1-C6-O6	-5.46	116.62	119.90
21	AA	566	G	N3-C4-C5	-5.46	125.87	128.60
21	AA	593	U	N1-C2-N3	5.46	118.18	114.90
21	AA	1056	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	1878	G	C5-C6-N1	5.46	114.23	111.50
3	AD	46	ARG	NE-CZ-NH1	5.46	123.03	120.30
21	AA	115	G	N3-C4-C5	-5.46	125.87	128.60
21	AA	914	A	C5-C6-N6	5.46	128.07	123.70
21	AA	1342	C	O4'-C1'-N1	5.46	112.57	108.20
36	BN	12	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	2702	G	N3-C2-N2	-5.46	116.08	119.90
21	AA	848	C	N1-C2-O2	5.46	122.18	118.90
21	AA	1386	G	C5-C6-N1	5.46	114.23	111.50
54	BA	421	C	C2'-C3'-O3'	5.46	122.44	113.70
21	AA	1379	G	N1-C6-O6	-5.46	116.62	119.90
21	AA	1510	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	437	U	C5-C6-N1	-5.46	119.97	122.70
54	BA	1339	G	C8-N9-C4	-5.46	104.22	106.40
54	BA	2706	A	N7-C8-N9	5.46	116.53	113.80
21	AA	848	C	N3-C4-C5	5.46	124.08	121.90
54	BA	576	U	O4'-C1'-N1	5.46	112.56	108.20
54	BA	796	C	O4'-C1'-N1	5.46	112.57	108.20
54	BA	1965	C	N1-C2-O2	5.46	122.17	118.90
54	BA	2461	A	C4-C5-C6	-5.46	114.27	117.00
55	BB	76	G	N3-C4-C5	-5.46	125.87	128.60
21	AA	1072	G	C5-C6-N1	5.46	114.23	111.50
21	AA	784	A	C6-C5-N7	5.45	136.12	132.30
21	AA	1111	A	C5-C6-N1	5.45	120.43	117.70
54	BA	13	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	1707	G	C5-C6-N1	5.45	114.23	111.50
54	BA	1789	A	C6-C5-N7	5.45	136.12	132.30
54	BA	1908	C	N3-C2-O2	-5.45	118.08	121.90
55	BB	62	C	N1-C2-O2	5.45	122.17	118.90
21	AA	1113	C	N3-C4-C5	5.45	124.08	121.90
54	BA	287	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	1426	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	2640	G	N1-C6-O6	-5.45	116.63	119.90
55	BB	76	G	N1-C6-O6	-5.45	116.63	119.90
21	AA	226	G	C8-N9-C4	-5.45	104.22	106.40
21	AA	235	C	N3-C4-C5	5.45	124.08	121.90
21	AA	438	U	C4-C5-C6	5.45	122.97	119.70
21	AA	807	A	C6-C5-N7	5.45	136.12	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1394	A	N1-C6-N6	-5.45	115.33	118.60
22	A1	9	A	O4'-C1'-N9	5.45	112.56	108.20
24	A3	26	C	N3-C2-O2	-5.45	118.08	121.90
54	BA	102	U	O4'-C1'-N1	5.45	112.56	108.20
54	BA	1329	U	O4'-C4'-C3'	5.45	110.46	106.10
54	BA	1389	G	O4'-C1'-N9	5.45	112.56	108.20
54	BA	2073	C	O4'-C1'-N1	5.45	112.56	108.20
54	BA	2546	U	N3-C2-O2	-5.45	118.39	122.20
21	AA	71	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	1240	U	N3-C2-O2	-5.45	118.39	122.20
21	AA	1406	U	C5-C6-N1	-5.45	119.98	122.70
54	BA	1463	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	1512	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	2576	G	N9-C4-C5	5.45	107.58	105.40
11	AL	55	ARG	NE-CZ-NH2	-5.45	117.58	120.30
54	BA	770	G	C5-C6-N1	5.45	114.22	111.50
54	BA	1159	U	O4'-C1'-N1	5.45	112.56	108.20
21	AA	152	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	734	G	O4'-C4'-C3'	5.45	110.46	106.10
54	BA	114	U	N1-C2-N3	5.45	118.17	114.90
54	BA	1332	G	O4'-C1'-N9	5.45	112.56	108.20
54	BA	1826	G	N3-C4-C5	-5.45	125.88	128.60
54	BA	2339	C	N3-C4-C5	5.45	124.08	121.90
21	AA	234	C	N3-C4-C5	5.44	124.08	121.90
54	BA	109	C	N1-C2-O2	5.44	122.17	118.90
54	BA	650	C	O4'-C1'-N1	5.44	112.56	108.20
54	BA	1269	A	C5-C6-N1	5.44	120.42	117.70
54	BA	2313	C	C1'-O4'-C4'	-5.44	105.55	109.90
11	AL	13	ARG	NH1-CZ-NH2	-5.44	113.41	119.40
18	AS	54	ARG	NE-CZ-NH1	5.44	123.02	120.30
21	AA	142	G	N1-C6-O6	-5.44	116.64	119.90
21	AA	201	G	N1-C6-O6	-5.44	116.63	119.90
54	BA	102	U	N3-C2-O2	-5.44	118.39	122.20
54	BA	116	C	O4'-C1'-N1	5.44	112.56	108.20
54	BA	368	A	C6-C5-N7	5.44	136.11	132.30
54	BA	1589	U	O4'-C1'-N1	5.44	112.56	108.20
54	BA	1674	G	C3'-C2'-C1'	5.44	105.85	101.50
54	BA	2527	C	N1-C2-O2	5.44	122.17	118.90
55	BB	30	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	172	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	308	C	C3'-C2'-C1'	5.44	105.85	101.50
21	AA	473	U	C3'-C2'-C1'	5.44	105.85	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	738	C	N1-C2-O2	5.44	122.17	118.90
23	A2	89	U	C5-C6-N1	-5.44	119.98	122.70
54	BA	947	A	C6-C5-N7	5.44	136.11	132.30
54	BA	1460	U	N3-C2-O2	-5.44	118.39	122.20
54	BA	1546	G	C4'-C3'-C2'	-5.44	97.16	102.60
54	BA	1748	C	N1-C2-O2	5.44	122.16	118.90
54	BA	2069	G	C5'-C4'-O4'	5.44	115.63	109.10
54	BA	2689	U	O4'-C1'-N1	5.44	112.55	108.20
55	BB	60	C	O4'-C1'-N1	5.44	112.55	108.20
55	BB	4	C	N1-C2-O2	5.44	122.16	118.90
12	AM	78	ARG	NE-CZ-NH1	5.44	123.02	120.30
21	AA	931	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	932	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	1051	C	N1-C2-O2	5.44	122.16	118.90
21	AA	1457	G	N9-C4-C5	5.44	107.58	105.40
24	A3	17	C	N3-C4-C5	5.44	124.08	121.90
54	BA	125	A	C6-C5-N7	5.44	136.11	132.30
54	BA	193	U	C4-C5-C6	5.44	122.96	119.70
54	BA	1305	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	2165	C	N3-C4-C5	5.44	124.08	121.90
54	BA	2473	U	C5-C6-N1	-5.44	119.98	122.70
55	BB	41	G	C5-C6-N1	5.44	114.22	111.50
21	AA	938	A	O4'-C1'-N9	5.44	112.55	108.20
21	AA	1372	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	685	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	1708	C	N1-C2-O2	5.44	122.16	118.90
54	BA	2054	A	O4'-C1'-N9	5.44	112.55	108.20
54	BA	83	A	C6-C5-N7	5.43	136.10	132.30
54	BA	306	U	O4'-C1'-N1	5.43	112.55	108.20
54	BA	2124	G	N1-C6-O6	-5.43	116.64	119.90
55	BB	90	C	N3-C4-C5	5.43	124.07	121.90
21	AA	340	U	C5-C6-N1	-5.43	119.98	122.70
21	AA	868	C	N3-C2-O2	-5.43	118.10	121.90
21	AA	949	A	C6-C5-N7	5.43	136.10	132.30
21	AA	1396	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	142	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	1415	G	C8-N9-C4	-5.43	104.23	106.40
54	BA	1634	A	C5-C6-N1	5.43	120.42	117.70
21	AA	439	U	O4'-C1'-N1	5.43	112.54	108.20
21	AA	1194	U	C5-C6-N1	-5.43	119.98	122.70
54	BA	711	G	N7-C8-N9	5.43	115.81	113.10
54	BA	961	C	N1-C2-O2	5.43	122.16	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1318	U	N3-C2-O2	-5.43	118.40	122.20
54	BA	2661	G	O4'-C1'-N9	5.43	112.54	108.20
21	AA	664	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	685	G	C5-C6-N1	5.43	114.21	111.50
54	BA	461	C	N3-C4-N4	-5.43	114.20	118.00
54	BA	1558	C	N3-C4-C5	5.43	124.07	121.90
54	BA	2132	U	C5-C6-N1	-5.43	119.99	122.70
21	AA	115	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	220	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	703	G	N3-C4-C5	-5.43	125.89	128.60
21	AA	907	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	1139	G	N3-C2-N2	-5.43	116.10	119.90
21	AA	1231	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	1311	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	1379	G	C5-C6-N1	5.43	114.21	111.50
52	B3	44	ARG	NE-CZ-NH2	-5.43	117.59	120.30
54	BA	208	C	O4'-C1'-N1	5.43	112.54	108.20
54	BA	855	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1482	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1874	C	O4'-C1'-N1	5.43	112.54	108.20
54	BA	2520	C	N3-C4-C5	5.43	124.07	121.90
21	AA	585	G	N1-C6-O6	-5.42	116.65	119.90
21	AA	827	U	N3-C2-O2	-5.42	118.40	122.20
21	AA	1081	A	C6-C5-N7	5.42	136.10	132.30
21	AA	1471	U	O4'-C1'-N1	5.42	112.54	108.20
24	A3	3	C	N1-C2-O2	5.42	122.15	118.90
54	BA	1374	G	N1-C6-O6	-5.42	116.64	119.90
54	BA	1724	G	C8-N9-C4	-5.42	104.23	106.40
54	BA	2016	U	N3-C2-O2	-5.42	118.40	122.20
54	BA	2359	C	N3-C4-C5	5.42	124.07	121.90
54	BA	2440	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	2542	A	O4'-C1'-N9	5.42	112.54	108.20
21	AA	394	G	N3-C2-N2	-5.42	116.10	119.90
21	AA	934	C	N3-C2-O2	-5.42	118.10	121.90
54	BA	977	G	C8-N9-C4	-5.42	104.23	106.40
54	BA	1563	U	C5-C6-N1	-5.42	119.99	122.70
54	BA	2116	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	2359	C	N1-C2-O2	5.42	122.15	118.90
21	AA	233	C	N3-C4-C5	5.42	124.07	121.90
21	AA	423	G	O4'-C1'-N9	5.42	112.54	108.20
21	AA	863	U	N3-C2-O2	-5.42	118.41	122.20
21	AA	1265	C	N3-C2-O2	-5.42	118.11	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1269	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	1507	A	C4-C5-C6	-5.42	114.29	117.00
38	BP	108	ARG	NE-CZ-NH2	5.42	123.01	120.30
54	BA	1570	A	C5-C6-N1	5.42	120.41	117.70
54	BA	1681	G	C8-N9-C4	-5.42	104.23	106.40
21	AA	1062	U	C5-C6-N1	-5.42	119.99	122.70
54	BA	668	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2124	G	N3-C4-C5	-5.42	125.89	128.60
21	AA	649	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	1441	A	C6-C5-N7	5.42	136.09	132.30
21	AA	1477	U	O4'-C1'-N1	5.42	112.53	108.20
54	BA	878	A	C5-C6-N1	5.42	120.41	117.70
54	BA	1117	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	1129	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1452	G	N3-C4-C5	-5.42	125.89	128.60
54	BA	1957	C	N3-C2-O2	-5.42	118.11	121.90
55	BB	81	G	C5-C6-N1	5.42	114.21	111.50
21	AA	490	C	N3-C4-C5	5.42	124.07	121.90
21	AA	831	A	C5-C6-N1	5.42	120.41	117.70
21	AA	1171	A	C5-C6-N1	5.42	120.41	117.70
21	AA	1189	U	C5-C6-N1	-5.42	119.99	122.70
54	BA	2774	C	N1-C2-O2	5.42	122.15	118.90
54	BA	455	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	1453	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2270	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	176	C	N1-C2-O2	5.41	122.15	118.90
54	BA	40	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	101	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	437	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1000	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	2556	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	2854	G	N9-C4-C5	5.41	107.57	105.40
21	AA	275	G	N3-C4-C5	-5.41	125.89	128.60
21	AA	1511	G	N9-C4-C5	5.41	107.56	105.40
54	BA	2323	G	N3-C2-N2	-5.41	116.11	119.90
21	AA	1167	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1114	C	N3-C4-C5	5.41	124.06	121.90
54	BA	1436	G	N3-C4-C5	-5.41	125.89	128.60
54	BA	1615	C	N1-C2-O2	5.41	122.15	118.90
54	BA	1776	G	N3-C4-C5	-5.41	125.89	128.60
54	BA	1924	C	O4'-C1'-N1	5.41	112.53	108.20
21	AA	879	C	N1-C2-O2	5.41	122.14	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	17	U	C5-C6-N1	-5.41	120.00	122.70
54	BA	1527	G	N1-C6-O6	-5.41	116.66	119.90
54	BA	1728	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	2816	G	C3'-C2'-C1'	5.41	105.83	101.50
21	AA	632	U	O4'-C1'-N1	5.41	112.53	108.20
21	AA	1273	C	N1-C2-O2	5.41	122.14	118.90
54	BA	677	A	N1-C6-N6	-5.41	115.36	118.60
55	BB	24	G	N1-C6-O6	-5.41	116.66	119.90
54	BA	151	C	N3-C2-O2	-5.41	118.12	121.90
54	BA	352	A	C5-C6-N1	5.41	120.40	117.70
54	BA	606	U	N3-C2-O2	-5.41	118.42	122.20
54	BA	646	U	N1-C2-N3	5.41	118.14	114.90
54	BA	715	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	791	C	N1-C2-O2	5.41	122.14	118.90
54	BA	912	C	N3-C2-O2	-5.41	118.12	121.90
54	BA	2367	G	N1-C6-O6	-5.41	116.66	119.90
8	AI	118	ARG	NE-CZ-NH1	5.40	123.00	120.30
21	AA	975	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	523	C	N1-C2-O2	5.40	122.14	118.90
54	BA	1237	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1994	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	1701	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	2306	C	N1-C2-O2	5.40	122.14	118.90
21	AA	262	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	1224	U	N3-C2-O2	-5.40	118.42	122.20
21	AA	1466	C	N1-C2-O2	5.40	122.14	118.90
54	BA	758	C	O4'-C1'-N1	5.40	112.52	108.20
55	BB	39	A	C5-C6-N1	5.40	120.40	117.70
21	AA	1207	G	N9-C4-C5	5.40	107.56	105.40
54	BA	502	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	809	G	N3-C4-C5	-5.40	125.90	128.60
54	BA	2415	G	N1-C6-O6	-5.40	116.66	119.90
55	BB	110	C	N3-C4-N4	-5.40	114.22	118.00
21	AA	236	A	C5-C6-N1	5.40	120.40	117.70
21	AA	346	G	C5-C6-N1	5.40	114.20	111.50
21	AA	402	G	N3-C4-C5	-5.40	125.90	128.60
21	AA	925	G	C5-C6-N1	5.40	114.20	111.50
22	A1	6	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1150	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	1193	G	N1-C6-O6	-5.40	116.66	119.90
54	BA	2381	A	C6-C5-N7	5.40	136.08	132.30
55	BB	64	G	C8-N9-C4	-5.40	104.24	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	29	A	C5-C6-N1	5.40	120.40	117.70
55	BB	79	G	C8-N9-C4	-5.40	104.24	106.40
21	AA	204	G	N9-C4-C5	5.39	107.56	105.40
21	AA	365	U	C1'-O4'-C4'	-5.39	105.58	109.90
21	AA	1062	U	N3-C2-O2	-5.39	118.42	122.20
54	BA	285	G	C8-N9-C4	-5.39	104.24	106.40
54	BA	1343	G	N3-C2-N2	-5.39	116.12	119.90
54	BA	1520	U	C5-C6-N1	-5.39	120.00	122.70
54	BA	2305	U	C5-C6-N1	-5.39	120.00	122.70
54	BA	2825	G	C2-N3-C4	5.39	114.60	111.90
21	AA	521	G	C5-C6-N1	5.39	114.20	111.50
21	AA	536	C	N1-C2-O2	5.39	122.14	118.90
21	AA	1223	C	N3-C2-O2	-5.39	118.12	121.90
54	BA	744	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1236	G	C3'-C2'-C1'	5.39	105.81	101.50
54	BA	1543	G	N3-C2-N2	-5.39	116.12	119.90
54	BA	2018	G	C5-C6-N1	5.39	114.20	111.50
55	BB	31	C	N3-C2-O2	-5.39	118.12	121.90
21	AA	1099	G	N1-C6-O6	-5.39	116.67	119.90
54	BA	2422	C	N1-C2-O2	5.39	122.13	118.90
54	BA	2866	U	C5-C6-N1	-5.39	120.00	122.70
3	AD	183	ARG	NE-CZ-NH1	5.39	123.00	120.30
21	AA	530	G	N1-C6-O6	-5.39	116.67	119.90
21	AA	1439	G	C5-C6-N1	5.39	114.19	111.50
54	BA	310	A	N1-C6-N6	-5.39	115.37	118.60
54	BA	464	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1665	A	O4'-C1'-N9	5.39	112.51	108.20
54	BA	2406	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	2558	C	N1-C2-O2	5.39	122.13	118.90
55	BB	92	C	O4'-C1'-N1	5.39	112.51	108.20
21	AA	1163	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	84	A	C4-C5-C6	-5.39	114.31	117.00
21	AA	124	C	N3-C4-C5	5.39	124.06	121.90
21	AA	734	G	N7-C8-N9	5.39	115.79	113.10
54	BA	429	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	2049	G	O4'-C1'-N9	5.39	112.51	108.20
54	BA	2155	U	O4'-C1'-N1	5.39	112.51	108.20
21	AA	34	C	N3-C4-C5	5.38	124.05	121.90
21	AA	215	C	O4'-C1'-N1	5.38	112.51	108.20
21	AA	1284	C	N3-C2-O2	-5.38	118.13	121.90
21	AA	1332	A	C4-C5-C6	-5.38	114.31	117.00
41	BS	11	ARG	NE-CZ-NH1	5.38	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	286	U	N1-C2-N3	5.38	118.13	114.90
54	BA	1785	A	C6-C5-N7	5.38	136.07	132.30
21	AA	356	A	C6-C5-N7	5.38	136.07	132.30
54	BA	1597	A	C3'-C2'-C1'	5.38	105.81	101.50
54	BA	1827	U	N3-C2-O2	-5.38	118.43	122.20
55	BB	46	A	N1-C6-N6	-5.38	115.37	118.60
21	AA	479	U	N3-C2-O2	-5.38	118.43	122.20
21	AA	1430	A	C3'-C2'-C1'	5.38	105.81	101.50
54	BA	1317	G	C1'-O4'-C4'	-5.38	105.59	109.90
54	BA	1559	U	O4'-C1'-N1	5.38	112.50	108.20
55	BB	105	G	N3-C4-C5	-5.38	125.91	128.60
54	BA	1205	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	2064	C	N3-C2-O2	-5.38	118.13	121.90
55	BB	104	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	1467	C	N3-C4-C5	5.38	124.05	121.90
54	BA	890	C	O4'-C1'-N1	5.38	112.50	108.20
54	BA	949	G	N7-C8-N9	5.38	115.79	113.10
54	BA	1567	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	1692	U	C5-C6-N1	-5.38	120.01	122.70
54	BA	2344	U	N3-C2-O2	-5.38	118.44	122.20
54	BA	2628	C	C6-N1-C2	-5.38	118.15	120.30
39	BQ	5	ARG	NE-CZ-NH1	5.38	122.99	120.30
54	BA	317	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	1766	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	2323	G	C8-N9-C4	-5.38	104.25	106.40
54	BA	2342	C	N1-C2-O2	5.38	122.13	118.90
54	BA	2620	C	N3-C2-O2	-5.38	118.14	121.90
21	AA	1053	G	C8-N9-C4	-5.38	104.25	106.40
54	BA	1576	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	2678	C	O4'-C1'-N1	5.38	112.50	108.20
21	AA	284	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	679	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	803	G	N3-C4-C5	-5.37	125.91	128.60
21	AA	1138	G	C5-C6-N1	5.37	114.19	111.50
21	AA	1417	G	C5-C6-N1	5.37	114.19	111.50
22	A1	23	A	C4-C5-C6	-5.37	114.31	117.00
24	A3	53	G	C8-N9-C4	-5.37	104.25	106.40
54	BA	1290	C	N1-C2-O2	5.37	122.12	118.90
54	BA	1604	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	1962	C	N1-C2-O2	5.37	122.12	118.90
54	BA	2057	G	C5-C6-N1	5.37	114.19	111.50
21	AA	370	C	N1-C2-O2	5.37	122.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	639	G	N3-C4-C5	-5.37	125.91	128.60
21	AA	806	C	O4'-C1'-N1	5.37	112.50	108.20
21	AA	1011	C	N1-C2-O2	5.37	122.12	118.90
54	BA	209	C	O4'-C1'-N1	5.37	112.50	108.20
54	BA	910	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	1414	C	O4'-C1'-N1	5.37	112.50	108.20
54	BA	1782	U	N3-C2-O2	-5.37	118.44	122.20
54	BA	2610	C	N1-C2-O2	5.37	122.12	118.90
21	AA	335	C	N1-C2-O2	5.37	122.12	118.90
54	BA	2068	U	C5-C6-N1	-5.37	120.02	122.70
54	BA	2498	C	N3-C4-C5	5.37	124.05	121.90
54	BA	2590	A	C4-C5-C6	-5.37	114.31	117.00
55	BB	65	U	N3-C2-O2	-5.37	118.44	122.20
21	AA	5	U	C1'-O4'-C4'	-5.37	105.61	109.90
21	AA	82	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	777	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	1452	C	N3-C2-O2	-5.37	118.14	121.90
24	A3	29	C	N1-C2-O2	5.37	122.12	118.90
54	BA	172	A	C6-C5-N7	5.37	136.06	132.30
54	BA	427	U	C4-C5-C6	5.37	122.92	119.70
54	BA	1066	U	C5-C6-N1	-5.37	120.02	122.70
54	BA	1899	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	469	C	O4'-C1'-N1	5.37	112.49	108.20
24	A3	6	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	549	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	1295	C	C5'-C4'-O4'	5.37	115.54	109.10
21	AA	481	G	N3-C4-C5	-5.37	125.92	128.60
54	BA	335	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	377	G	C5-C6-N1	5.37	114.18	111.50
54	BA	2521	C	N3-C4-C5	5.37	124.05	121.90
54	BA	2785	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	269	C	N3-C2-O2	-5.36	118.14	121.90
54	BA	1875	G	C8-N9-C4	-5.36	104.25	106.40
54	BA	1888	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	2124	G	C5-C6-N1	5.36	114.18	111.50
54	BA	2146	C	N1-C2-O2	5.36	122.12	118.90
54	BA	2717	C	N3-C4-C5	5.36	124.05	121.90
21	AA	311	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	196	A	C5-C6-N1	5.36	120.38	117.70
21	AA	917	G	C8-N9-C4	-5.36	104.26	106.40
32	BJ	95	ARG	NE-CZ-NH1	5.36	122.98	120.30
46	BX	17	ARG	NH1-CZ-NH2	-5.36	113.50	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	11	C	N3-C4-C5	5.36	124.04	121.90
54	BA	1509	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	1810	A	C6-C5-N7	5.36	136.05	132.30
54	BA	2644	G	N1-C6-O6	-5.36	116.68	119.90
21	AA	605	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	831	G	O4'-C1'-N9	5.36	112.49	108.20
54	BA	1464	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	1729	U	N3-C2-O2	-5.36	118.45	122.20
54	BA	2229	U	C5-C6-N1	-5.36	120.02	122.70
21	AA	15	G	N1-C6-O6	-5.36	116.69	119.90
21	AA	72	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	418	C	N1-C2-O2	5.36	122.11	118.90
21	AA	605	U	N1-C2-N3	5.36	118.11	114.90
21	AA	1433	A	C5-C6-N1	5.36	120.38	117.70
22	A1	21	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2116	G	N9-C4-C5	5.36	107.54	105.40
21	AA	1534	A	C4-C5-C6	-5.36	114.32	117.00
23	A2	90	U	C5-C6-N1	-5.36	120.02	122.70
54	BA	561	G	N1-C6-O6	-5.36	116.69	119.90
54	BA	1317	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	1430	G	C8-N9-C4	-5.36	104.26	106.40
54	BA	1832	C	N3-C4-C5	5.36	124.04	121.90
21	AA	151	A	C4-C5-C6	-5.35	114.32	117.00
54	BA	777	G	C5-C6-N1	5.35	114.18	111.50
54	BA	2353	G	C8-N9-C4	-5.35	104.26	106.40
21	AA	116	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	166	U	N3-C2-O2	-5.35	118.45	122.20
21	AA	308	C	O4'-C4'-C3'	5.35	110.38	106.10
21	AA	397	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	692	U	N3-C2-O2	-5.35	118.45	122.20
21	AA	1183	U	N3-C2-O2	-5.35	118.45	122.20
54	BA	552	U	O4'-C1'-N1	5.35	112.48	108.20
54	BA	846	U	N3-C2-O2	-5.35	118.45	122.20
54	BA	2086	U	C5'-C4'-O4'	5.35	115.52	109.10
54	BA	2092	U	C5-C6-N1	-5.35	120.02	122.70
21	AA	539	A	C6-C5-N7	5.35	136.05	132.30
54	BA	1967	C	O4'-C1'-N1	5.35	112.48	108.20
6	AG	4	ARG	NE-CZ-NH1	5.35	122.97	120.30
21	AA	496	A	O4'-C1'-N9	5.35	112.48	108.20
21	AA	571	U	O4'-C4'-C3'	5.35	110.38	106.10
21	AA	1141	C	N1-C2-O2	5.35	122.11	118.90
21	AA	1314	C	O4'-C1'-N1	5.35	112.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	54	G	N3-C4-C5	-5.35	125.93	128.60
54	BA	659	G	C5-C6-N1	5.35	114.17	111.50
54	BA	2138	G	O4'-C1'-N9	5.35	112.48	108.20
55	BB	54	G	C5-C6-N1	5.35	114.17	111.50
20	AU	44	ARG	NE-CZ-NH1	5.35	122.97	120.30
21	AA	308	C	N1-C2-O2	5.35	122.11	118.90
21	AA	396	C	N1-C2-O2	5.35	122.11	118.90
21	AA	568	G	N3-C2-N2	-5.35	116.16	119.90
21	AA	912	C	N1-C2-O2	5.35	122.11	118.90
21	AA	1200	C	N3-C2-O2	-5.35	118.16	121.90
21	AA	1524	C	N1-C2-O2	5.35	122.11	118.90
24	A3	50	G	C5-C6-N1	5.35	114.17	111.50
54	BA	321	U	C5-C6-N1	-5.35	120.03	122.70
54	BA	381	G	N9-C4-C5	5.35	107.54	105.40
54	BA	597	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	1438	U	N3-C2-O2	-5.35	118.46	122.20
54	BA	2110	G	C5-C6-N1	5.35	114.17	111.50
54	BA	2130	U	N1-C2-N3	5.35	118.11	114.90
54	BA	1318	U	C3'-C2'-C1'	5.35	105.78	101.50
54	BA	2101	A	C4-C5-C6	-5.35	114.33	117.00
1	AB	73	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	AB	224	ARG	NE-CZ-NH1	5.34	122.97	120.30
21	AA	771	G	N1-C6-O6	-5.34	116.69	119.90
22	A1	67	U	N3-C2-O2	-5.34	118.46	122.20
54	BA	605	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	664	G	C5-C6-N1	5.34	114.17	111.50
54	BA	867	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1209	U	N1-C2-N3	5.34	118.11	114.90
54	BA	2432	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2890	G	C5-C6-N1	5.34	114.17	111.50
55	BB	114	C	N3-C2-O2	-5.34	118.16	121.90
21	AA	851	G	C8-N9-C4	-5.34	104.26	106.40
21	AA	1028	C	N1-C2-O2	5.34	122.11	118.90
54	BA	142	A	C5-C6-N1	5.34	120.37	117.70
54	BA	1539	U	C5-C6-N1	-5.34	120.03	122.70
54	BA	2650	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	2715	C	O4'-C1'-N1	5.34	112.47	108.20
21	AA	1044	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	1066	C	N1-C2-O2	5.34	122.11	118.90
54	BA	159	G	N3-C4-C5	-5.34	125.93	128.60
54	BA	247	G	O4'-C1'-N9	5.34	112.47	108.20
54	BA	765	C	N1-C2-O2	5.34	122.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1389	G	C8-N9-C4	-5.34	104.26	106.40
54	BA	1702	G	N1-C6-O6	-5.34	116.69	119.90
55	BB	116	G	O4'-C1'-N9	5.34	112.47	108.20
21	AA	995	C	O4'-C1'-N1	5.34	112.47	108.20
25	BC	155	ARG	NE-CZ-NH2	-5.34	117.63	120.30
54	BA	383	C	N3-C4-C5	5.34	124.04	121.90
54	BA	1488	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1941	C	N1-C2-O2	5.34	122.10	118.90
21	AA	1308	U	C5-C6-N1	-5.34	120.03	122.70
54	BA	517	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1167	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1951	U	C5-C6-N1	-5.34	120.03	122.70
54	BA	2129	C	N1-C2-O2	5.34	122.10	118.90
21	AA	245	U	C5-C6-N1	-5.34	120.03	122.70
21	AA	263	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	878	A	C5-C6-N1	5.34	120.37	117.70
21	AA	899	C	N3-C2-O2	-5.34	118.16	121.90
21	AA	1115	U	N1-C2-N3	5.34	118.10	114.90
54	BA	32	C	N1-C2-O2	5.34	122.10	118.90
54	BA	90	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	774	G	N9-C4-C5	5.34	107.53	105.40
21	AA	1400	C	O4'-C4'-C3'	5.33	110.37	106.10
54	BA	37	C	N3-C4-C5	5.33	124.03	121.90
54	BA	914	G	C5-C6-N1	5.33	114.17	111.50
54	BA	2819	G	N1-C6-O6	-5.33	116.70	119.90
21	AA	145	G	C8-N9-C4	-5.33	104.27	106.40
21	AA	664	G	C5-C6-N1	5.33	114.17	111.50
21	AA	1080	A	C4-C5-C6	-5.33	114.33	117.00
22	A1	11	C	N1-C2-O2	5.33	122.10	118.90
54	BA	15	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	236	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	377	G	O4'-C1'-N9	5.33	112.47	108.20
54	BA	1027	A	C4-C5-C6	-5.33	114.33	117.00
54	BA	1562	U	N3-C2-O2	-5.33	118.47	122.20
54	BA	2092	U	C4-C5-C6	5.33	122.90	119.70
54	BA	2761	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	1030	U	N1-C2-N3	5.33	118.10	114.90
54	BA	468	G	C5-C6-N1	5.33	114.17	111.50
54	BA	651	G	N9-C4-C5	5.33	107.53	105.40
54	BA	657	U	N1-C2-N3	5.33	118.10	114.90
54	BA	856	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	1431	A	C6-C5-N7	5.33	136.03	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1904	G	C8-N9-C4	-5.33	104.27	106.40
54	BA	2361	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	2841	C	N3-C2-O2	-5.33	118.17	121.90
55	BB	92	C	C4'-C3'-C2'	-5.33	97.27	102.60
21	AA	422	C	C5'-C4'-C3'	-5.33	107.47	116.00
54	BA	106	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	156	A	C6-C5-N7	5.33	136.03	132.30
54	BA	427	U	N1-C2-N3	5.33	118.10	114.90
4	AE	68	ARG	NE-CZ-NH1	5.33	122.97	120.30
21	AA	408	A	C6-C5-N7	5.33	136.03	132.30
21	AA	677	U	N1-C2-N3	5.33	118.10	114.90
23	A2	87	U	C4-C5-C6	5.33	122.90	119.70
28	BF	79	ARG	NE-CZ-NH2	-5.33	117.64	120.30
54	BA	698	C	C3'-C2'-C1'	5.33	105.76	101.50
54	BA	755	U	C4'-C3'-C2'	-5.33	97.27	102.60
54	BA	1804	C	N3-C4-C5	5.33	124.03	121.90
54	BA	2137	U	N1-C2-O2	5.33	126.53	122.80
54	BA	2178	C	N3-C2-O2	-5.33	118.17	121.90
21	AA	373	A	C2-N3-C4	5.33	113.26	110.60
21	AA	1077	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	1301	A	C4-C5-C6	-5.33	114.34	117.00
54	BA	1739	A	C5-C6-N1	5.33	120.36	117.70
54	BA	1799	G	C5-C6-N1	5.33	114.16	111.50
21	AA	44	A	C4-C5-C6	-5.33	114.34	117.00
54	BA	51	G	C8-N9-C4	-5.33	104.27	106.40
54	BA	599	A	C6-C5-N7	5.33	136.03	132.30
54	BA	1481	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	1509	A	C2-N3-C4	5.33	113.26	110.60
54	BA	1541	C	N1-C2-O2	5.33	122.09	118.90
54	BA	2074	U	N3-C2-O2	-5.33	118.47	122.20
28	BF	101	ARG	NE-CZ-NH1	5.32	122.96	120.30
54	BA	98	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	945	A	C6-C5-N7	5.32	136.03	132.30
54	BA	1030	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	1481	U	N1-C2-N3	5.32	118.09	114.90
54	BA	1833	C	N3-C4-C5	5.32	124.03	121.90
54	BA	2240	U	N1-C2-N3	5.32	118.09	114.90
54	BA	2824	C	O4'-C1'-N1	5.32	112.46	108.20
21	AA	995	C	N1-C2-O2	5.32	122.09	118.90
22	A1	68	C	N3-C2-O2	-5.32	118.17	121.90
54	BA	1679	A	C6-C5-N7	5.32	136.03	132.30
54	BA	1817	G	N3-C2-N2	-5.32	116.17	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2428	G	N3-C4-C5	-5.32	125.94	128.60
10	AK	124	LYS	C-N-CA	5.32	135.00	121.70
21	AA	232	G	C5-C6-N1	5.32	114.16	111.50
21	AA	715	A	C6-C5-N7	5.32	136.02	132.30
21	AA	1094	G	N3-C2-N2	-5.32	116.18	119.90
21	AA	1178	G	C5-C6-N1	5.32	114.16	111.50
54	BA	1125	G	C5-C6-N1	5.32	114.16	111.50
54	BA	1306	C	N1-C2-O2	5.32	122.09	118.90
54	BA	1390	U	O4'-C1'-N1	5.32	112.46	108.20
54	BA	1656	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	1816	C	N1-C2-O2	5.32	122.09	118.90
54	BA	2260	C	N3-C2-O2	-5.32	118.17	121.90
21	AA	485	U	C5-C6-N1	-5.32	120.04	122.70
21	AA	630	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	1078	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	280	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	412	A	O4'-C1'-N9	5.32	112.45	108.20
54	BA	1089	A	O4'-C1'-C2'	-5.32	100.48	105.80
54	BA	1291	C	N3-C2-O2	-5.32	118.18	121.90
21	AA	131	A	C6-C5-N7	5.32	136.02	132.30
21	AA	170	U	C5-C6-N1	-5.32	120.04	122.70
21	AA	475	C	N1-C2-O2	5.32	122.09	118.90
21	AA	544	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	1298	U	O4'-C1'-N1	5.32	112.45	108.20
21	AA	1300	G	P-O3'-C3'	5.32	126.08	119.70
34	BL	48	ARG	NE-CZ-NH1	5.32	122.96	120.30
54	BA	835	C	N3-C2-O2	-5.32	118.18	121.90
54	BA	1584	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	1972	G	C8-N9-C4	-5.32	104.27	106.40
54	BA	2101	A	C5-C6-N1	5.32	120.36	117.70
21	AA	418	C	N3-C4-C5	5.32	124.03	121.90
21	AA	582	C	N3-C4-C5	5.32	124.03	121.90
21	AA	939	G	C8-N9-C4	-5.32	104.27	106.40
49	B0	51	ARG	NE-CZ-NH2	-5.32	117.64	120.30
54	BA	810	U	N3-C2-O2	-5.32	118.48	122.20
21	AA	1318	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	647	G	N3-C4-C5	-5.31	125.94	128.60
21	AA	793	U	N3-C2-O2	-5.31	118.48	122.20
24	A3	49	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	201	C	N1-C2-O2	5.31	122.09	118.90
54	BA	890	C	C3'-C2'-C1'	-5.31	97.25	101.50
54	BA	989	G	O4'-C1'-N9	5.31	112.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1089	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	2049	G	N9-C4-C5	5.31	107.53	105.40
54	BA	2255	G	C5-C6-N1	5.31	114.16	111.50
54	BA	2117	A	C4-C5-C6	-5.31	114.34	117.00
21	AA	787	A	C5-C6-N1	5.31	120.36	117.70
21	AA	1335	U	O4'-C4'-C3'	5.31	110.35	106.10
33	BK	49	ARG	NE-CZ-NH1	5.31	122.95	120.30
54	BA	86	G	N1-C6-O6	-5.31	116.71	119.90
54	BA	123	G	C5-C6-N1	5.31	114.16	111.50
54	BA	876	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	888	C	N1-C2-O2	5.31	122.08	118.90
54	BA	1937	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	2169	A	C8-N9-C4	-5.31	103.68	105.80
54	BA	2428	G	O4'-C1'-N9	5.31	112.45	108.20
21	AA	1432	G	C5-C6-N1	5.31	114.15	111.50
54	BA	516	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	1964	G	N3-C4-C5	-5.31	125.95	128.60
54	BA	2385	C	N1-C2-O2	5.31	122.08	118.90
54	BA	2390	U	C5-C6-N1	-5.31	120.05	122.70
21	AA	1249	C	N3-C2-O2	-5.31	118.19	121.90
21	AA	1333	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	548	G	C8-N9-C4	-5.31	104.28	106.40
21	AA	305	G	O4'-C1'-N9	5.30	112.44	108.20
21	AA	433	G	N3-C4-C5	-5.30	125.95	128.60
21	AA	701	U	N3-C2-O2	-5.30	118.49	122.20
21	AA	842	U	C5-C6-N1	-5.30	120.05	122.70
21	AA	1173	U	C5-C6-N1	-5.30	120.05	122.70
21	AA	1155	A	C5-C6-N1	5.30	120.35	117.70
54	BA	1474	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2737	G	N3-C4-C5	-5.30	125.95	128.60
21	AA	756	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	1221	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	1548	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	1703	G	C5-C6-N1	5.30	114.15	111.50
54	BA	1868	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2618	G	C5'-C4'-O4'	5.30	115.46	109.10
21	AA	507	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	529	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	1559	U	N3-C2-O2	-5.30	118.49	122.20
54	BA	2428	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	429	U	N1-C2-N3	5.30	118.08	114.90
54	BA	901	C	N3-C2-O2	-5.30	118.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2063	C	C2-N3-C4	-5.30	117.25	119.90
54	BA	2281	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	2383	G	C8-N9-C4	-5.30	104.28	106.40
21	AA	257	G	C5-C6-N1	5.30	114.15	111.50
21	AA	322	C	N3-C2-O2	-5.30	118.19	121.90
21	AA	403	C	N3-C4-C5	5.30	124.02	121.90
21	AA	1369	C	N1-C2-O2	5.30	122.08	118.90
21	AA	1450	U	N1-C2-N3	5.30	118.08	114.90
54	BA	330	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	446	G	O4'-C4'-C3'	5.30	110.34	106.10
54	BA	808	G	C3'-C2'-C1'	5.30	105.74	101.50
54	BA	1536	C	C5'-C4'-C3'	-5.30	107.53	116.00
54	BA	1669	A	C5-C6-N1	5.30	120.35	117.70
54	BA	2175	C	N3-C4-C5	5.30	124.02	121.90
54	BA	2515	C	N1-C2-O2	5.30	122.08	118.90
21	AA	327	A	O4'-C1'-N9	5.29	112.44	108.20
54	BA	394	C	N1-C2-O2	5.29	122.08	118.90
54	BA	948	C	N1-C2-O2	5.29	122.08	118.90
54	BA	2693	G	C5-C6-N1	5.29	114.15	111.50
21	AA	1126	U	C5-C6-N1	-5.29	120.05	122.70
54	BA	57	C	N3-C2-O2	-5.29	118.19	121.90
54	BA	427	U	C5-C6-N1	-5.29	120.05	122.70
54	BA	1112	G	C8-N9-C4	-5.29	104.28	106.40
54	BA	2047	C	C4'-C3'-C2'	-5.29	97.31	102.60
54	BA	2235	G	C4'-C3'-C2'	-5.29	97.31	102.60
54	BA	2374	C	N3-C4-C5	5.29	124.02	121.90
54	BA	2803	G	C5-C6-N1	5.29	114.15	111.50
54	BA	2830	C	N3-C2-O2	-5.29	118.19	121.90
21	AA	97	G	N3-C4-C5	-5.29	125.95	128.60
21	AA	1036	A	C6-C5-N7	5.29	136.00	132.30
54	BA	175	G	N3-C2-N2	-5.29	116.20	119.90
54	BA	445	C	N1-C2-O2	5.29	122.08	118.90
54	BA	2513	A	C6-C5-N7	5.29	136.00	132.30
54	BA	2602	A	C1'-O4'-C4'	-5.29	105.67	109.90
54	BA	2867	G	O4'-C1'-N9	5.29	112.43	108.20
22	A1	67	U	C5-C6-N1	-5.29	120.06	122.70
54	BA	2890	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	921	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1518	C	N3-C2-O2	-5.29	118.20	121.90
55	BB	105	G	C8-N9-C4	-5.29	104.28	106.40
21	AA	1478	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	136	G	C5-C6-N1	5.29	114.14	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1580	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	2002	G	N1-C6-O6	-5.29	116.73	119.90
21	AA	166	U	C5-C6-N1	-5.29	120.06	122.70
21	AA	267	C	C3'-C2'-C1'	5.29	105.73	101.50
22	A1	71	C	O4'-C1'-N1	5.29	112.43	108.20
28	BF	109	ARG	NE-CZ-NH2	-5.29	117.66	120.30
54	BA	149	A	O4'-C1'-N9	5.29	112.43	108.20
54	BA	761	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	943	A	C4-C5-C6	-5.29	114.36	117.00
21	AA	248	C	O4'-C1'-N1	5.28	112.43	108.20
21	AA	379	C	N3-C4-C5	5.28	124.01	121.90
54	BA	345	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	513	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1818	U	C5-C6-N1	-5.28	120.06	122.70
54	BA	1984	G	C8-N9-C4	-5.28	104.29	106.40
54	BA	2347	C	N3-C2-O2	-5.28	118.20	121.90
54	BA	2571	U	N3-C2-O2	-5.28	118.50	122.20
21	AA	1117	A	C6-C5-N7	5.28	136.00	132.30
54	BA	446	G	C3'-C2'-C1'	5.28	105.73	101.50
54	BA	734	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	916	G	N3-C4-C5	-5.28	125.96	128.60
54	BA	1585	C	C2-N3-C4	-5.28	117.26	119.90
54	BA	2085	U	C5-C6-N1	-5.28	120.06	122.70
54	BA	2820	A	C4-C5-C6	-5.28	114.36	117.00
55	BB	117	G	N9-C4-C5	5.28	107.51	105.40
21	AA	94	G	N3-C2-N2	-5.28	116.20	119.90
21	AA	164	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	802	A	N1-C6-N6	-5.28	115.43	118.60
54	BA	1041	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	1071	G	C3'-C2'-C1'	5.28	105.72	101.50
54	BA	2305	U	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2679	A	O4'-C1'-N9	5.28	112.42	108.20
54	BA	2699	C	N1-C2-O2	5.28	122.07	118.90
21	AA	725	G	C5'-C4'-C3'	-5.28	107.55	116.00
54	BA	1545	A	C6-C5-N7	5.28	136.00	132.30
21	AA	80	A	C6-C5-N7	5.28	136.00	132.30
21	AA	113	G	N7-C8-N9	5.28	115.74	113.10
24	A3	16	C	N1-C2-O2	5.28	122.07	118.90
24	A3	58	A	C6-C5-N7	5.28	136.00	132.30
54	BA	348	A	O4'-C1'-N9	5.28	112.42	108.20
54	BA	1714	U	N3-C2-O2	-5.28	118.51	122.20
21	AA	220	G	N9-C4-C5	5.28	107.51	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1370	G	O4'-C1'-N9	5.28	112.42	108.20
54	BA	1887	C	N3-C2-O2	-5.28	118.21	121.90
55	BB	112	G	C5-C6-N1	5.28	114.14	111.50
54	BA	210	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	456	C	N3-C4-N4	-5.27	114.31	118.00
54	BA	846	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	1248	G	O4'-C1'-N9	5.27	112.42	108.20
55	BB	17	C	N3-C2-O2	-5.27	118.21	121.90
21	AA	1097	C	C1'-O4'-C4'	-5.27	105.68	109.90
21	AA	1176	A	C5-C6-N1	5.27	120.34	117.70
38	BP	88	ARG	NE-CZ-NH1	5.27	122.94	120.30
54	BA	130	C	N3-C4-C5	5.27	124.01	121.90
54	BA	518	G	C8-N9-C4	-5.27	104.29	106.40
54	BA	541	A	C6-C5-N7	5.27	135.99	132.30
54	BA	1036	G	C5-C6-N1	5.27	114.14	111.50
54	BA	1169	A	C6-C5-N7	5.27	135.99	132.30
54	BA	1979	U	N3-C2-O2	-5.27	118.51	122.20
54	BA	2583	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	2847	U	N1-C2-N3	5.27	118.06	114.90
55	BB	5	U	C4'-C3'-C2'	-5.27	97.33	102.60
21	AA	1460	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	1172	C	N3-C2-O2	-5.27	118.21	121.90
21	AA	34	C	N1-C2-O2	5.27	122.06	118.90
21	AA	622	A	C6-C5-N7	5.27	135.99	132.30
21	AA	979	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2240	U	O4'-C1'-N1	5.27	112.42	108.20
21	AA	139	A	C5-C6-N1	5.27	120.33	117.70
21	AA	364	A	C6-C5-N7	5.27	135.99	132.30
21	AA	503	C	N3-C2-O2	-5.27	118.21	121.90
21	AA	521	G	O4'-C1'-N9	5.27	112.41	108.20
21	AA	1097	C	N3-C2-O2	-5.27	118.21	121.90
21	AA	1184	G	N3-C4-C5	-5.27	125.97	128.60
21	AA	1342	C	N3-C4-C5	5.27	124.01	121.90
54	BA	994	C	N1-C2-O2	5.27	122.06	118.90
54	BA	1613	G	O4'-C1'-N9	5.27	112.41	108.20
54	BA	2138	G	N1-C6-O6	-5.27	116.74	119.90
21	AA	116	A	C6-C5-N7	5.27	135.99	132.30
21	AA	443	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	726	G	O4'-C1'-N9	5.27	112.41	108.20
54	BA	935	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	1489	C	N1-C2-O2	5.27	122.06	118.90
54	BA	2341	G	C4'-C3'-C2'	-5.27	97.33	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	187	G	C5-C6-N1	5.26	114.13	111.50
21	AA	204	G	C8-N9-C4	-5.26	104.29	106.40
21	AA	426	U	N1-C2-N3	5.26	118.06	114.90
21	AA	809	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	343	C	O4'-C1'-N1	5.26	112.41	108.20
54	BA	1841	U	O4'-C1'-N1	5.26	112.41	108.20
55	BB	117	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	872	A	C2-N3-C4	5.26	113.23	110.60
21	AA	40	C	N1-C2-O2	5.26	122.06	118.90
21	AA	1215	G	N9-C4-C5	5.26	107.50	105.40
21	AA	1276	G	N7-C8-N9	5.26	115.73	113.10
21	AA	1482	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	666	A	C5-C6-N1	5.26	120.33	117.70
54	BA	775	G	O4'-C1'-N9	5.26	112.41	108.20
54	BA	1624	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	2745	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	504	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	547	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	861	G	N7-C8-N9	5.26	115.73	113.10
21	AA	897	C	O4'-C1'-N1	5.26	112.41	108.20
21	AA	923	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	1233	G	C5-C6-N1	5.26	114.13	111.50
21	AA	1487	G	O4'-C1'-N9	5.26	112.41	108.20
54	BA	1082	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	1462	C	N3-C2-O2	-5.26	118.22	121.90
54	BA	1725	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	1831	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	2065	C	N3-C2-O2	-5.26	118.22	121.90
54	BA	2131	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	2317	A	C6-C5-N7	5.26	135.98	132.30
54	BA	2813	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	33	A	C6-C5-N7	5.26	135.98	132.30
54	BA	1422	G	N1-C6-O6	-5.26	116.75	119.90
54	BA	2624	G	N1-C6-O6	-5.26	116.75	119.90
17	AR	47	ARG	NE-CZ-NH2	-5.26	117.67	120.30
21	AA	631	C	N1-C2-O2	5.26	122.05	118.90
21	AA	1387	G	C5-C6-N1	5.26	114.13	111.50
21	AA	1519	A	C6-C5-N7	5.26	135.98	132.30
54	BA	514	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	1618	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	2243	U	O4'-C1'-N1	5.26	112.41	108.20
55	BB	24	G	C8-N9-C4	-5.26	104.30	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2222	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2638	G	C8-N9-C4	-5.25	104.30	106.40
55	BB	59	A	C4-C5-C6	-5.25	114.37	117.00
21	AA	1085	U	C5-C6-N1	-5.25	120.07	122.70
21	AA	1528	U	N3-C2-O2	-5.25	118.52	122.20
54	BA	532	A	O4'-C1'-N9	5.25	112.40	108.20
54	BA	920	A	C6-C5-N7	5.25	135.98	132.30
54	BA	1084	A	C6-C5-N7	5.25	135.98	132.30
54	BA	1795	C	N3-C2-O2	-5.25	118.22	121.90
54	BA	2537	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2546	U	C5-C6-N1	-5.25	120.07	122.70
21	AA	248	C	N1-C2-O2	5.25	122.05	118.90
21	AA	764	C	N1-C2-O2	5.25	122.05	118.90
54	BA	410	G	N9-C4-C5	5.25	107.50	105.40
54	BA	1257	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1911	U	C5'-C4'-O4'	5.25	115.40	109.10
54	BA	2424	C	O4'-C1'-N1	5.25	112.40	108.20
21	AA	21	G	C5-C6-N1	5.25	114.12	111.50
21	AA	359	G	N3-C4-C5	-5.25	125.97	128.60
21	AA	426	U	N3-C2-O2	-5.25	118.53	122.20
54	BA	869	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	2611	C	O4'-C1'-N1	5.25	112.40	108.20
21	AA	494	G	N3-C4-C5	-5.25	125.97	128.60
21	AA	610	U	O4'-C1'-N1	5.25	112.40	108.20
21	AA	1432	G	C3'-C2'-C1'	5.25	105.70	101.50
21	AA	1502	A	O4'-C1'-N9	5.25	112.40	108.20
54	BA	2757	A	C5'-C4'-O4'	5.25	115.40	109.10
55	BB	82	U	C5-C6-N1	-5.25	120.08	122.70
21	AA	1380	U	C5-C6-N1	-5.25	120.08	122.70
21	AA	1392	G	C5-C6-N1	5.25	114.12	111.50
54	BA	721	A	C6-C5-N7	5.25	135.97	132.30
54	BA	2805	C	N1-C2-O2	5.25	122.05	118.90
55	BB	42	C	N3-C2-O2	-5.25	118.23	121.90
21	AA	501	C	N3-C4-C5	5.25	124.00	121.90
54	BA	47	C	N3-C2-O2	-5.25	118.23	121.90
21	AA	75	G	C5-C6-N1	5.24	114.12	111.50
21	AA	811	C	O4'-C1'-N1	5.24	112.39	108.20
21	AA	1093	A	C5-C6-N1	5.24	120.32	117.70
54	BA	171	U	C5-C6-N1	-5.24	120.08	122.70
54	BA	1888	G	C8-N9-C4	-5.24	104.30	106.40
54	BA	2196	C	C1'-O4'-C4'	-5.24	105.71	109.90
54	BA	2636	C	O4'-C1'-N1	5.24	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AP	14	ARG	NE-CZ-NH1	5.24	122.92	120.30
54	BA	578	G	N1-C6-O6	-5.24	116.75	119.90
54	BA	702	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	1129	A	C5-C6-N1	5.24	120.32	117.70
21	AA	253	A	C5-C6-N1	5.24	120.32	117.70
21	AA	816	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	1472	U	N3-C2-O2	-5.24	118.53	122.20
54	BA	37	C	N1-C2-O2	5.24	122.04	118.90
54	BA	505	A	O4'-C1'-N9	5.24	112.39	108.20
54	BA	1041	G	C5-C6-N1	5.24	114.12	111.50
54	BA	1088	A	C6-C5-N7	5.24	135.97	132.30
54	BA	2831	G	N1-C6-O6	-5.24	116.76	119.90
21	AA	572	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	701	U	P-O3'-C3'	5.24	125.98	119.70
21	AA	744	C	N1-C2-O2	5.24	122.04	118.90
21	AA	1001	C	N3-C2-O2	-5.24	118.23	121.90
21	AA	1067	A	P-O3'-C3'	5.24	125.99	119.70
21	AA	1405	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	59	U	N1-C2-N3	5.24	118.04	114.90
54	BA	504	A	C1'-O4'-C4'	-5.24	105.71	109.90
54	BA	1214	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	1222	U	C5-C6-N1	-5.24	120.08	122.70
54	BA	2030	A	C6-C5-N7	5.24	135.97	132.30
55	BB	76	G	O4'-C1'-N9	5.24	112.39	108.20
21	AA	1121	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	1330	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	774	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	1639	C	N3-C4-N4	-5.24	114.33	118.00
15	AP	51	ARG	NE-CZ-NH2	-5.24	117.68	120.30
21	AA	747	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	755	G	O4'-C1'-N9	5.24	112.39	108.20
21	AA	818	G	N3-C2-N2	-5.24	116.23	119.90
24	A3	3	C	N3-C4-C5	5.24	124.00	121.90
54	BA	570	G	N3-C2-N2	-5.24	116.23	119.90
54	BA	948	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	1281	G	C5'-C4'-O4'	5.24	115.38	109.10
54	BA	1316	U	N1-C2-N3	5.24	118.04	114.90
54	BA	1350	C	C4'-C3'-C2'	-5.24	97.36	102.60
54	BA	1351	C	C6-N1-C2	-5.24	118.21	120.30
54	BA	2077	A	N1-C6-N6	-5.24	115.46	118.60
54	BA	2557	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	370	C	N3-C4-C5	5.23	123.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	773	G	C5-C6-N1	5.23	114.12	111.50
21	AA	1300	G	O4'-C1'-N9	5.23	112.39	108.20
21	AA	1514	G	C5-C6-N1	5.23	114.12	111.50
54	BA	1033	U	N3-C2-O2	-5.23	118.54	122.20
54	BA	1834	U	C3'-C2'-C1'	5.23	105.69	101.50
54	BA	2066	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	2168	G	C4'-C3'-C2'	-5.23	97.37	102.60
54	BA	2463	C	N3-C2-O2	-5.23	118.24	121.90
21	AA	146	G	C5-C6-N1	5.23	114.12	111.50
21	AA	719	C	N3-C2-O2	-5.23	118.24	121.90
21	AA	1237	C	N1-C2-O2	5.23	122.04	118.90
54	BA	860	U	O4'-C1'-N1	5.23	112.38	108.20
54	BA	874	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	1088	A	C2-N3-C4	5.23	113.22	110.60
54	BA	2563	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2809	A	C4-C5-C6	-5.23	114.38	117.00
54	BA	2890	G	N3-C4-C5	-5.23	125.98	128.60
54	BA	838	C	C5'-C4'-O4'	5.23	115.38	109.10
54	BA	1505	A	C6-C5-N7	5.23	135.96	132.30
54	BA	2323	G	N7-C8-N9	5.23	115.72	113.10
54	BA	2626	C	N3-C2-O2	-5.23	118.24	121.90
55	BB	64	G	N3-C4-C5	-5.23	125.99	128.60
54	BA	1378	A	C3'-C2'-C1'	5.23	105.68	101.50
20	AU	46	ARG	NE-CZ-NH1	5.23	122.91	120.30
21	AA	799	G	C5-C6-N1	5.23	114.11	111.50
21	AA	813	U	O4'-C1'-N1	5.23	112.38	108.20
24	A3	43	G	N9-C4-C5	5.23	107.49	105.40
54	BA	108	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	651	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	47	C	N3-C2-O2	-5.22	118.24	121.90
21	AA	918	A	C5-C6-N6	5.22	127.88	123.70
21	AA	1340	A	O4'-C1'-N9	5.22	112.38	108.20
27	BE	44	ARG	NE-CZ-NH1	5.22	122.91	120.30
54	BA	249	C	P-O3'-C3'	5.22	125.97	119.70
54	BA	676	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	1714	U	C1'-O4'-C4'	-5.22	105.72	109.90
54	BA	2197	U	N3-C2-O2	-5.22	118.54	122.20
21	AA	212	G	O4'-C1'-N9	5.22	112.38	108.20
21	AA	444	G	N3-C4-C5	-5.22	125.99	128.60
21	AA	799	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	1504	G	O4'-C1'-N9	5.22	112.38	108.20
22	A1	33	U	N3-C2-O2	-5.22	118.54	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A2	86	U	C5'-C4'-C3'	-5.22	107.64	116.00
54	BA	204	A	C6-C5-N7	5.22	135.96	132.30
54	BA	1646	C	N3-C4-C5	5.22	123.99	121.90
54	BA	1767	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	1100	C	N1-C2-O2	5.22	122.03	118.90
21	AA	1119	C	O4'-C1'-N1	5.22	112.38	108.20
21	AA	1139	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	122	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	810	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	1158	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1635	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	1644	C	N3-C2-O2	-5.22	118.25	121.90
54	BA	2417	C	C4'-C3'-C2'	-5.22	97.38	102.60
21	AA	531	U	C5-C6-N1	-5.22	120.09	122.70
21	AA	843	U	O4'-C1'-N1	5.22	112.37	108.20
22	A1	43	G	N1-C6-O6	-5.22	116.77	119.90
55	BB	63	C	N3-C2-O2	-5.22	118.25	121.90
21	AA	1192	C	N1-C2-O2	5.22	122.03	118.90
21	AA	1434	A	C6-C5-N7	5.22	135.95	132.30
54	BA	1850	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	420	U	N1-C2-N3	5.21	118.03	114.90
21	AA	883	C	C1'-O4'-C4'	-5.21	105.73	109.90
21	AA	1126	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1764	C	N3-C2-O2	-5.21	118.25	121.90
54	BA	2689	U	C1'-O4'-C4'	-5.21	105.73	109.90
54	BA	1397	U	N1-C2-N3	5.21	118.03	114.90
54	BA	2246	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	2337	G	N3-C4-C5	-5.21	125.99	128.60
54	BA	2343	U	C5-C6-N1	-5.21	120.09	122.70
21	AA	155	A	C6-C5-N7	5.21	135.95	132.30
21	AA	428	G	N1-C6-O6	-5.21	116.77	119.90
21	AA	679	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	220	G	N3-C4-C5	-5.21	125.99	128.60
54	BA	660	C	C3'-C2'-C1'	5.21	105.67	101.50
54	BA	1989	G	N7-C8-N9	5.21	115.71	113.10
21	AA	176	C	N3-C4-C5	5.21	123.98	121.90
22	A1	56	C	N1-C2-O2	5.21	122.03	118.90
54	BA	1594	U	N3-C2-O2	-5.21	118.55	122.20
54	BA	1806	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2229	U	N1-C2-N3	5.21	118.03	114.90
54	BA	2755	C	N1-C2-O2	5.21	122.03	118.90
11	AL	120	ARG	NE-CZ-NH1	5.21	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1023	U	O4'-C1'-N1	5.21	112.37	108.20
21	AA	1204	A	C6-C5-N7	5.21	135.94	132.30
21	AA	1364	U	N1-C2-N3	5.21	118.03	114.90
21	AA	1482	G	C8-N9-C4	-5.21	104.32	106.40
54	BA	35	G	N3-C4-C5	-5.21	126.00	128.60
54	BA	116	C	N1-C2-O2	5.21	122.03	118.90
54	BA	154	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1776	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	2145	C	N3-C4-C5	5.21	123.98	121.90
54	BA	2338	C	N3-C4-C5	5.21	123.98	121.90
54	BA	2679	A	C5-C6-N1	5.21	120.30	117.70
55	BB	9	G	N1-C6-O6	-5.21	116.77	119.90
21	AA	34	C	C5'-C4'-O4'	5.21	115.35	109.10
21	AA	513	C	N1-C2-O2	5.21	122.02	118.90
21	AA	517	G	C5-C6-N1	5.21	114.10	111.50
21	AA	524	G	C5-C6-N1	5.21	114.10	111.50
21	AA	1432	G	N3-C4-C5	-5.21	126.00	128.60
24	A3	64	G	N7-C8-N9	5.21	115.70	113.10
54	BA	458	G	O4'-C1'-N9	5.21	112.36	108.20
54	BA	571	U	O4'-C1'-C2'	-5.21	100.59	105.80
54	BA	884	U	C5-C6-N1	-5.21	120.10	122.70
54	BA	1576	U	C5-C6-N1	-5.21	120.10	122.70
54	BA	2391	G	C5-C6-N1	5.21	114.10	111.50
54	BA	2743	U	C5-C6-N1	-5.21	120.10	122.70
54	BA	2862	G	N1-C6-O6	-5.21	116.78	119.90
21	AA	536	C	N3-C4-C5	5.21	123.98	121.90
21	AA	872	A	C4-C5-C6	-5.21	114.40	117.00
21	AA	984	C	N1-C2-O2	5.21	122.02	118.90
54	BA	422	A	C5-C6-N1	5.21	120.30	117.70
54	BA	1569	A	C5-C6-N1	5.21	120.30	117.70
54	BA	2697	G	C4'-C3'-C2'	-5.21	97.39	102.60
9	AJ	89	ARG	NE-CZ-NH2	-5.20	117.70	120.30
21	AA	1167	A	C3'-C2'-C1'	5.20	105.66	101.50
21	AA	1324	A	C4-C5-C6	-5.20	114.40	117.00
34	BL	69	ARG	NE-CZ-NH1	5.20	122.90	120.30
54	BA	104	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1228	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	1711	A	C2-N3-C4	5.20	113.20	110.60
54	BA	646	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1572	A	C4-C5-C6	-5.20	114.40	117.00
21	AA	1104	G	C5-C6-N1	5.20	114.10	111.50
21	AA	1251	A	C6-C5-N7	5.20	135.94	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1105	U	N1-C2-N3	5.20	118.02	114.90
54	BA	2234	G	N3-C4-C5	-5.20	126.00	128.60
54	BA	2894	G	C5-C6-N1	5.20	114.10	111.50
21	AA	177	G	C5-C6-N1	5.20	114.10	111.50
21	AA	434	U	N3-C2-O2	-5.20	118.56	122.20
54	BA	548	G	N7-C8-N9	5.20	115.70	113.10
54	BA	583	G	C5-C6-N1	5.20	114.10	111.50
54	BA	616	A	O4'-C1'-N9	5.20	112.36	108.20
54	BA	680	C	C2-N3-C4	-5.20	117.30	119.90
54	BA	1793	C	C5'-C4'-O4'	5.20	115.34	109.10
54	BA	2617	U	O4'-C1'-N1	5.20	112.36	108.20
21	AA	411	A	C5-C6-N1	5.20	120.30	117.70
21	AA	652	U	C5-C6-N1	-5.20	120.10	122.70
54	BA	123	G	C5'-C4'-O4'	5.20	115.34	109.10
54	BA	2160	C	N1-C2-O2	5.20	122.02	118.90
21	AA	1027	C	N3-C2-O2	-5.20	118.26	121.90
22	A1	57	G	C5-C6-N1	5.20	114.10	111.50
54	BA	296	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	716	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1392	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1713	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	2005	A	C5-C6-N1	5.20	120.30	117.70
54	BA	2056	G	C5-C6-N1	5.20	114.10	111.50
54	BA	2311	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	2804	U	C5-C6-N1	-5.20	120.10	122.70
54	BA	637	A	C4-C5-C6	-5.19	114.40	117.00
54	BA	1579	A	O4'-C1'-N9	5.19	112.36	108.20
54	BA	2165	C	N1-C2-O2	5.19	122.02	118.90
21	AA	847	G	C5-C6-N1	5.19	114.10	111.50
24	A3	54	G	O4'-C1'-N9	5.19	112.35	108.20
54	BA	28	A	O4'-C1'-N9	5.19	112.35	108.20
54	BA	371	A	C4-C5-C6	-5.19	114.40	117.00
54	BA	433	C	N3-C4-C5	5.19	123.98	121.90
54	BA	1545	A	C4-C5-C6	-5.19	114.40	117.00
54	BA	1567	G	C5-C6-N1	5.19	114.10	111.50
54	BA	1823	G	C5-C6-N1	5.19	114.10	111.50
54	BA	1843	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	1859	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	2135	A	C4-C5-C6	-5.19	114.40	117.00
54	BA	2328	A	C5-C6-N1	5.19	120.30	117.70
21	AA	392	C	N3-C4-C5	5.19	123.98	121.90
54	BA	82	U	O4'-C1'-N1	5.19	112.35	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	239	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	509	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	795	C	C6-N1-C2	-5.19	118.22	120.30
54	BA	1503	A	C5-C6-N1	5.19	120.30	117.70
54	BA	1792	G	N9-C4-C5	5.19	107.48	105.40
21	AA	494	G	C8-N9-C4	-5.19	104.32	106.40
21	AA	1483	A	C5-C6-N1	5.19	120.30	117.70
54	BA	281	C	N1-C2-O2	5.19	122.01	118.90
54	BA	646	U	C4-C5-C6	5.19	122.81	119.70
21	AA	136	C	O4'-C1'-N1	5.19	112.35	108.20
21	AA	186	C	N3-C4-C5	5.19	123.97	121.90
21	AA	1246	A	C6-C5-N7	5.19	135.93	132.30
21	AA	1382	C	N1-C2-O2	5.19	122.01	118.90
21	AA	1534	A	C5-C6-N1	5.19	120.29	117.70
23	A2	81	U	N3-C2-O2	-5.19	118.57	122.20
54	BA	398	C	N1-C2-O2	5.19	122.01	118.90
54	BA	544	C	N3-C4-C5	5.19	123.97	121.90
54	BA	873	C	C5'-C4'-O4'	5.19	115.33	109.10
54	BA	1634	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	1797	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	1910	G	O4'-C1'-N9	5.19	112.35	108.20
54	BA	2029	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	2496	C	C1'-O4'-C4'	-5.19	105.75	109.90
54	BA	2706	A	C5-C6-N1	5.19	120.29	117.70
21	AA	367	U	O4'-C1'-N1	5.19	112.35	108.20
21	AA	772	U	N3-C2-O2	-5.19	118.57	122.20
24	A3	62	C	N1-C2-O2	5.19	122.01	118.90
54	BA	1678	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	2416	C	N1-C2-O2	5.19	122.01	118.90
21	AA	49	U	C5-C6-N1	-5.18	120.11	122.70
21	AA	366	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	1147	C	C2-N3-C4	-5.18	117.31	119.90
54	BA	219	A	C6-C5-N7	5.18	135.93	132.30
54	BA	598	U	O4'-C1'-N1	5.18	112.35	108.20
54	BA	803	U	O4'-C1'-N1	5.18	112.35	108.20
54	BA	1140	C	N1-C2-O2	5.18	122.01	118.90
54	BA	1229	C	O4'-C1'-N1	5.18	112.35	108.20
54	BA	2868	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	108	G	C2-N3-C4	5.18	114.49	111.90
21	AA	593	U	N3-C2-O2	-5.18	118.57	122.20
21	AA	1364	U	C5-C6-N1	-5.18	120.11	122.70
21	AA	1473	G	C5-C6-N1	5.18	114.09	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	724	U	N3-C2-O2	-5.18	118.57	122.20
54	BA	939	G	C5'-C4'-C3'	-5.18	107.71	116.00
54	BA	1376	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	1873	G	C5-C6-N1	5.18	114.09	111.50
54	BA	2031	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2130	U	C5-C6-N1	-5.18	120.11	122.70
54	BA	2326	C	N3-C4-C5	5.18	123.97	121.90
54	BA	2589	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	497	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	936	C	O4'-C1'-N1	5.18	112.34	108.20
21	AA	1188	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	381	G	C8-N9-C4	-5.18	104.33	106.40
54	BA	1332	G	N3-C4-C5	-5.18	126.01	128.60
54	BA	2664	G	C5-C6-N1	5.18	114.09	111.50
55	BB	12	C	C2-N3-C4	-5.18	117.31	119.90
21	AA	79	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	253	A	C1'-O4'-C4'	-5.18	105.76	109.90
21	AA	329	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	778	G	O4'-C1'-N9	5.18	112.34	108.20
23	A2	87	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	1145	C	N3-C2-O2	-5.18	118.28	121.90
54	BA	1267	U	C5-C6-N1	-5.18	120.11	122.70
54	BA	1387	A	N1-C6-N6	-5.18	115.49	118.60
54	BA	1565	C	N3-C2-O2	-5.18	118.28	121.90
54	BA	1871	A	C2-N3-C4	5.18	113.19	110.60
54	BA	2839	G	C5-C6-N1	5.18	114.09	111.50
21	AA	5	U	P-O3'-C3'	5.17	125.91	119.70
21	AA	452	A	O4'-C1'-N9	5.17	112.34	108.20
21	AA	782	A	C4-C5-C6	-5.17	114.41	117.00
21	AA	823	C	N3-C2-O2	-5.17	118.28	121.90
21	AA	1089	G	C8-N9-C4	-5.17	104.33	106.40
21	AA	1162	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	292	U	O4'-C1'-N1	5.17	112.34	108.20
54	BA	1168	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1461	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	2097	A	C4-C5-C6	-5.17	114.41	117.00
21	AA	378	G	C5-C6-N1	5.17	114.09	111.50
21	AA	469	C	C2-N3-C4	-5.17	117.31	119.90
54	BA	145	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	584	C	N3-C4-C5	5.17	123.97	121.90
54	BA	711	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1325	U	C5-C6-N1	-5.17	120.11	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	158	G	C5-C6-N1	5.17	114.08	111.50
21	AA	271	C	N3-C4-C5	5.17	123.97	121.90
54	BA	985	C	N1-C2-O2	5.17	122.00	118.90
54	BA	998	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1667	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1719	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	2104	C	C2-N3-C4	-5.17	117.31	119.90
54	BA	2767	C	O4'-C1'-N1	5.17	112.34	108.20
21	AA	201	G	C5-C6-N1	5.17	114.08	111.50
21	AA	421	U	N1-C2-O2	5.17	126.42	122.80
21	AA	1128	C	N3-C4-C5	5.17	123.97	121.90
21	AA	1243	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	152	A	C5-C6-N1	5.17	120.28	117.70
54	BA	281	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	1040	A	C4-C5-C6	-5.17	114.42	117.00
54	BA	1049	C	N3-C2-O2	-5.17	118.28	121.90
21	AA	677	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	801	G	C5-C6-N1	5.17	114.08	111.50
54	BA	826	U	C5-C4-O4	-5.17	122.80	125.90
54	BA	1210	G	O4'-C1'-N9	5.17	112.33	108.20
21	AA	880	C	O4'-C1'-N1	5.17	112.33	108.20
54	BA	712	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1379	U	C3'-C2'-C1'	5.17	105.63	101.50
54	BA	2162	G	N9-C4-C5	5.17	107.47	105.40
54	BA	2364	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	2583	G	C5-C6-N1	5.17	114.08	111.50
21	AA	61	G	C5-C6-N1	5.17	114.08	111.50
21	AA	969	A	C2-N3-C4	5.17	113.18	110.60
21	AA	1361	G	N3-C4-C5	-5.17	126.02	128.60
21	AA	1453	G	N7-C8-N9	5.17	115.68	113.10
54	BA	1819	A	C6-C5-N7	5.17	135.92	132.30
54	BA	2193	G	O4'-C1'-N9	5.17	112.33	108.20
54	BA	2278	A	C1'-O4'-C4'	-5.16	105.77	109.90
54	BA	2638	G	N7-C8-N9	5.16	115.68	113.10
54	BA	2887	A	C6-C5-N7	5.16	135.91	132.30
54	BA	844	A	C5-C6-N1	5.16	120.28	117.70
54	BA	1143	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1835	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	2113	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	2331	G	N1-C6-O6	-5.16	116.80	119.90
21	AA	111	G	C5-C6-N1	5.16	114.08	111.50
21	AA	344	A	C3'-C2'-C1'	5.16	105.63	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	531	U	N1-C2-N3	5.16	118.00	114.90
21	AA	840	C	N1-C2-O2	5.16	122.00	118.90
21	AA	1144	G	O4'-C1'-N9	5.16	112.33	108.20
22	A1	1	G	N3-C4-C5	-5.16	126.02	128.60
28	BF	91	ARG	NE-CZ-NH1	5.16	122.88	120.30
32	BJ	37	ARG	CD-NE-CZ	5.16	130.82	123.60
54	BA	417	C	N3-C2-O2	-5.16	118.29	121.90
54	BA	516	C	N3-C4-C5	5.16	123.96	121.90
54	BA	1248	G	N3-C2-N2	-5.16	116.29	119.90
21	AA	722	G	O4'-C1'-N9	5.16	112.33	108.20
21	AA	909	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	1134	G	C5-C6-N1	5.16	114.08	111.50
23	A2	88	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	722	A	C5-C6-N1	5.16	120.28	117.70
54	BA	950	G	N3-C2-N2	-5.16	116.29	119.90
54	BA	1045	C	N3-C4-C5	5.16	123.96	121.90
54	BA	1662	U	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1953	A	C6-C5-N7	5.16	135.91	132.30
54	BA	2655	G	N3-C2-N2	-5.16	116.29	119.90
54	BA	2698	U	N1-C2-N3	5.16	118.00	114.90
21	AA	1230	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	1320	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	1439	G	N1-C6-O6	-5.16	116.81	119.90
21	AA	1520	C	N1-C2-O2	5.16	121.99	118.90
54	BA	1124	G	O4'-C1'-N9	5.16	112.33	108.20
54	BA	2130	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	2681	C	N3-C2-O2	-5.16	118.29	121.90
21	AA	614	C	N3-C2-O2	-5.16	118.29	121.90
21	AA	1430	A	O4'-C4'-C3'	5.16	110.22	106.10
54	BA	738	G	C8-N9-C4	-5.16	104.34	106.40
54	BA	1079	C	C6-N1-C2	-5.16	118.24	120.30
54	BA	1258	U	C5-C6-N1	-5.16	120.12	122.70
54	BA	1639	C	O4'-C1'-N1	5.16	112.33	108.20
54	BA	2487	G	P-O3'-C3'	5.16	125.89	119.70
54	BA	2708	G	O4'-C1'-N9	5.16	112.33	108.20
21	AA	191	G	N3-C4-C5	-5.15	126.02	128.60
54	BA	660	C	N1-C2-O2	5.15	121.99	118.90
21	AA	91	U	O4'-C1'-N1	5.15	112.32	108.20
21	AA	1221	G	C5-C6-N1	5.15	114.08	111.50
21	AA	1223	C	N1-C2-O2	5.15	121.99	118.90
54	BA	214	G	C5-C6-N1	5.15	114.08	111.50
54	BA	1319	C	O4'-C1'-N1	5.15	112.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1329	U	N3-C2-O2	-5.15	118.59	122.20
54	BA	1966	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	2080	A	C2-N3-C4	5.15	113.18	110.60
54	BA	2238	G	C8-N9-C4	-5.15	104.34	106.40
21	AA	10	A	C6-C5-N7	5.15	135.91	132.30
21	AA	18	C	N3-C2-O2	-5.15	118.30	121.90
24	A3	2	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	55	G	N3-C4-C5	-5.15	126.03	128.60
54	BA	107	G	N7-C8-N9	5.15	115.67	113.10
54	BA	707	G	C5-C6-N1	5.15	114.08	111.50
54	BA	1267	U	N3-C2-O2	-5.15	118.59	122.20
54	BA	1284	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	1559	U	C5-C6-N1	-5.15	120.12	122.70
54	BA	1781	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2854	G	C8-N9-C4	-5.15	104.34	106.40
55	BB	91	C	N3-C4-C5	5.15	123.96	121.90
21	AA	755	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1595	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2206	C	N3-C2-O2	-5.15	118.30	121.90
54	BA	2207	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2503	A	C4-C5-C6	-5.15	114.43	117.00
21	AA	805	C	N3-C2-O2	-5.15	118.30	121.90
21	AA	1084	G	C8-N9-C4	-5.15	104.34	106.40
21	AA	1477	U	N1-C2-N3	5.15	117.99	114.90
54	BA	354	A	C6-C5-N7	5.15	135.90	132.30
54	BA	436	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	1890	A	C4-C5-C6	-5.15	114.43	117.00
54	BA	1905	C	N3-C2-O2	-5.15	118.30	121.90
21	AA	35	G	N3-C2-N2	-5.15	116.30	119.90
54	BA	144	A	C4-C5-C6	-5.15	114.43	117.00
54	BA	736	C	N3-C2-O2	-5.15	118.30	121.90
54	BA	2222	C	N3-C4-C5	5.15	123.96	121.90
55	BB	93	C	N3-C2-O2	-5.15	118.30	121.90
54	BA	980	A	C6-C5-N7	5.14	135.90	132.30
54	BA	1378	A	O4'-C4'-C3'	5.14	110.22	106.10
54	BA	1447	C	N3-C4-C5	5.14	123.96	121.90
54	BA	1756	G	C5-C6-N1	5.14	114.07	111.50
54	BA	1869	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	2100	G	C5-C6-N1	5.14	114.07	111.50
54	BA	2175	C	N1-C2-O2	5.14	121.99	118.90
21	AA	297	G	N3-C4-C5	-5.14	126.03	128.60
21	AA	441	A	C6-C5-N7	5.14	135.90	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	526	C	N3-C2-O2	-5.14	118.30	121.90
21	AA	849	G	C5-C6-N1	5.14	114.07	111.50
21	AA	980	C	N1-C2-O2	5.14	121.99	118.90
54	BA	69	C	N3-C4-C5	5.14	123.96	121.90
54	BA	329	G	C3'-C2'-C1'	5.14	105.61	101.50
54	BA	1368	G	N3-C4-C5	-5.14	126.03	128.60
54	BA	1389	G	N9-C4-C5	5.14	107.46	105.40
54	BA	1532	A	C6-C5-N7	5.14	135.90	132.30
54	BA	2539	C	N1-C2-O2	5.14	121.99	118.90
21	AA	101	A	C6-C5-N7	5.14	135.90	132.30
21	AA	601	G	C5-C6-N1	5.14	114.07	111.50
8	AI	105	ARG	CD-NE-CZ	5.14	130.80	123.60
21	AA	971	G	C5-C6-N1	5.14	114.07	111.50
22	A1	57	G	O4'-C1'-N9	5.14	112.31	108.20
24	A3	19	G	O4'-C1'-N9	5.14	112.31	108.20
54	BA	21	A	C6-C5-N7	5.14	135.90	132.30
54	BA	830	G	O4'-C1'-N9	5.14	112.31	108.20
54	BA	958	U	N1-C2-N3	5.14	117.98	114.90
54	BA	1334	G	C5-C6-N1	5.14	114.07	111.50
54	BA	1651	G	C5-C6-N1	5.14	114.07	111.50
54	BA	2202	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2500	U	C5'-C4'-O4'	5.14	115.27	109.10
55	BB	50	A	C5-C6-N1	5.14	120.27	117.70
2	AC	131	ARG	NE-CZ-NH1	5.14	122.87	120.30
54	BA	178	G	C8-N9-C4	-5.14	104.34	106.40
54	BA	2324	U	N3-C2-O2	-5.14	118.60	122.20
54	BA	2776	A	C6-C5-N7	5.14	135.90	132.30
21	AA	180	U	N3-C2-O2	-5.14	118.60	122.20
21	AA	446	G	C5-C6-N1	5.14	114.07	111.50
21	AA	782	A	C5-C6-N1	5.14	120.27	117.70
54	BA	826	U	N3-C4-O4	5.14	123.00	119.40
54	BA	986	C	N1-C2-O2	5.14	121.98	118.90
54	BA	2093	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	2098	U	C5-C6-N1	-5.14	120.13	122.70
54	BA	2232	C	C4'-C3'-C2'	-5.14	97.46	102.60
54	BA	2500	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2600	A	C5-C6-N1	5.14	120.27	117.70
55	BB	82	U	N3-C2-O2	-5.14	118.60	122.20
21	AA	1121	U	O4'-C1'-N1	5.13	112.31	108.20
21	AA	1302	C	N3-C4-C5	5.13	123.95	121.90
21	AA	1423	G	C5-C6-N1	5.13	114.07	111.50
21	AA	1472	U	N1-C2-N3	5.13	117.98	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BO	15	ARG	NE-CZ-NH1	5.13	122.87	120.30
47	BY	48	ARG	NE-CZ-NH1	5.13	122.87	120.30
54	BA	149	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	758	C	N3-C4-C5	5.13	123.95	121.90
54	BA	1506	U	N3-C2-O2	-5.13	118.61	122.20
21	AA	371	A	C6-C5-N7	5.13	135.89	132.30
21	AA	869	G	N3-C4-C5	-5.13	126.03	128.60
54	BA	2100	G	C5'-C4'-O4'	5.13	115.26	109.10
54	BA	492	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	588	U	C5-C6-N1	-5.13	120.13	122.70
54	BA	745	G	O4'-C1'-N9	5.13	112.31	108.20
54	BA	1128	G	C5'-C4'-O4'	5.13	115.26	109.10
54	BA	1467	U	O4'-C1'-N1	5.13	112.31	108.20
54	BA	2577	A	C4-C5-C6	-5.13	114.43	117.00
21	AA	41	G	C5-C6-N1	5.13	114.06	111.50
54	BA	691	C	O4'-C1'-N1	5.13	112.30	108.20
54	BA	1242	U	N1-C2-N3	5.13	117.98	114.90
54	BA	1429	G	C8-N9-C4	-5.13	104.35	106.40
54	BA	1986	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2157	G	O4'-C1'-N9	5.13	112.30	108.20
54	BA	2319	G	N3-C4-C5	-5.13	126.03	128.60
21	AA	798	U	O4'-C1'-N1	5.13	112.30	108.20
21	AA	1353	G	C8-N9-C4	-5.13	104.35	106.40
21	AA	1397	C	C6-N1-C2	-5.13	118.25	120.30
54	BA	359	G	C5-C6-N1	5.13	114.06	111.50
54	BA	918	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	1677	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	1963	U	O4'-C1'-N1	5.13	112.30	108.20
54	BA	2626	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2850	A	C8-N9-C4	-5.13	103.75	105.80
21	AA	1091	U	N3-C2-O2	-5.13	118.61	122.20
54	BA	1448	G	C4'-C3'-C2'	-5.13	97.47	102.60
54	BA	1608	A	C5-C6-N1	5.13	120.26	117.70
54	BA	1724	G	N3-C4-C5	-5.13	126.04	128.60
54	BA	2240	U	C5-C6-N1	-5.13	120.14	122.70
54	BA	2283	C	C2-N3-C4	-5.13	117.34	119.90
54	BA	2735	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	1469	C	N3-C4-C5	5.12	123.95	121.90
54	BA	1888	G	N7-C8-N9	5.12	115.66	113.10
6	AG	52	ARG	NE-CZ-NH1	5.12	122.86	120.30
21	AA	463	U	C5-C6-N1	-5.12	120.14	122.70
21	AA	761	G	O4'-C1'-N9	5.12	112.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1207	G	C8-N9-C4	-5.12	104.35	106.40
21	AA	1213	A	C6-C5-N7	5.12	135.89	132.30
21	AA	1390	U	C4-C5-C6	5.12	122.77	119.70
54	BA	738	G	C5-C6-N1	5.12	114.06	111.50
54	BA	1527	G	C5-C6-N1	5.12	114.06	111.50
54	BA	1854	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2215	C	C6-N1-C2	-5.12	118.25	120.30
54	BA	2310	C	N3-C2-O2	-5.12	118.31	121.90
54	BA	2830	C	N1-C2-O2	5.12	121.97	118.90
55	BB	44	G	N7-C8-N9	5.12	115.66	113.10
21	AA	295	C	N3-C2-O2	-5.12	118.31	121.90
21	AA	558	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	1484	C	N3-C4-N4	-5.12	114.42	118.00
54	BA	620	G	N3-C4-C5	-5.12	126.04	128.60
54	BA	1071	G	C8-N9-C4	-5.12	104.35	106.40
54	BA	1373	A	C5-C6-N1	5.12	120.26	117.70
54	BA	1853	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	1988	G	C4'-C3'-C2'	-5.12	97.48	102.60
54	BA	2895	G	C5-C6-N1	5.12	114.06	111.50
55	BB	104	A	C5-C6-N1	5.12	120.26	117.70
21	AA	1211	U	C1'-O4'-C4'	-5.12	105.80	109.90
54	BA	249	C	N3-C2-O2	-5.12	118.32	121.90
54	BA	757	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	357	G	N7-C8-N9	5.12	115.66	113.10
21	AA	468	A	C2-N3-C4	5.12	113.16	110.60
54	BA	1459	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1869	G	C8-N9-C4	-5.12	104.35	106.40
54	BA	2033	A	C5-C6-N1	5.12	120.26	117.70
54	BA	2435	A	C4-C5-C6	-5.12	114.44	117.00
55	BB	49	C	N3-C2-O2	-5.12	118.32	121.90
21	AA	26	A	C6-C5-N7	5.12	135.88	132.30
21	AA	23	C	N1-C2-O2	5.12	121.97	118.90
21	AA	903	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	1117	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	127	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2062	A	C8-N9-C4	-5.12	103.75	105.80
54	BA	2086	U	O4'-C1'-N1	5.12	112.29	108.20
54	BA	2897	U	O4'-C1'-N1	5.12	112.29	108.20
55	BB	68	C	O4'-C1'-N1	5.12	112.29	108.20
10	AK	105	ARG	NE-CZ-NH1	5.11	122.86	120.30
21	AA	429	U	C4-C5-C6	5.11	122.77	119.70
21	AA	742	G	N3-C4-C5	-5.11	126.04	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	985	C	N3-C4-C5	5.11	123.94	121.90
21	AA	1261	A	C4-C5-C6	-5.11	114.44	117.00
21	AA	1434	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	624	C	N1-C2-O2	5.11	121.97	118.90
54	BA	977	G	N7-C8-N9	5.11	115.66	113.10
54	BA	1014	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	1220	G	C8-N9-C4	-5.11	104.36	106.40
54	BA	1882	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	2072	C	N3-C2-O2	-5.11	118.32	121.90
54	BA	2253	G	C8-N9-C4	-5.11	104.35	106.40
21	AA	72	A	C5-C6-N1	5.11	120.26	117.70
21	AA	674	G	N9-C4-C5	5.11	107.44	105.40
54	BA	213	A	C6-C5-N7	5.11	135.88	132.30
54	BA	705	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	1305	C	N3-C4-C5	5.11	123.94	121.90
54	BA	2381	A	C4'-C3'-C2'	-5.11	97.49	102.60
2	AC	106	ARG	NE-CZ-NH1	5.11	122.86	120.30
21	AA	68	G	N3-C4-C5	-5.11	126.05	128.60
21	AA	1209	C	N3-C4-N4	-5.11	114.42	118.00
22	A1	12	U	C5'-C4'-O4'	5.11	115.23	109.10
54	BA	985	C	N3-C4-C5	5.11	123.94	121.90
54	BA	1131	G	C5-C6-N1	5.11	114.06	111.50
54	BA	1528	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	1809	A	C5-C6-N1	5.11	120.25	117.70
54	BA	2063	C	N1-C2-O2	5.11	121.97	118.90
54	BA	2365	G	N7-C8-N9	5.11	115.66	113.10
55	BB	93	C	O4'-C1'-N1	5.11	112.29	108.20
21	AA	808	C	N1-C2-O2	5.11	121.97	118.90
21	AA	957	U	O4'-C1'-N1	5.11	112.28	108.20
54	BA	621	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	2020	A	C1'-O4'-C4'	-5.11	105.81	109.90
54	BA	2667	C	O4'-C1'-N1	5.11	112.28	108.20
21	AA	1093	A	C4-C5-C6	-5.11	114.45	117.00
24	A3	7	G	N1-C6-O6	-5.11	116.84	119.90
54	BA	418	C	N3-C2-O2	-5.11	118.33	121.90
54	BA	484	C	O4'-C1'-N1	5.11	112.28	108.20
54	BA	808	G	O4'-C1'-N9	5.11	112.28	108.20
54	BA	1288	G	N1-C6-O6	-5.11	116.84	119.90
54	BA	1306	C	N3-C4-C5	5.11	123.94	121.90
21	AA	1438	G	N3-C2-N2	-5.10	116.33	119.90
54	BA	308	G	C5-C6-N1	5.10	114.05	111.50
54	BA	1297	C	N3-C2-O2	-5.10	118.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2403	C	N3-C4-C5	5.10	123.94	121.90
21	AA	30	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	514	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1126	U	N1-C2-N3	5.10	117.96	114.90
21	AA	1350	A	C6-C5-N7	5.10	135.87	132.30
54	BA	48	G	C8-N9-C4	-5.10	104.36	106.40
54	BA	536	G	N9-C4-C5	5.10	107.44	105.40
54	BA	1019	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	1272	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	1356	G	N3-C4-C5	-5.10	126.05	128.60
54	BA	2252	G	C5-C6-N1	5.10	114.05	111.50
21	AA	1434	A	O4'-C1'-N9	5.10	112.28	108.20
21	AA	1445	U	C5-C6-N1	-5.10	120.15	122.70
21	AA	1506	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	809	G	N7-C8-N9	5.10	115.65	113.10
54	BA	1682	G	C5-C6-N1	5.10	114.05	111.50
21	AA	102	G	C5-C6-N1	5.10	114.05	111.50
21	AA	153	C	N3-C2-O2	-5.10	118.33	121.90
21	AA	284	C	N1-C2-O2	5.10	121.96	118.90
21	AA	525	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1114	C	N3-C2-O2	-5.10	118.33	121.90
24	A3	71	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	2780	G	C1'-O4'-C4'	-5.10	105.82	109.90
55	BB	41	G	N3-C4-C5	-5.10	126.05	128.60
21	AA	640	A	C6-C5-N7	5.10	135.87	132.30
21	AA	1192	C	N3-C2-O2	-5.10	118.33	121.90
22	A1	61	C	N3-C4-C5	5.10	123.94	121.90
54	BA	135	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	784	G	C8-N9-C4	-5.10	104.36	106.40
54	BA	1525	A	C5-C6-N1	5.10	120.25	117.70
54	BA	1612	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	1800	C	N3-C4-C5	5.10	123.94	121.90
54	BA	1828	G	C5-C6-N1	5.10	114.05	111.50
54	BA	1847	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	1857	G	N3-C2-N2	-5.10	116.33	119.90
54	BA	1874	C	N1-C2-O2	5.10	121.96	118.90
54	BA	2047	C	N3-C2-O2	-5.10	118.33	121.90
54	BA	2598	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2737	G	N1-C6-O6	-5.10	116.84	119.90
21	AA	1411	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	42	A	C6-C5-N7	5.10	135.87	132.30
54	BA	2497	A	O4'-C1'-N9	5.10	112.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	369	G	C8-N9-C4	-5.09	104.36	106.40
21	AA	535	A	C4-C5-C6	-5.09	114.45	117.00
21	AA	939	G	N7-C8-N9	5.09	115.65	113.10
21	AA	1134	G	N1-C6-O6	-5.09	116.84	119.90
21	AA	1336	C	N1-C2-O2	5.09	121.96	118.90
54	BA	557	C	N3-C4-C5	5.09	123.94	121.90
54	BA	1592	C	N3-C2-O2	-5.09	118.33	121.90
54	BA	1925	C	O4'-C1'-N1	5.09	112.28	108.20
54	BA	2135	A	C5-C6-N1	5.09	120.25	117.70
54	BA	2307	G	C5-C6-N1	5.09	114.05	111.50
54	BA	2510	C	N3-C2-O2	-5.09	118.33	121.90
54	BA	2719	G	N7-C8-N9	5.09	115.65	113.10
54	BA	427	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2029	G	C3'-C2'-C1'	5.09	105.57	101.50
21	AA	419	C	N3-C2-O2	-5.09	118.34	121.90
21	AA	741	G	C8-N9-C4	-5.09	104.36	106.40
21	AA	1127	G	C5-C6-N1	5.09	114.05	111.50
54	BA	122	G	C4'-C3'-C2'	-5.09	97.51	102.60
54	BA	481	G	C8-N9-C4	-5.09	104.36	106.40
54	BA	523	C	C5'-C4'-O4'	5.09	115.21	109.10
54	BA	1656	C	N3-C2-O2	-5.09	118.33	121.90
54	BA	1990	C	N3-C4-N4	-5.09	114.44	118.00
54	BA	2240	U	C4-C5-C6	5.09	122.75	119.70
54	BA	2521	C	N1-C2-O2	5.09	121.95	118.90
54	BA	2590	A	C6-C5-N7	5.09	135.86	132.30
54	BA	2633	G	N3-C2-N2	-5.09	116.33	119.90
21	AA	213	G	C5-C6-N1	5.09	114.05	111.50
54	BA	36	G	C5-C6-N1	5.09	114.05	111.50
54	BA	412	A	C6-C5-N7	5.09	135.86	132.30
54	BA	1868	C	N3-C2-O2	-5.09	118.34	121.90
54	BA	2519	U	N3-C2-O2	-5.09	118.64	122.20
21	AA	434	U	C5-C6-N1	-5.09	120.16	122.70
54	BA	484	C	N1-C2-O2	5.09	121.95	118.90
54	BA	1950	G	N3-C2-N2	-5.09	116.34	119.90
54	BA	2555	U	O4'-C1'-N1	5.09	112.27	108.20
2	AC	131	ARG	NE-CZ-NH2	-5.09	117.76	120.30
21	AA	363	A	C6-C5-N7	5.09	135.86	132.30
21	AA	425	G	C8-N9-C4	-5.09	104.37	106.40
21	AA	723	U	N3-C2-O2	-5.09	118.64	122.20
21	AA	1466	C	N3-C4-C5	5.09	123.94	121.90
54	BA	126	A	O4'-C1'-N9	5.09	112.27	108.20
54	BA	164	C	N3-C4-C5	5.09	123.94	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	346	A	C6-C5-N7	5.09	135.86	132.30
54	BA	730	A	C6-C5-N7	5.09	135.86	132.30
54	BA	772	C	N3-C2-O2	-5.09	118.34	121.90
54	BA	1436	G	C8-N9-C4	-5.09	104.36	106.40
54	BA	1508	A	C1'-O4'-C4'	-5.09	105.83	109.90
21	AA	953	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	1489	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	730	A	C1'-O4'-C4'	-5.08	105.83	109.90
54	BA	2825	G	C5-C6-N1	5.08	114.04	111.50
21	AA	318	G	N3-C4-C5	-5.08	126.06	128.60
21	AA	621	A	O4'-C1'-N9	5.08	112.27	108.20
21	AA	825	A	C4-C5-C6	-5.08	114.46	117.00
21	AA	898	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	1119	C	N3-C2-O2	-5.08	118.34	121.90
21	AA	1482	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	455	C	O4'-C4'-C3'	5.08	110.17	106.10
54	BA	607	U	C5-C6-N1	-5.08	120.16	122.70
54	BA	819	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1071	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	1435	G	N7-C8-N9	5.08	115.64	113.10
54	BA	1510	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1637	A	C6-C5-N7	5.08	135.86	132.30
54	BA	2424	C	C5'-C4'-C3'	-5.08	107.87	116.00
21	AA	79	G	C5-C6-N1	5.08	114.04	111.50
21	AA	591	U	C5'-C4'-C3'	-5.08	107.87	116.00
22	A1	63	G	N7-C8-N9	5.08	115.64	113.10
22	A1	70	C	C5'-C4'-O4'	5.08	115.20	109.10
39	BQ	29	ARG	NE-CZ-NH1	5.08	122.84	120.30
54	BA	432	A	C6-C5-N7	5.08	135.86	132.30
54	BA	547	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	711	G	N9-C4-C5	5.08	107.43	105.40
54	BA	777	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	1443	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	1549	A	C6-C5-N7	5.08	135.86	132.30
54	BA	2573	C	C6-N1-C2	-5.08	118.27	120.30
21	AA	280	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2190	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	2276	G	C5-C6-N1	5.08	114.04	111.50
21	AA	683	G	C5-C6-N1	5.08	114.04	111.50
42	BT	12	ARG	NE-CZ-NH1	5.08	122.84	120.30
54	BA	157	C	N3-C2-O2	-5.08	118.34	121.90
54	BA	350	G	C5-C6-N1	5.08	114.04	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	389	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	506	G	N7-C8-N9	5.08	115.64	113.10
54	BA	1298	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1308	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1418	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	2852	G	C5-C6-N1	5.08	114.04	111.50
21	AA	943	U	C5-C6-N1	-5.08	120.16	122.70
21	AA	281	G	N3-C4-C5	-5.08	126.06	128.60
21	AA	384	G	N3-C2-N2	-5.08	116.35	119.90
21	AA	429	U	N3-C2-O2	-5.08	118.65	122.20
21	AA	805	C	O4'-C1'-N1	5.08	112.26	108.20
21	AA	1169	A	C6-C5-N7	5.08	135.85	132.30
21	AA	1490	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	52	A	N1-C6-N6	-5.08	115.56	118.60
54	BA	1541	C	N3-C4-C5	5.08	123.93	121.90
54	BA	1648	U	N3-C2-O2	-5.08	118.65	122.20
21	AA	775	G	C8-N9-C4	-5.07	104.37	106.40
21	AA	993	G	O4'-C4'-C3'	5.07	110.16	106.10
21	AA	1003	G	O4'-C1'-N9	5.07	112.26	108.20
54	BA	33	C	N3-C2-O2	-5.07	118.35	121.90
54	BA	161	A	C6-C5-N7	5.07	135.85	132.30
54	BA	844	A	C4-C5-C6	-5.07	114.46	117.00
54	BA	957	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1465	G	N3-C4-C5	-5.07	126.06	128.60
54	BA	2443	C	C2-N3-C4	-5.07	117.36	119.90
21	AA	467	U	N3-C2-O2	-5.07	118.65	122.20
21	AA	1257	A	C4-C5-C6	-5.07	114.46	117.00
21	AA	1421	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1142	A	C6-C5-N7	5.07	135.85	132.30
21	AA	16	A	C2-N3-C4	5.07	113.14	110.60
21	AA	172	A	C3'-C2'-C1'	5.07	105.56	101.50
21	AA	239	U	N3-C2-O2	-5.07	118.65	122.20
21	AA	673	A	C4-C5-C6	-5.07	114.46	117.00
21	AA	712	A	N1-C6-N6	-5.07	115.56	118.60
21	AA	812	G	C5-C6-N1	5.07	114.04	111.50
21	AA	1355	G	N3-C4-C5	-5.07	126.06	128.60
54	BA	358	U	N1-C2-N3	5.07	117.94	114.90
54	BA	1237	A	C4'-C3'-C2'	-5.07	97.53	102.60
54	BA	1555	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1674	G	N3-C4-C5	-5.07	126.06	128.60
54	BA	1958	C	N3-C2-O2	-5.07	118.35	121.90
54	BA	2300	C	N1-C2-O2	5.07	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2618	G	C5-C6-N1	5.07	114.03	111.50
21	AA	921	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	170	U	C4'-C3'-C2'	-5.07	97.53	102.60
54	BA	2271	G	C5-C6-N1	5.07	114.03	111.50
54	BA	2510	C	O4'-C1'-N1	5.07	112.25	108.20
21	AA	463	U	O4'-C1'-N1	5.07	112.25	108.20
21	AA	1049	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	567	U	O4'-C1'-N1	5.07	112.25	108.20
54	BA	764	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	876	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	1093	G	N3-C2-N2	-5.07	116.35	119.90
54	BA	1356	G	C8-N9-C4	-5.07	104.37	106.40
21	AA	976	G	N1-C6-O6	-5.07	116.86	119.90
22	A1	61	C	C5'-C4'-O4'	5.07	115.18	109.10
54	BA	1226	A	C6-C5-N7	5.07	135.84	132.30
54	BA	1281	G	C5-C6-N1	5.07	114.03	111.50
54	BA	2291	U	O4'-C1'-N1	5.07	112.25	108.20
55	BB	9	G	N3-C4-C5	-5.07	126.07	128.60
55	BB	22	U	N1-C2-N3	5.07	117.94	114.90
55	BB	86	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1758	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	156	C	N1-C2-O2	5.06	121.94	118.90
21	AA	267	C	N1-C2-O2	5.06	121.94	118.90
21	AA	1380	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1289	C	N1-C2-O2	5.06	121.94	118.90
54	BA	1408	G	C5-C6-N1	5.06	114.03	111.50
54	BA	1649	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	2413	G	N3-C2-N2	-5.06	116.36	119.90
54	BA	2873	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	887	G	N3-C2-N2	-5.06	116.36	119.90
21	AA	1152	A	C6-C5-N7	5.06	135.84	132.30
54	BA	2039	U	C5-C6-N1	-5.06	120.17	122.70
54	BA	2488	G	N1-C6-O6	-5.06	116.86	119.90
21	AA	606	G	N1-C6-O6	-5.06	116.86	119.90
21	AA	1129	C	N1-C2-O2	5.06	121.94	118.90
54	BA	122	G	C5-C6-N1	5.06	114.03	111.50
54	BA	360	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	397	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1269	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	1710	G	N9-C4-C5	5.06	107.42	105.40
54	BA	2538	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2739	U	O4'-C1'-N1	5.06	112.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	355	C	C5'-C4'-O4'	5.06	115.17	109.10
21	AA	612	C	N1-C2-O2	5.06	121.94	118.90
54	BA	14	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	1114	C	C2-N3-C4	-5.06	117.37	119.90
54	BA	1447	C	N1-C2-O2	5.06	121.93	118.90
54	BA	1741	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2453	A	C5-C6-N1	5.06	120.23	117.70
54	BA	2477	U	N1-C2-N3	5.06	117.94	114.90
54	BA	2851	A	C6-C5-N7	5.06	135.84	132.30
21	AA	659	U	O4'-C4'-C3'	5.06	110.14	106.10
21	AA	674	G	O4'-C1'-N9	5.06	112.25	108.20
54	BA	653	U	C1'-O4'-C4'	-5.06	105.86	109.90
54	BA	2078	C	C4'-C3'-C2'	-5.06	97.54	102.60
54	BA	2099	U	C5-C6-N1	-5.06	120.17	122.70
54	BA	2603	G	N1-C6-O6	-5.06	116.87	119.90
55	BB	14	U	C5-C6-N1	-5.06	120.17	122.70
55	BB	25	U	O4'-C1'-N1	5.06	112.25	108.20
11	AL	82	ARG	NE-CZ-NH1	5.05	122.83	120.30
21	AA	402	G	C5-C6-N1	5.05	114.03	111.50
54	BA	584	C	N3-C2-O2	-5.05	118.36	121.90
54	BA	642	U	C5-C6-N1	-5.05	120.17	122.70
54	BA	2122	U	N1-C2-N3	5.05	117.93	114.90
54	BA	2180	U	N3-C2-O2	-5.05	118.66	122.20
21	AA	664	G	N3-C4-C5	-5.05	126.07	128.60
54	BA	573	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	1294	U	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	1807	G	O4'-C1'-N9	5.05	112.24	108.20
54	BA	2056	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	2582	G	N3-C4-C5	-5.05	126.07	128.60
16	AQ	63	CYS	O-C-N	-5.05	114.62	122.70
21	AA	6	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	270	A	C6-C5-N7	5.05	135.84	132.30
21	AA	293	G	N3-C2-N2	-5.05	116.36	119.90
21	AA	572	A	C3'-C2'-C1'	5.05	105.54	101.50
21	AA	671	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	699	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1532	U	C1'-O4'-C4'	-5.05	105.86	109.90
54	BA	185	G	C8-N9-C4	-5.05	104.38	106.40
54	BA	817	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1343	G	N9-C4-C5	5.05	107.42	105.40
54	BA	1398	C	O4'-C4'-C3'	5.05	110.14	106.10
54	BA	1704	C	N3-C2-O2	-5.05	118.36	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1986	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2423	U	O4'-C1'-N1	5.05	112.24	108.20
21	AA	1409	C	N3-C2-O2	-5.05	118.37	121.90
54	BA	445	C	N3-C4-C5	5.05	123.92	121.90
54	BA	489	G	C5-C6-N1	5.05	114.03	111.50
54	BA	877	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	1154	G	N3-C4-C5	-5.05	126.08	128.60
54	BA	1374	G	C5-C6-N1	5.05	114.03	111.50
54	BA	2160	C	N3-C4-C5	5.05	123.92	121.90
21	AA	326	G	C8-N9-C4	-5.05	104.38	106.40
26	BD	124	ARG	NE-CZ-NH1	5.05	122.82	120.30
54	BA	826	U	C4-C5-C6	5.05	122.73	119.70
54	BA	1238	G	C5-C6-N1	5.05	114.02	111.50
54	BA	2380	C	N1-C2-O2	5.05	121.93	118.90
21	AA	147	G	N3-C4-C5	-5.05	126.08	128.60
21	AA	914	A	C4-C5-C6	-5.05	114.48	117.00
21	AA	1277	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1476	U	C5-C6-N1	-5.05	120.18	122.70
54	BA	1817	G	C5-C6-N1	5.05	114.02	111.50
54	BA	2006	C	O4'-C1'-N1	5.05	112.24	108.20
21	AA	296	U	N1-C2-N3	5.04	117.93	114.90
21	AA	1226	C	C5'-C4'-C3'	-5.04	107.93	116.00
22	A1	20	G	N3-C4-C5	-5.04	126.08	128.60
54	BA	1388	G	N3-C2-N2	-5.04	116.37	119.90
54	BA	2824	C	N3-C4-C5	5.04	123.92	121.90
15	AP	25	ARG	NE-CZ-NH2	-5.04	117.78	120.30
21	AA	166	U	C5'-C4'-O4'	5.04	115.15	109.10
21	AA	403	C	N1-C2-O2	5.04	121.93	118.90
21	AA	549	C	N1-C2-O2	5.04	121.93	118.90
21	AA	1502	A	C8-N9-C4	-5.04	103.78	105.80
54	BA	874	G	C5-C6-N1	5.04	114.02	111.50
54	BA	1857	G	N9-C4-C5	5.04	107.42	105.40
54	BA	2365	G	C8-N9-C4	-5.04	104.38	106.40
21	AA	178	C	N3-C2-O2	-5.04	118.37	121.90
21	AA	1367	C	O4'-C1'-N1	5.04	112.23	108.20
21	AA	1496	C	N3-C4-C5	5.04	123.92	121.90
22	A1	8	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	286	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	706	A	C8-N9-C4	-5.04	103.78	105.80
54	BA	879	G	N9-C4-C5	5.04	107.42	105.40
54	BA	2122	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	2511	U	N1-C2-N3	5.04	117.92	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2567	G	C5-C6-N1	5.04	114.02	111.50
54	BA	2678	C	N3-C2-O2	-5.04	118.37	121.90
54	BA	2885	G	N9-C4-C5	5.04	107.42	105.40
55	BB	12	C	C3'-C2'-C1'	-5.04	97.47	101.50
21	AA	610	U	C1'-O4'-C4'	-5.04	105.87	109.90
54	BA	423	A	C6-C5-N7	5.04	135.83	132.30
54	BA	1096	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	2844	G	N1-C6-O6	-5.04	116.88	119.90
21	AA	914	A	C6-C5-N7	5.04	135.83	132.30
54	BA	568	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	1954	G	C3'-C2'-C1'	5.04	105.53	101.50
54	BA	2305	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	2861	U	C4-C5-C6	5.04	122.72	119.70
21	AA	876	C	C1'-O4'-C4'	-5.04	105.87	109.90
54	BA	114	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	118	A	C5'-C4'-O4'	5.04	115.14	109.10
54	BA	285	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	657	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	2006	C	N3-C4-C5	5.04	123.92	121.90
54	BA	2756	U	N1-C1'-C2'	5.04	120.55	114.00
21	AA	390	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	776	G	N9-C4-C5	5.04	107.41	105.40
21	AA	1090	U	C4-C5-C6	5.04	122.72	119.70
54	BA	821	A	C6-C5-N7	5.04	135.82	132.30
54	BA	2777	G	C8-N9-C4	-5.04	104.39	106.40
21	AA	603	U	O4'-C1'-N1	5.03	112.23	108.20
54	BA	4	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	1209	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	1721	G	N7-C8-N9	5.03	115.62	113.10
55	BB	3	C	N3-C4-C5	5.03	123.91	121.90
21	AA	569	C	N3-C2-O2	-5.03	118.38	121.90
21	AA	803	G	N9-C4-C5	5.03	107.41	105.40
22	A1	42	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	676	A	C6-C5-N7	5.03	135.82	132.30
54	BA	1186	G	O4'-C1'-N9	5.03	112.22	108.20
54	BA	1471	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	2021	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2076	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	2283	C	O4'-C1'-N1	5.03	112.23	108.20
54	BA	2651	C	O4'-C1'-N1	5.03	112.23	108.20
54	BA	2794	C	N3-C4-C5	5.03	123.91	121.90
55	BB	51	G	N9-C4-C5	5.03	107.41	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	638	U	N3-C2-O2	-5.03	118.68	122.20
21	AA	686	U	N3-C2-O2	-5.03	118.68	122.20
21	AA	911	U	C5-C6-N1	-5.03	120.19	122.70
21	AA	1203	C	O4'-C1'-N1	5.03	112.22	108.20
35	BM	59	ARG	NE-CZ-NH1	5.03	122.81	120.30
54	BA	266	G	C5-C6-N1	5.03	114.02	111.50
54	BA	1288	G	C1'-O4'-C4'	-5.03	105.88	109.90
54	BA	1365	A	C4-C5-C6	-5.03	114.48	117.00
54	BA	1763	G	C5-C6-N1	5.03	114.02	111.50
54	BA	2162	G	N3-C4-C5	-5.03	126.08	128.60
54	BA	2850	A	C4'-C3'-C2'	-5.03	97.57	102.60
55	BB	71	C	N1-C2-O2	5.03	121.92	118.90
21	AA	223	A	C6-C5-N7	5.03	135.82	132.30
21	AA	1355	G	O4'-C1'-N9	5.03	112.22	108.20
21	AA	1398	A	C2-N3-C4	5.03	113.11	110.60
54	BA	90	U	N1-C2-N3	5.03	117.92	114.90
54	BA	687	C	N3-C2-O2	-5.03	118.38	121.90
54	BA	2086	U	C4'-C3'-C2'	-5.03	97.57	102.60
54	BA	2768	U	O4'-C1'-N1	5.03	112.22	108.20
21	AA	211	G	O4'-C1'-N9	5.03	112.22	108.20
21	AA	415	A	C2-N3-C4	5.03	113.11	110.60
21	AA	1139	G	N9-C4-C5	5.03	107.41	105.40
21	AA	1231	G	C8-N9-C4	-5.03	104.39	106.40
54	BA	114	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	216	A	C5-C6-N1	5.03	120.21	117.70
54	BA	731	C	N1-C2-O2	5.03	121.92	118.90
54	BA	1363	C	N3-C4-C5	5.03	123.91	121.90
54	BA	1459	G	C5'-C4'-O4'	5.03	115.13	109.10
54	BA	1704	C	N1-C2-O2	5.03	121.92	118.90
54	BA	1746	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	2853	C	O4'-C1'-N1	5.03	112.22	108.20
21	AA	21	G	N1-C6-O6	-5.03	116.89	119.90
21	AA	359	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	1182	G	N3-C4-C5	-5.03	126.09	128.60
54	BA	152	A	C4'-C3'-C2'	-5.03	97.58	102.60
54	BA	292	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	519	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1237	A	O4'-C1'-N9	5.03	112.22	108.20
54	BA	2045	C	N3-C4-C5	5.03	123.91	121.90
54	BA	2362	C	C2-N3-C4	-5.03	117.39	119.90
54	BA	2812	G	C8-N9-C4	-5.03	104.39	106.40
55	BB	34	A	O4'-C1'-N9	5.03	112.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1391	U	N3-C2-O2	-5.02	118.68	122.20
54	BA	95	A	O4'-C1'-N9	5.02	112.22	108.20
54	BA	440	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1305	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1360	G	O4'-C1'-N9	5.02	112.22	108.20
54	BA	2352	A	C4'-C3'-C2'	-5.02	97.58	102.60
55	BB	67	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	381	C	C3'-C2'-C1'	5.02	105.52	101.50
21	AA	846	G	C5-C6-N1	5.02	114.01	111.50
21	AA	1140	C	N1-C2-O2	5.02	121.91	118.90
21	AA	1253	G	C5-C6-N1	5.02	114.01	111.50
54	BA	159	G	C5'-C4'-O4'	5.02	115.13	109.10
54	BA	547	A	C5'-C4'-O4'	5.02	115.13	109.10
54	BA	1299	G	C5-C6-N1	5.02	114.01	111.50
54	BA	1554	U	N1-C2-N3	5.02	117.91	114.90
54	BA	1690	A	C6-C5-N7	5.02	135.81	132.30
54	BA	1943	U	N3-C2-O2	-5.02	118.68	122.20
54	BA	2010	G	C5-C6-N1	5.02	114.01	111.50
54	BA	2108	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	2120	G	C5-C6-N1	5.02	114.01	111.50
21	AA	56	U	N3-C2-O2	-5.02	118.69	122.20
21	AA	1188	A	C6-C5-N7	5.02	135.81	132.30
21	AA	1371	G	N7-C8-N9	5.02	115.61	113.10
54	BA	456	C	N3-C4-C5	5.02	123.91	121.90
54	BA	1291	C	N3-C4-C5	5.02	123.91	121.90
54	BA	2368	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2815	C	N1-C2-O2	5.02	121.91	118.90
21	AA	287	U	C5-C6-N1	-5.02	120.19	122.70
21	AA	924	C	N1-C2-O2	5.02	121.91	118.90
21	AA	1042	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	1762	A	C4'-C3'-C2'	-5.02	97.58	102.60
21	AA	1160	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	1366	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	264	C	C1'-O4'-C4'	-5.02	105.89	109.90
54	BA	445	C	N3-C4-N4	-5.02	114.49	118.00
54	BA	544	C	N1-C2-O2	5.02	121.91	118.90
54	BA	681	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	1091	G	C5-C6-N1	5.02	114.01	111.50
54	BA	1616	A	C6-C5-N7	5.02	135.81	132.30
54	BA	1954	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	431	U	N1-C2-N3	5.02	117.91	114.90
54	BA	1369	G	C4'-C3'-C2'	-5.02	97.58	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2069	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	2379	G	O4'-C1'-N9	5.02	112.21	108.20
21	AA	312	C	N1-C2-O2	5.01	121.91	118.90
21	AA	530	G	C5-C6-N1	5.01	114.01	111.50
21	AA	599	C	N1-C2-O2	5.01	121.91	118.90
21	AA	812	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	1193	G	C8-N9-C4	-5.01	104.39	106.40
21	AA	1491	G	C5'-C4'-C3'	-5.01	107.97	116.00
54	BA	2608	G	N1-C6-O6	-5.01	116.89	119.90
55	BB	7	G	C8-N9-C4	-5.01	104.39	106.40
21	AA	20	U	C4-C5-C6	5.01	122.71	119.70
21	AA	96	U	N1-C2-N3	5.01	117.91	114.90
54	BA	578	G	N3-C4-C5	-5.01	126.09	128.60
21	AA	235	C	N3-C2-O2	-5.01	118.39	121.90
21	AA	457	G	C5-C6-N1	5.01	114.01	111.50
21	AA	570	G	C5-C6-N1	5.01	114.01	111.50
21	AA	755	G	N9-C4-C5	5.01	107.40	105.40
46	BX	71	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
54	BA	590	A	C1'-O4'-C4'	-5.01	105.89	109.90
54	BA	1066	U	N3-C2-O2	-5.01	118.69	122.20
54	BA	1124	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	1385	A	O4'-C1'-N9	5.01	112.21	108.20
54	BA	2176	A	C2-N3-C4	5.01	113.11	110.60
54	BA	2867	G	N3-C2-N2	-5.01	116.39	119.90
21	AA	1074	G	C8-N9-C4	-5.01	104.40	106.40
21	AA	1136	C	N1-C2-O2	5.01	121.91	118.90
22	A1	42	G	C5-C6-N1	5.01	114.00	111.50
24	A3	23	G	N9-C4-C5	5.01	107.40	105.40
24	A3	67	C	C2-N3-C4	-5.01	117.39	119.90
39	BQ	10	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	638	G	C5'-C4'-C3'	-5.01	107.98	116.00
54	BA	663	G	C5-C6-N1	5.01	114.00	111.50
54	BA	1379	U	P-O3'-C3'	5.01	125.71	119.70
54	BA	1450	G	C3'-C2'-C1'	5.01	105.51	101.50
54	BA	2113	U	C5-C6-N1	-5.01	120.19	122.70
54	BA	2415	G	C5-C6-N1	5.01	114.00	111.50
54	BA	2544	G	C8-N9-C4	-5.01	104.40	106.40
54	BA	2812	G	N7-C8-N9	5.01	115.60	113.10
21	AA	599	C	O4'-C1'-N1	5.01	112.21	108.20
54	BA	296	U	N1-C2-N3	5.01	117.91	114.90
54	BA	1398	C	N3-C4-C5	5.01	123.90	121.90
54	BA	1907	G	C5-C6-N1	5.01	114.00	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2102	G	C4'-C3'-C2'	-5.01	97.59	102.60
55	BB	23	G	N3-C4-C5	-5.01	126.10	128.60
21	AA	37	U	O4'-C1'-N1	5.01	112.20	108.20
21	AA	992	U	C1'-O4'-C4'	-5.01	105.89	109.90
21	AA	1361	G	C8-N9-C4	-5.01	104.40	106.40
54	BA	631	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	943	A	C6-C5-N7	5.01	135.81	132.30
54	BA	1338	G	C8-N9-C4	-5.01	104.40	106.40
54	BA	1605	C	N1-C2-O2	5.01	121.90	118.90
54	BA	1872	A	C4'-C3'-C2'	-5.01	97.59	102.60
54	BA	2087	G	N7-C8-N9	5.01	115.60	113.10
54	BA	2645	G	O4'-C1'-N9	5.01	112.20	108.20
54	BA	2659	G	N1-C6-O6	-5.01	116.90	119.90
54	BA	2745	C	N1-C2-O2	5.01	121.90	118.90
21	AA	293	G	C5-C6-N1	5.00	114.00	111.50
21	AA	341	C	N1-C2-O2	5.00	121.90	118.90
21	AA	789	U	N3-C2-O2	-5.00	118.70	122.20
21	AA	846	G	N1-C6-O6	-5.00	116.90	119.90
24	A3	70	C	N1-C2-O2	5.00	121.90	118.90
54	BA	2133	G	C8-N9-C4	-5.00	104.40	106.40
54	BA	2592	G	C5-C6-N1	5.00	114.00	111.50
54	BA	2705	A	C6-C5-N7	5.00	135.80	132.30
21	AA	182	A	C2-N3-C4	5.00	113.10	110.60
21	AA	545	C	O4'-C1'-N1	5.00	112.20	108.20
21	AA	1056	U	N1-C2-N3	5.00	117.90	114.90
22	A1	18	G	N3-C2-N2	-5.00	116.40	119.90
54	BA	275	C	N1-C2-O2	5.00	121.90	118.90
54	BA	287	G	C5-C6-N1	5.00	114.00	111.50
54	BA	747	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	807	U	C3'-C2'-C1'	5.00	105.50	101.50
54	BA	903	C	O4'-C1'-N1	5.00	112.20	108.20
54	BA	1011	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	1436	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	1755	A	C5-C6-N1	5.00	120.20	117.70
54	BA	2104	C	N3-C4-C5	5.00	123.90	121.90
54	BA	2373	G	C5-C6-N1	5.00	114.00	111.50
54	BA	2442	C	N3-C4-C5	5.00	123.90	121.90
55	BB	80	U	N1-C2-N3	5.00	117.90	114.90
55	BB	109	A	C6-C5-N7	5.00	135.80	132.30
21	AA	417	G	C5-C6-N1	5.00	114.00	111.50
54	BA	724	U	N1-C2-N3	5.00	117.90	114.90
54	BA	1852	U	O4'-C1'-N1	5.00	112.20	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1940	U	C4-C5-C6	5.00	122.70	119.70
54	BA	2221	G	N3-C4-C5	-5.00	126.10	128.60
55	BB	18	G	C5-C6-N1	5.00	114.00	111.50

There are no chirality outliers.

All (1054) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	16	C	Sidechain
22	A1	25	C	Sidechain
22	A1	29	U	Sidechain
22	A1	32	C	Sidechain
22	A1	33	U	Sidechain
22	A1	39	G	Sidechain
22	A1	45	G	Sidechain
22	A1	6	A	Sidechain
22	A1	62	C	Sidechain
22	A1	65	C	Sidechain
22	A1	74	C	Sidechain
22	A1	75	C	Sidechain
22	A1	76	A	Sidechain
23	A2	80	C	Sidechain
23	A2	81	U	Sidechain
23	A2	82	A	Sidechain
23	A2	83	U	Sidechain
23	A2	86	U	Sidechain
24	A3	11	A	Sidechain
24	A3	2	G	Sidechain
24	A3	22	A	Sidechain
24	A3	25	U	Sidechain
24	A3	26	C	Sidechain
24	A3	31	G	Sidechain
24	A3	32	G	Sidechain
24	A3	46	G	Sidechain
24	A3	54	G	Sidechain
24	A3	57	C	Sidechain
24	A3	64	G	Sidechain
24	A3	69	C	Sidechain
24	A3	70	C	Sidechain
24	A3	71	G	Sidechain
24	A3	73	A	Sidechain
24	A3	74	A	Sidechain

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Mol	Chain	Res	Type	Group
24	A3	75	C	Sidechain
24	A3	76	C	Sidechain
24	A3	77	A	Sidechain
21	AA	1000	A	Sidechain
21	AA	1012	A	Sidechain
21	AA	1016	A	Sidechain
21	AA	1017	U	Sidechain
21	AA	1029	U	Sidechain
21	AA	1031	C	Sidechain
21	AA	1038	C	Sidechain
21	AA	1046	A	Sidechain
21	AA	1053	G	Sidechain
21	AA	1055	A	Sidechain
21	AA	1057	G	Sidechain
21	AA	1065	U	Sidechain
21	AA	1072	G	Sidechain
21	AA	1076	U	Sidechain
21	AA	1077	G	Sidechain
21	AA	1079	G	Sidechain
21	AA	1088	G	Sidechain
21	AA	1092	A	Sidechain
21	AA	1093	A	Sidechain
21	AA	1094	G	Sidechain
21	AA	1101	A	Sidechain
21	AA	1102	A	Sidechain
21	AA	1105	A	Sidechain
21	AA	1108	G	Sidechain
21	AA	1119	C	Sidechain
21	AA	1123	U	Sidechain
21	AA	1130	A	Sidechain
21	AA	1131	G	Sidechain
21	AA	1132	C	Sidechain
21	AA	1150	A	Sidechain
21	AA	1153	G	Sidechain
21	AA	1155	A	Sidechain
21	AA	1159	U	Sidechain
21	AA	1162	C	Sidechain
21	AA	1163	A	Sidechain
21	AA	1164	G	Sidechain
21	AA	1176	A	Sidechain
21	AA	1178	G	Sidechain
21	AA	1184	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1198	G	Sidechain
21	AA	12	U	Sidechain
21	AA	120	A	Sidechain
21	AA	1206	G	Sidechain
21	AA	1212	U	Sidechain
21	AA	1213	A	Sidechain
21	AA	1215	G	Sidechain
21	AA	1219	A	Sidechain
21	AA	122	G	Sidechain
21	AA	123	U	Sidechain
21	AA	1245	C	Sidechain
21	AA	1249	C	Sidechain
21	AA	125	U	Sidechain
21	AA	1256	A	Sidechain
21	AA	1264	U	Sidechain
21	AA	1266	G	Sidechain
21	AA	1276	G	Sidechain
21	AA	1278	G	Sidechain
21	AA	1279	G	Sidechain
21	AA	1280	A	Sidechain
21	AA	1282	C	Sidechain
21	AA	1285	A	Sidechain
21	AA	1288	A	Sidechain
21	AA	129	A	Sidechain
21	AA	1291	U	Sidechain
21	AA	1296	C	Sidechain
21	AA	1297	G	Sidechain
21	AA	1299	A	Sidechain
21	AA	13	U	Sidechain
21	AA	1300	G	Sidechain
21	AA	1307	U	Sidechain
21	AA	1316	G	Sidechain
21	AA	1319	A	Sidechain
21	AA	1321	U	Sidechain
21	AA	1329	A	Sidechain
21	AA	1331	G	Sidechain
21	AA	1335	U	Sidechain
21	AA	1337	G	Sidechain
21	AA	1343	G	Sidechain
21	AA	1358	U	Sidechain
21	AA	1359	C	Sidechain
21	AA	1363	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1364	U	Sidechain
21	AA	1367	C	Sidechain
21	AA	1370	G	Sidechain
21	AA	1374	A	Sidechain
21	AA	1376	U	Sidechain
21	AA	1382	C	Sidechain
21	AA	1383	C	Sidechain
21	AA	1391	U	Sidechain
21	AA	1406	U	Sidechain
21	AA	1412	C	Sidechain
21	AA	1414	U	Sidechain
21	AA	1418	A	Sidechain
21	AA	1424	U	Sidechain
21	AA	1425	U	Sidechain
21	AA	1430	A	Sidechain
21	AA	1432	G	Sidechain
21	AA	1435	G	Sidechain
21	AA	1436	U	Sidechain
21	AA	1438	G	Sidechain
21	AA	1446	A	Sidechain
21	AA	1450	U	Sidechain
21	AA	1460	C	Sidechain
21	AA	1468	A	Sidechain
21	AA	1483	A	Sidechain
21	AA	1487	G	Sidechain
21	AA	1488	G	Sidechain
21	AA	149	A	Sidechain
21	AA	1491	G	Sidechain
21	AA	1498	U	Sidechain
21	AA	1501	C	Sidechain
21	AA	1505	G	Sidechain
21	AA	1514	G	Sidechain
21	AA	1516	G	Sidechain
21	AA	1518	A	Sidechain
21	AA	152	A	Sidechain
21	AA	1525	G	Sidechain
21	AA	1527	U	Sidechain
21	AA	153	C	Sidechain
21	AA	1530	G	Sidechain
21	AA	1532	U	Sidechain
21	AA	1533	C	Sidechain
21	AA	1534	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	154	U	Sidechain
21	AA	155	A	Sidechain
21	AA	159	G	Sidechain
21	AA	161	A	Sidechain
21	AA	163	C	Sidechain
21	AA	164	G	Sidechain
21	AA	171	A	Sidechain
21	AA	174	A	Sidechain
21	AA	176	C	Sidechain
21	AA	181	A	Sidechain
21	AA	182	A	Sidechain
21	AA	187	G	Sidechain
21	AA	188	C	Sidechain
21	AA	194	C	Sidechain
21	AA	197	A	Sidechain
21	AA	198	G	Sidechain
21	AA	20	U	Sidechain
21	AA	202	G	Sidechain
21	AA	203	G	Sidechain
21	AA	211	G	Sidechain
21	AA	215	C	Sidechain
21	AA	229	U	Sidechain
21	AA	230	G	Sidechain
21	AA	236	A	Sidechain
21	AA	237	G	Sidechain
21	AA	238	A	Sidechain
21	AA	249	U	Sidechain
21	AA	252	U	Sidechain
21	AA	257	G	Sidechain
21	AA	260	G	Sidechain
21	AA	264	C	Sidechain
21	AA	268	U	Sidechain
21	AA	270	A	Sidechain
21	AA	272	C	Sidechain
21	AA	277	C	Sidechain
21	AA	278	G	Sidechain
21	AA	279	A	Sidechain
21	AA	291	U	Sidechain
21	AA	292	G	Sidechain
21	AA	297	G	Sidechain
21	AA	309	A	Sidechain
21	AA	324	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	326	G	Sidechain
21	AA	331	G	Sidechain
21	AA	336	A	Sidechain
21	AA	337	G	Sidechain
21	AA	340	U	Sidechain
21	AA	343	U	Sidechain
21	AA	344	A	Sidechain
21	AA	347	G	Sidechain
21	AA	348	G	Sidechain
21	AA	350	G	Sidechain
21	AA	353	A	Sidechain
21	AA	355	C	Sidechain
21	AA	357	G	Sidechain
21	AA	36	C	Sidechain
21	AA	362	G	Sidechain
21	AA	365	U	Sidechain
21	AA	368	U	Sidechain
21	AA	376	G	Sidechain
21	AA	377	G	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	382	A	Sidechain
21	AA	387	U	Sidechain
21	AA	39	G	Sidechain
21	AA	394	G	Sidechain
21	AA	399	G	Sidechain
21	AA	40	C	Sidechain
21	AA	403	C	Sidechain
21	AA	405	U	Sidechain
21	AA	406	G	Sidechain
21	AA	409	U	Sidechain
21	AA	413	G	Sidechain
21	AA	427	U	Sidechain
21	AA	429	U	Sidechain
21	AA	436	C	Sidechain
21	AA	442	G	Sidechain
21	AA	449	G	Sidechain
21	AA	452	A	Sidechain
21	AA	455	G	Sidechain
21	AA	462	G	Sidechain
21	AA	464	U	Sidechain
21	AA	468	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	476	U	Sidechain
21	AA	477	C	Sidechain
21	AA	479	U	Sidechain
21	AA	480	U	Sidechain
21	AA	485	U	Sidechain
21	AA	491	G	Sidechain
21	AA	492	C	Sidechain
21	AA	493	A	Sidechain
21	AA	5	U	Sidechain
21	AA	50	A	Sidechain
21	AA	51	A	Sidechain
21	AA	510	A	Sidechain
21	AA	514	C	Sidechain
21	AA	516	U	Sidechain
21	AA	521	G	Sidechain
21	AA	527	G	Sidechain
21	AA	529	G	Sidechain
21	AA	530	G	Sidechain
21	AA	535	A	Sidechain
21	AA	537	G	Sidechain
21	AA	547	A	Sidechain
21	AA	557	G	Sidechain
21	AA	558	G	Sidechain
21	AA	562	U	Sidechain
21	AA	564	C	Sidechain
21	AA	566	G	Sidechain
21	AA	571	U	Sidechain
21	AA	572	A	Sidechain
21	AA	586	C	Sidechain
21	AA	588	G	Sidechain
21	AA	590	U	Sidechain
21	AA	597	G	Sidechain
21	AA	598	U	Sidechain
21	AA	6	G	Sidechain
21	AA	60	A	Sidechain
21	AA	61	G	Sidechain
21	AA	611	C	Sidechain
21	AA	613	C	Sidechain
21	AA	617	G	Sidechain
21	AA	623	C	Sidechain
21	AA	626	G	Sidechain
21	AA	635	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	636	U	Sidechain
21	AA	641	U	Sidechain
21	AA	646	G	Sidechain
21	AA	65	A	Sidechain
21	AA	653	U	Sidechain
21	AA	657	U	Sidechain
21	AA	660	C	Sidechain
21	AA	663	A	Sidechain
21	AA	670	G	Sidechain
21	AA	671	G	Sidechain
21	AA	68	G	Sidechain
21	AA	682	G	Sidechain
21	AA	688	G	Sidechain
21	AA	690	G	Sidechain
21	AA	691	G	Sidechain
21	AA	692	U	Sidechain
21	AA	696	A	Sidechain
21	AA	698	G	Sidechain
21	AA	699	C	Sidechain
21	AA	704	A	Sidechain
21	AA	710	G	Sidechain
21	AA	712	A	Sidechain
21	AA	715	A	Sidechain
21	AA	716	A	Sidechain
21	AA	722	G	Sidechain
21	AA	727	G	Sidechain
21	AA	728	A	Sidechain
21	AA	735	C	Sidechain
21	AA	740	U	Sidechain
21	AA	741	G	Sidechain
21	AA	742	G	Sidechain
21	AA	747	A	Sidechain
21	AA	751	U	Sidechain
21	AA	752	G	Sidechain
21	AA	754	C	Sidechain
21	AA	755	G	Sidechain
21	AA	760	G	Sidechain
21	AA	763	G	Sidechain
21	AA	776	G	Sidechain
21	AA	787	A	Sidechain
21	AA	791	G	Sidechain
21	AA	795	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	802	A	Sidechain
21	AA	809	G	Sidechain
21	AA	811	C	Sidechain
21	AA	812	G	Sidechain
21	AA	813	U	Sidechain
21	AA	818	G	Sidechain
21	AA	820	U	Sidechain
21	AA	826	C	Sidechain
21	AA	827	U	Sidechain
21	AA	828	U	Sidechain
21	AA	83	C	Sidechain
21	AA	830	G	Sidechain
21	AA	833	G	Sidechain
21	AA	844	G	Sidechain
21	AA	864	A	Sidechain
21	AA	873	A	Sidechain
21	AA	874	G	Sidechain
21	AA	882	C	Sidechain
21	AA	883	C	Sidechain
21	AA	886	G	Sidechain
21	AA	887	G	Sidechain
21	AA	890	G	Sidechain
21	AA	892	A	Sidechain
21	AA	894	G	Sidechain
21	AA	898	G	Sidechain
21	AA	90	C	Sidechain
21	AA	900	A	Sidechain
21	AA	901	A	Sidechain
21	AA	904	U	Sidechain
21	AA	914	A	Sidechain
21	AA	922	G	Sidechain
21	AA	926	G	Sidechain
21	AA	927	G	Sidechain
21	AA	928	G	Sidechain
21	AA	933	G	Sidechain
21	AA	938	A	Sidechain
21	AA	94	G	Sidechain
21	AA	944	G	Sidechain
21	AA	95	C	Sidechain
21	AA	954	G	Sidechain
21	AA	968	A	Sidechain
21	AA	97	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	971	G	Sidechain
21	AA	973	G	Sidechain
21	AA	976	G	Sidechain
21	AA	978	A	Sidechain
21	AA	99	C	Sidechain
21	AA	994	A	Sidechain
21	AA	995	C	Sidechain
21	AA	997	U	Sidechain
21	AA	998	C	Sidechain
3	AD	44	LYS	Peptide
4	AE	148	SER	Peptide
13	AN	69	ARG	Sidechain
14	AO	68	TYR	Sidechain
56	B5	21	TYR	Sidechain
54	BA	1008	A	Sidechain
54	BA	1012	U	Sidechain
54	BA	1016	G	Sidechain
54	BA	1023	U	Sidechain
54	BA	1024	G	Sidechain
54	BA	1035	U	Sidechain
54	BA	1048	A	Sidechain
54	BA	1051	G	Sidechain
54	BA	1052	C	Sidechain
54	BA	1058	U	Sidechain
54	BA	1067	A	Sidechain
54	BA	1071	G	Sidechain
54	BA	1073	A	Sidechain
54	BA	108	G	Sidechain
54	BA	1083	U	Sidechain
54	BA	1087	G	Sidechain
54	BA	1088	A	Sidechain
54	BA	1093	G	Sidechain
54	BA	1100	C	Sidechain
54	BA	1108	U	Sidechain
54	BA	111	A	Sidechain
54	BA	1123	C	Sidechain
54	BA	1125	G	Sidechain
54	BA	1126	A	Sidechain
54	BA	1127	A	Sidechain
54	BA	1134	A	Sidechain
54	BA	1140	C	Sidechain
54	BA	1142	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1147	A	Sidechain
54	BA	1149	G	Sidechain
54	BA	1151	A	Sidechain
54	BA	1155	A	Sidechain
54	BA	1156	A	Sidechain
54	BA	116	C	Sidechain
54	BA	1160	G	Sidechain
54	BA	1162	G	Sidechain
54	BA	1166	G	Sidechain
54	BA	1167	C	Sidechain
54	BA	1175	A	Sidechain
54	BA	1181	U	Sidechain
54	BA	1182	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	1188	U	Sidechain
54	BA	1191	G	Sidechain
54	BA	1195	G	Sidechain
54	BA	1197	G	Sidechain
54	BA	1205	A	Sidechain
54	BA	1206	G	Sidechain
54	BA	1208	C	Sidechain
54	BA	1210	G	Sidechain
54	BA	1215	G	Sidechain
54	BA	1218	G	Sidechain
54	BA	1221	C	Sidechain
54	BA	1223	G	Sidechain
54	BA	1224	U	Sidechain
54	BA	1230	A	Sidechain
54	BA	1236	G	Sidechain
54	BA	1237	A	Sidechain
54	BA	1242	U	Sidechain
54	BA	1251	C	Sidechain
54	BA	1252	G	Sidechain
54	BA	1258	U	Sidechain
54	BA	1263	U	Sidechain
54	BA	1267	U	Sidechain
54	BA	1273	U	Sidechain
54	BA	1279	G	Sidechain
54	BA	1281	G	Sidechain
54	BA	1283	G	Sidechain
54	BA	1307	A	Sidechain
54	BA	1309	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1312	U	Sidechain
54	BA	1313	U	Sidechain
54	BA	1315	C	Sidechain
54	BA	1317	G	Sidechain
54	BA	1320	C	Sidechain
54	BA	1326	U	Sidechain
54	BA	1330	C	Sidechain
54	BA	1334	G	Sidechain
54	BA	1336	A	Sidechain
54	BA	1343	G	Sidechain
54	BA	1344	U	Sidechain
54	BA	1345	C	Sidechain
54	BA	1351	C	Sidechain
54	BA	1360	G	Sidechain
54	BA	1364	G	Sidechain
54	BA	1366	A	Sidechain
54	BA	1373	A	Sidechain
54	BA	1376	C	Sidechain
54	BA	1377	G	Sidechain
54	BA	1378	A	Sidechain
54	BA	1384	A	Sidechain
54	BA	1386	C	Sidechain
54	BA	1388	G	Sidechain
54	BA	1389	G	Sidechain
54	BA	139	U	Sidechain
54	BA	1392	A	Sidechain
54	BA	1399	C	Sidechain
54	BA	14	A	Sidechain
54	BA	140	C	Sidechain
54	BA	1405	U	Sidechain
54	BA	1407	G	Sidechain
54	BA	141	G	Sidechain
54	BA	1415	U	Sidechain
54	BA	1422	G	Sidechain
54	BA	1426	G	Sidechain
54	BA	1434	A	Sidechain
54	BA	1437	C	Sidechain
54	BA	144	A	Sidechain
54	BA	1442	U	Sidechain
54	BA	1444	G	Sidechain
54	BA	1445	G	Sidechain
54	BA	1447	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1448	G	Sidechain
54	BA	1454	C	Sidechain
54	BA	1455	G	Sidechain
54	BA	1456	G	Sidechain
54	BA	1461	C	Sidechain
54	BA	1469	A	Sidechain
54	BA	1473	G	Sidechain
54	BA	1492	G	Sidechain
54	BA	1499	C	Sidechain
54	BA	150	U	Sidechain
54	BA	1502	A	Sidechain
54	BA	1507	C	Sidechain
54	BA	1519	G	Sidechain
54	BA	1520	U	Sidechain
54	BA	1527	G	Sidechain
54	BA	1528	A	Sidechain
54	BA	1530	G	Sidechain
54	BA	1532	A	Sidechain
54	BA	1534	U	Sidechain
54	BA	1535	A	Sidechain
54	BA	1544	A	Sidechain
54	BA	1546	G	Sidechain
54	BA	155	A	Sidechain
54	BA	1553	A	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1562	U	Sidechain
54	BA	1563	U	Sidechain
54	BA	1573	G	Sidechain
54	BA	1576	U	Sidechain
54	BA	1577	C	Sidechain
54	BA	158	U	Sidechain
54	BA	1586	A	Sidechain
54	BA	159	G	Sidechain
54	BA	1593	A	Sidechain
54	BA	1596	A	Sidechain
54	BA	160	A	Sidechain
54	BA	1600	C	Sidechain
54	BA	1602	U	Sidechain
54	BA	161	A	Sidechain
54	BA	1610	A	Sidechain
54	BA	1611	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1616	A	Sidechain
54	BA	1618	A	Sidechain
54	BA	1620	G	Sidechain
54	BA	1628	G	Sidechain
54	BA	1631	G	Sidechain
54	BA	1638	C	Sidechain
54	BA	1642	G	Sidechain
54	BA	1652	A	Sidechain
54	BA	1661	G	Sidechain
54	BA	1662	U	Sidechain
54	BA	1664	A	Sidechain
54	BA	1665	A	Sidechain
54	BA	1667	G	Sidechain
54	BA	1671	U	Sidechain
54	BA	1681	G	Sidechain
54	BA	1682	G	Sidechain
54	BA	1683	U	Sidechain
54	BA	1697	G	Sidechain
54	BA	17	G	Sidechain
54	BA	1701	A	Sidechain
54	BA	1702	G	Sidechain
54	BA	1703	G	Sidechain
54	BA	1704	C	Sidechain
54	BA	1706	C	Sidechain
54	BA	1708	C	Sidechain
54	BA	1713	A	Sidechain
54	BA	1731	G	Sidechain
54	BA	1733	G	Sidechain
54	BA	1734	G	Sidechain
54	BA	1738	G	Sidechain
54	BA	1739	A	Sidechain
54	BA	1744	A	Sidechain
54	BA	1747	U	Sidechain
54	BA	1749	A	Sidechain
54	BA	1751	U	Sidechain
54	BA	1754	A	Sidechain
54	BA	1758	U	Sidechain
54	BA	1760	C	Sidechain
54	BA	1762	A	Sidechain
54	BA	1770	G	Sidechain
54	BA	1774	C	Sidechain
54	BA	1785	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1787	A	Sidechain
54	BA	1789	A	Sidechain
54	BA	1791	A	Sidechain
54	BA	1792	G	Sidechain
54	BA	1802	A	Sidechain
54	BA	1820	U	Sidechain
54	BA	1826	G	Sidechain
54	BA	1827	U	Sidechain
54	BA	1828	G	Sidechain
54	BA	1837	C	Sidechain
54	BA	1840	G	Sidechain
54	BA	1854	A	Sidechain
54	BA	1857	G	Sidechain
54	BA	1858	A	Sidechain
54	BA	1860	G	Sidechain
54	BA	1869	G	Sidechain
54	BA	1870	C	Sidechain
54	BA	1883	U	Sidechain
54	BA	1887	C	Sidechain
54	BA	1888	G	Sidechain
54	BA	1890	A	Sidechain
54	BA	1893	C	Sidechain
54	BA	1894	C	Sidechain
54	BA	1897	G	Sidechain
54	BA	1903	G	Sidechain
54	BA	1905	C	Sidechain
54	BA	1910	G	Sidechain
54	BA	1914	C	Sidechain
54	BA	1927	A	Sidechain
54	BA	1932	A	Sidechain
54	BA	1945	G	Sidechain
54	BA	1956	U	Sidechain
54	BA	196	A	Sidechain
54	BA	1960	A	Sidechain
54	BA	1961	C	Sidechain
54	BA	1962	C	Sidechain
54	BA	1971	U	Sidechain
54	BA	1976	U	Sidechain
54	BA	198	C	Sidechain
54	BA	1983	G	Sidechain
54	BA	1989	G	Sidechain
54	BA	1993	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1995	U	Sidechain
54	BA	1997	C	Sidechain
54	BA	20	C	Sidechain
54	BA	2002	G	Sidechain
54	BA	2004	G	Sidechain
54	BA	2007	U	Sidechain
54	BA	2012	G	Sidechain
54	BA	2013	A	Sidechain
54	BA	2018	G	Sidechain
54	BA	2019	A	Sidechain
54	BA	202	U	Sidechain
54	BA	2029	G	Sidechain
54	BA	2055	C	Sidechain
54	BA	2056	G	Sidechain
54	BA	2058	A	Sidechain
54	BA	2059	A	Sidechain
54	BA	206	U	Sidechain
54	BA	2062	A	Sidechain
54	BA	2066	C	Sidechain
54	BA	2067	G	Sidechain
54	BA	207	A	Sidechain
54	BA	2072	C	Sidechain
54	BA	2078	C	Sidechain
54	BA	2079	U	Sidechain
54	BA	2082	A	Sidechain
54	BA	2088	A	Sidechain
54	BA	2091	C	Sidechain
54	BA	2104	C	Sidechain
54	BA	2107	G	Sidechain
54	BA	2109	U	Sidechain
54	BA	2111	U	Sidechain
54	BA	2113	U	Sidechain
54	BA	2114	A	Sidechain
54	BA	2115	G	Sidechain
54	BA	2121	G	Sidechain
54	BA	2125	G	Sidechain
54	BA	2128	G	Sidechain
54	BA	2132	U	Sidechain
54	BA	2140	G	Sidechain
54	BA	2153	C	Sidechain
54	BA	2157	G	Sidechain
54	BA	2160	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2167	U	Sidechain
54	BA	2168	G	Sidechain
54	BA	2172	U	Sidechain
54	BA	2175	C	Sidechain
54	BA	2176	A	Sidechain
54	BA	2181	U	Sidechain
54	BA	2189	U	Sidechain
54	BA	2196	C	Sidechain
54	BA	2197	U	Sidechain
54	BA	2198	A	Sidechain
54	BA	2202	U	Sidechain
54	BA	2207	C	Sidechain
54	BA	2211	A	Sidechain
54	BA	2212	A	Sidechain
54	BA	2217	G	Sidechain
54	BA	2219	U	Sidechain
54	BA	2224	G	Sidechain
54	BA	2225	A	Sidechain
54	BA	2230	G	Sidechain
54	BA	2236	U	Sidechain
54	BA	2242	G	Sidechain
54	BA	2244	U	Sidechain
54	BA	2245	U	Sidechain
54	BA	2248	C	Sidechain
54	BA	2249	U	Sidechain
54	BA	2250	G	Sidechain
54	BA	2251	G	Sidechain
54	BA	2256	G	Sidechain
54	BA	2257	U	Sidechain
54	BA	2266	A	Sidechain
54	BA	2271	G	Sidechain
54	BA	2274	A	Sidechain
54	BA	2278	A	Sidechain
54	BA	2283	C	Sidechain
54	BA	2284	A	Sidechain
54	BA	2290	G	Sidechain
54	BA	2298	A	Sidechain
54	BA	2300	C	Sidechain
54	BA	2301	C	Sidechain
54	BA	2302	U	Sidechain
54	BA	2304	G	Sidechain
54	BA	2308	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	231	A	Sidechain
54	BA	2323	G	Sidechain
54	BA	2327	A	Sidechain
54	BA	2328	A	Sidechain
54	BA	2330	G	Sidechain
54	BA	2331	G	Sidechain
54	BA	2336	A	Sidechain
54	BA	2337	G	Sidechain
54	BA	2338	C	Sidechain
54	BA	234	U	Sidechain
54	BA	2344	U	Sidechain
54	BA	235	U	Sidechain
54	BA	2352	A	Sidechain
54	BA	2357	G	Sidechain
54	BA	2363	G	Sidechain
54	BA	2375	G	Sidechain
54	BA	2376	A	Sidechain
54	BA	238	C	Sidechain
54	BA	2389	G	Sidechain
54	BA	2391	G	Sidechain
54	BA	2392	A	Sidechain
54	BA	2396	G	Sidechain
54	BA	2399	G	Sidechain
54	BA	240	C	Sidechain
54	BA	2411	A	Sidechain
54	BA	2416	C	Sidechain
54	BA	2418	A	Sidechain
54	BA	2428	G	Sidechain
54	BA	2432	A	Sidechain
54	BA	2433	A	Sidechain
54	BA	2439	A	Sidechain
54	BA	2442	C	Sidechain
54	BA	2444	G	Sidechain
54	BA	2447	G	Sidechain
54	BA	2455	G	Sidechain
54	BA	2466	C	Sidechain
54	BA	2468	A	Sidechain
54	BA	2469	A	Sidechain
54	BA	247	G	Sidechain
54	BA	2478	A	Sidechain
54	BA	248	G	Sidechain
54	BA	2481	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2495	G	Sidechain
54	BA	2499	C	Sidechain
54	BA	250	G	Sidechain
54	BA	2500	U	Sidechain
54	BA	2504	U	Sidechain
54	BA	2505	G	Sidechain
54	BA	2508	G	Sidechain
54	BA	2512	C	Sidechain
54	BA	2516	A	Sidechain
54	BA	2517	C	Sidechain
54	BA	2519	U	Sidechain
54	BA	2523	G	Sidechain
54	BA	2527	C	Sidechain
54	BA	2529	G	Sidechain
54	BA	2532	G	Sidechain
54	BA	2543	G	Sidechain
54	BA	2564	A	Sidechain
54	BA	2566	A	Sidechain
54	BA	2567	G	Sidechain
54	BA	2572	A	Sidechain
54	BA	2576	G	Sidechain
54	BA	2579	C	Sidechain
54	BA	2581	G	Sidechain
54	BA	2588	G	Sidechain
54	BA	2596	U	Sidechain
54	BA	2597	G	Sidechain
54	BA	2598	A	Sidechain
54	BA	2600	A	Sidechain
54	BA	2601	C	Sidechain
54	BA	2603	G	Sidechain
54	BA	2606	C	Sidechain
54	BA	2607	G	Sidechain
54	BA	2611	C	Sidechain
54	BA	2614	A	Sidechain
54	BA	262	A	Sidechain
54	BA	2621	G	Sidechain
54	BA	2622	U	Sidechain
54	BA	2626	C	Sidechain
54	BA	2631	G	Sidechain
54	BA	2637	U	Sidechain
54	BA	2639	A	Sidechain
54	BA	264	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2640	G	Sidechain
54	BA	2644	G	Sidechain
54	BA	265	A	Sidechain
54	BA	2652	C	Sidechain
54	BA	2659	G	Sidechain
54	BA	2662	A	Sidechain
54	BA	2668	G	Sidechain
54	BA	2669	G	Sidechain
54	BA	2673	G	Sidechain
54	BA	2679	A	Sidechain
54	BA	2680	U	Sidechain
54	BA	2682	A	Sidechain
54	BA	2687	U	Sidechain
54	BA	27	G	Sidechain
54	BA	2701	U	Sidechain
54	BA	2710	C	Sidechain
54	BA	2711	A	Sidechain
54	BA	2716	C	Sidechain
54	BA	2733	A	Sidechain
54	BA	2737	G	Sidechain
54	BA	2750	A	Sidechain
54	BA	2756	U	Sidechain
54	BA	276	U	Sidechain
54	BA	2765	A	Sidechain
54	BA	2774	C	Sidechain
54	BA	2780	G	Sidechain
54	BA	2781	A	Sidechain
54	BA	2784	U	Sidechain
54	BA	2785	C	Sidechain
54	BA	2787	C	Sidechain
54	BA	2790	U	Sidechain
54	BA	2802	G	Sidechain
54	BA	2805	C	Sidechain
54	BA	2806	C	Sidechain
54	BA	2807	U	Sidechain
54	BA	2811	G	Sidechain
54	BA	2817	U	Sidechain
54	BA	2819	G	Sidechain
54	BA	2822	G	Sidechain
54	BA	2823	A	Sidechain
54	BA	2829	A	Sidechain
54	BA	283	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2832	U	Sidechain
54	BA	2839	G	Sidechain
54	BA	2852	G	Sidechain
54	BA	2857	G	Sidechain
54	BA	2859	G	Sidechain
54	BA	2861	U	Sidechain
54	BA	2868	A	Sidechain
54	BA	2871	U	Sidechain
54	BA	2873	A	Sidechain
54	BA	2874	C	Sidechain
54	BA	2879	A	Sidechain
54	BA	2883	A	Sidechain
54	BA	2886	A	Sidechain
54	BA	2887	A	Sidechain
54	BA	2888	C	Sidechain
54	BA	2895	G	Sidechain
54	BA	2903	U	Sidechain
54	BA	295	G	Sidechain
54	BA	297	G	Sidechain
54	BA	304	U	Sidechain
54	BA	305	C	Sidechain
54	BA	307	G	Sidechain
54	BA	308	G	Sidechain
54	BA	309	A	Sidechain
54	BA	313	G	Sidechain
54	BA	317	G	Sidechain
54	BA	32	C	Sidechain
54	BA	323	C	Sidechain
54	BA	325	G	Sidechain
54	BA	326	G	Sidechain
54	BA	327	G	Sidechain
54	BA	333	G	Sidechain
54	BA	334	C	Sidechain
54	BA	339	U	Sidechain
54	BA	340	A	Sidechain
54	BA	344	A	Sidechain
54	BA	355	U	Sidechain
54	BA	36	G	Sidechain
54	BA	364	C	Sidechain
54	BA	367	G	Sidechain
54	BA	385	C	Sidechain
54	BA	39	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	392	U	Sidechain
54	BA	393	C	Sidechain
54	BA	394	C	Sidechain
54	BA	4	U	Sidechain
54	BA	401	A	Sidechain
54	BA	402	A	Sidechain
54	BA	404	A	Sidechain
54	BA	416	U	Sidechain
54	BA	418	C	Sidechain
54	BA	420	C	Sidechain
54	BA	422	A	Sidechain
54	BA	434	U	Sidechain
54	BA	442	G	Sidechain
54	BA	446	G	Sidechain
54	BA	45	G	Sidechain
54	BA	450	G	Sidechain
54	BA	458	G	Sidechain
54	BA	463	G	Sidechain
54	BA	467	G	Sidechain
54	BA	471	A	Sidechain
54	BA	473	G	Sidechain
54	BA	476	G	Sidechain
54	BA	477	A	Sidechain
54	BA	478	A	Sidechain
54	BA	479	A	Sidechain
54	BA	481	G	Sidechain
54	BA	49	A	Sidechain
54	BA	493	G	Sidechain
54	BA	494	G	Sidechain
54	BA	495	G	Sidechain
54	BA	496	G	Sidechain
54	BA	499	U	Sidechain
54	BA	5	A	Sidechain
54	BA	500	G	Sidechain
54	BA	501	A	Sidechain
54	BA	505	A	Sidechain
54	BA	508	A	Sidechain
54	BA	510	C	Sidechain
54	BA	514	A	Sidechain
54	BA	518	G	Sidechain
54	BA	521	U	Sidechain
54	BA	522	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	523	C	Sidechain
54	BA	525	U	Sidechain
54	BA	527	C	Sidechain
54	BA	528	A	Sidechain
54	BA	53	A	Sidechain
54	BA	531	C	Sidechain
54	BA	538	A	Sidechain
54	BA	543	G	Sidechain
54	BA	547	A	Sidechain
54	BA	567	U	Sidechain
54	BA	573	U	Sidechain
54	BA	576	U	Sidechain
54	BA	579	G	Sidechain
54	BA	58	G	Sidechain
54	BA	587	C	Sidechain
54	BA	589	U	Sidechain
54	BA	59	U	Sidechain
54	BA	590	A	Sidechain
54	BA	595	C	Sidechain
54	BA	597	G	Sidechain
54	BA	600	G	Sidechain
54	BA	603	A	Sidechain
54	BA	608	A	Sidechain
54	BA	611	C	Sidechain
54	BA	614	A	Sidechain
54	BA	615	U	Sidechain
54	BA	628	G	Sidechain
54	BA	630	G	Sidechain
54	BA	632	A	Sidechain
54	BA	636	G	Sidechain
54	BA	637	A	Sidechain
54	BA	64	A	Sidechain
54	BA	65	U	Sidechain
54	BA	655	A	Sidechain
54	BA	659	G	Sidechain
54	BA	670	A	Sidechain
54	BA	687	C	Sidechain
54	BA	69	C	Sidechain
54	BA	693	A	Sidechain
54	BA	695	G	Sidechain
54	BA	703	U	Sidechain
54	BA	71	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	715	A	Sidechain
54	BA	716	A	Sidechain
54	BA	718	A	Sidechain
54	BA	722	A	Sidechain
54	BA	724	U	Sidechain
54	BA	725	G	Sidechain
54	BA	727	A	Sidechain
54	BA	737	C	Sidechain
54	BA	738	G	Sidechain
54	BA	74	A	Sidechain
54	BA	750	A	Sidechain
54	BA	752	A	Sidechain
54	BA	76	C	Sidechain
54	BA	760	G	Sidechain
54	BA	764	A	Sidechain
54	BA	765	C	Sidechain
54	BA	770	G	Sidechain
54	BA	774	G	Sidechain
54	BA	775	G	Sidechain
54	BA	777	G	Sidechain
54	BA	792	A	Sidechain
54	BA	793	A	Sidechain
54	BA	794	A	Sidechain
54	BA	795	C	Sidechain
54	BA	8	C	Sidechain
54	BA	800	A	Sidechain
54	BA	801	G	Sidechain
54	BA	802	A	Sidechain
54	BA	804	A	Sidechain
54	BA	805	G	Sidechain
54	BA	806	C	Sidechain
54	BA	810	U	Sidechain
54	BA	811	U	Sidechain
54	BA	813	U	Sidechain
54	BA	827	U	Sidechain
54	BA	828	U	Sidechain
54	BA	830	G	Sidechain
54	BA	834	G	Sidechain
54	BA	857	G	Sidechain
54	BA	858	G	Sidechain
54	BA	860	U	Sidechain
54	BA	862	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	880	G	Sidechain
54	BA	886	A	Sidechain
54	BA	888	C	Sidechain
54	BA	889	C	Sidechain
54	BA	895	U	Sidechain
54	BA	899	A	Sidechain
54	BA	90	U	Sidechain
54	BA	910	A	Sidechain
54	BA	912	C	Sidechain
54	BA	920	A	Sidechain
54	BA	925	A	Sidechain
54	BA	926	G	Sidechain
54	BA	929	U	Sidechain
54	BA	930	G	Sidechain
54	BA	931	U	Sidechain
54	BA	941	A	Sidechain
54	BA	942	G	Sidechain
54	BA	952	G	Sidechain
54	BA	956	G	Sidechain
54	BA	959	A	Sidechain
54	BA	96	C	Sidechain
54	BA	966	G	Sidechain
54	BA	97	C	Sidechain
54	BA	974	G	Sidechain
54	BA	975	A	Sidechain
54	BA	983	A	Sidechain
54	BA	984	A	Sidechain
54	BA	988	A	Sidechain
54	BA	993	G	Sidechain
54	BA	998	C	Sidechain
55	BB	106	G	Sidechain
55	BB	109	A	Sidechain
55	BB	112	G	Sidechain
55	BB	12	C	Sidechain
55	BB	13	G	Sidechain
55	BB	14	U	Sidechain
55	BB	15	A	Sidechain
55	BB	19	C	Sidechain
55	BB	23	G	Sidechain
55	BB	31	C	Sidechain
55	BB	35	C	Sidechain
55	BB	38	C	Sidechain

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Mol	Chain	Res	Type	Group
55	BB	39	A	Sidechain
55	BB	49	C	Sidechain
55	BB	50	A	Sidechain
55	BB	57	A	Sidechain
55	BB	6	G	Sidechain
55	BB	64	G	Sidechain
55	BB	66	A	Sidechain
55	BB	69	G	Sidechain
55	BB	75	G	Sidechain
55	BB	87	U	Sidechain
55	BB	96	G	Sidechain
46	BX	36	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	1	0
5	AF	818	0	808	1	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	1	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
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	1	0
21	AA	32828	0	16011	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A1	1627	0	802	0	0
23	A2	309	0	156	0	0
24	A3	1642	0	811	2	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	1	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	1	0
33	BK	939	0	1012	1	0
34	BL	1045	0	1117	2	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	1	0
38	BP	917	0	965	1	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	1	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	1	0
52	B3	504	0	574	3	0
53	B4	302	0	343	0	0
54	BA	62317	0	30495	12	0
55	BB	2504	0	1187	0	0
56	B5	1658	0	1751	1	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	98156	28	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 (28) 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)
34:BL:64:PHE:CE2	52:B3:24:LYS:HE2	2.40	0.56
20:AU:30:GLU:H	20:AU:31:VAL:HG22	1.72	0.54
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.30	0.49
56:B5:19:LYS:HE3	56:B5:21:TYR:CE2	2.46	0.49
52:B3:2:LYS:HE3	54:BA:242:G:C8	2.51	0.45
54:BA:780:G:C6	54:BA:782:A:C2	3.05	0.45
24:A3:75:C:H2'	24:A3:76:C:C5'	2.46	0.44
33:BK:106:GLU:CD	33:BK:106:GLU:H	2.20	0.44
45:BW:35:ILE:N	45:BW:35:ILE:HD12	2.33	0.44
21:AA:901:A:N7	21:AA:902:G:H1'	2.34	0.43
21:AA:539:A:H2'	21:AA:540:G:C8	2.54	0.42
54:BA:669:G:H2'	54:BA:670:A:C5	2.54	0.42
4:AE:155:LYS:HE2	7:AH:44:PHE:CE1	2.54	0.42
54:BA:639:U:H2'	54:BA:640:C:C6	2.55	0.42
51:B2:8:SER:HB3	54:BA:686:U:H3	1.85	0.42
21:AA:493:A:H2'	21:AA:494:G:C4	2.55	0.42
29:BG:93:TYR:CE2	29:BG:159:LYS:HE2	2.54	0.41
54:BA:2210:U:C2	54:BA:2212:A:H2'	2.55	0.41
54:BA:1050:A:C2	54:BA:2751:G:C4	3.08	0.41
54:BA:139:U:H3'	54:BA:140:C:C5'	2.51	0.41
34:BL:64:PHE:CZ	52:B3:24:LYS:HE2	2.56	0.41
54:BA:2291:U:H2'	54:BA:2292:U:C6	2.56	0.41
37:BO:5:SER:HA	37:BO:8:ILE:HG22	2.03	0.41
32:BJ:13:ARG:HB3	32:BJ:53:TYR:CD2	2.56	0.40
21:AA:713:G:H2'	21:AA:714:G:C8	2.57	0.40
38:BP:93:LYS:HE3	54:BA:1754:A:C8	2.57	0.40
24:A3:75:C:H1'	54:BA:2602:A:H2'	2.04	0.40
54:BA:449:A:O5'	54:BA:449:A:C8	2.75	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%)	199 (91%)	17 (8%)	2 (1%)	19	61
2	AC	205/208 (99%)	187 (91%)	15 (7%)	3 (2%)	11	51
3	AD	203/206 (98%)	184 (91%)	14 (7%)	5 (2%)	6	39
4	AE	150/152 (99%)	132 (88%)	14 (9%)	4 (3%)	5	38
5	AF	99/101 (98%)	88 (89%)	8 (8%)	3 (3%)	5	35
6	AG	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	8	45
7	AH	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	6	40
8	AI	126/128 (98%)	113 (90%)	7 (6%)	6 (5%)	2	26
9	AJ	98/100 (98%)	90 (92%)	4 (4%)	4 (4%)	3	29
10	AK	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	19	61
11	AL	121/124 (98%)	108 (89%)	7 (6%)	6 (5%)	2	26
12	AM	112/115 (97%)	100 (89%)	9 (8%)	3 (3%)	5	38
13	AN	98/101 (97%)	83 (85%)	12 (12%)	3 (3%)	4	35
14	AO	86/89 (97%)	76 (88%)	8 (9%)	2 (2%)	7	41
15	AP	79/81 (98%)	67 (85%)	8 (10%)	4 (5%)	2	25
16	AQ	80/82 (98%)	75 (94%)	3 (4%)	2 (2%)	6	39
17	AR	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
18	AS	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	13	54
19	AT	84/86 (98%)	76 (90%)	7 (8%)	1 (1%)	14	56
20	AU	51/53 (96%)	32 (63%)	9 (18%)	10 (20%)	0	2
25	BC	270/273 (99%)	246 (91%)	18 (7%)	6 (2%)	7	42
26	BD	207/209 (99%)	177 (86%)	19 (9%)	11 (5%)	2	25
27	BE	199/201 (99%)	179 (90%)	11 (6%)	9 (4%)	3	28
28	BF	176/179 (98%)	150 (85%)	20 (11%)	6 (3%)	4	33
29	BG	174/177 (98%)	156 (90%)	15 (9%)	3 (2%)	10	49
30	BH	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	12	52
31	BI	139/142 (98%)	130 (94%)	7 (5%)	2 (1%)	12	52
32	BJ	140/142 (99%)	122 (87%)	15 (11%)	3 (2%)	8	43
33	BK	121/123 (98%)	112 (93%)	9 (7%)	0	100	100
34	BL	141/144 (98%)	127 (90%)	10 (7%)	4 (3%)	5	37
35	BM	134/136 (98%)	118 (88%)	11 (8%)	5 (4%)	4	31
36	BN	119/121 (98%)	107 (90%)	10 (8%)	2 (2%)	10	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	19	61
38	BP	112/115 (97%)	94 (84%)	11 (10%)	7 (6%)	1	21
39	BQ	115/118 (98%)	109 (95%)	3 (3%)	3 (3%)	6	38
40	BR	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	8	45
41	BS	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	19	61
42	BT	92/94 (98%)	71 (77%)	17 (18%)	4 (4%)	3	28
43	BU	101/104 (97%)	88 (87%)	10 (10%)	3 (3%)	5	35
44	BV	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
45	BW	78/80 (98%)	60 (77%)	15 (19%)	3 (4%)	3	30
46	BX	75/79 (95%)	64 (85%)	9 (12%)	2 (3%)	5	38
47	BY	61/63 (97%)	53 (87%)	7 (12%)	1 (2%)	11	50
48	BZ	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	9	47
49	B0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	2	24
50	B1	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	3	29
51	B2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	B3	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	11	50
53	B4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	2	24
56	B5	221/234 (94%)	207 (94%)	12 (5%)	2 (1%)	19	61
All	All	5876/6008 (98%)	5263 (90%)	456 (8%)	157 (3%)	9	38

All (157) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	149	PRO
6	AG	11	ILE
6	AG	56	SER
8	AI	110	VAL
9	AJ	57	VAL
13	AN	56	SER
14	AO	18	ALA
18	AS	4	LEU
20	AU	9	GLU
20	AU	37	TYR
25	BC	136	VAL
26	BD	80	TRP
26	BD	170	VAL

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Mol	Chain	Res	Type
28	BF	103	ILE
34	BL	36	LYS
36	BN	47	VAL
39	BQ	87	VAL
42	BT	68	LYS
50	B1	50	GLU
2	AC	167	TYR
3	AD	24	VAL
4	AE	105	ILE
5	AF	6	ILE
6	AG	5	VAL
7	AH	77	VAL
8	AI	119	LYS
9	AJ	74	VAL
12	AM	42	VAL
15	AP	17	TYR
15	AP	79	ASN
19	AT	3	ILE
20	AU	15	LEU
20	AU	27	VAL
27	BE	49	ARG
30	BH	121	VAL
34	BL	25	SER
34	BL	101	ILE
35	BM	36	VAL
35	BM	58	LYS
35	BM	70	ASP
38	BP	31	VAL
39	BQ	86	SER
41	BS	29	VAL
42	BT	61	LEU
43	BU	43	LYS
45	BW	68	PHE
46	BX	17	ARG
46	BX	27	ARG
49	B0	52	LYS
50	B1	6	GLU
3	AD	28	ASP
3	AD	84	ASN
5	AF	63	ASN
11	AL	68	GLY
11	AL	78	VAL

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Mol	Chain	Res	Type
13	AN	55	SER
15	AP	50	THR
16	AQ	27	PHE
20	AU	13	VAL
20	AU	25	ALA
20	AU	31	VAL
25	BC	37	SER
25	BC	196	ASN
25	BC	260	LYS
26	BD	2	ILE
26	BD	22	ILE
26	BD	51	THR
26	BD	77	ARG
26	BD	131	ASP
26	BD	150	GLN
27	BE	43	THR
27	BE	96	VAL
27	BE	123	LYS
28	BF	87	LYS
28	BF	132	ARG
29	BG	22	VAL
32	BJ	15	TRP
34	BL	125	LEU
35	BM	117	PHE
38	BP	74	GLN
40	BR	53	PHE
43	BU	5	ARG
43	BU	45	GLN
47	BY	37	LEU
56	B5	91	GLY
1	AB	11	ALA
1	AB	18	GLN
4	AE	38	VAL
7	AH	65	PHE
8	AI	31	GLN
8	AI	57	VAL
9	AJ	75	ASP
12	AM	60	ALA
14	AO	43	ALA
16	AQ	64	ARG
26	BD	15	PHE
26	BD	75	ALA

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Mol	Chain	Res	Type
27	BE	71	GLY
32	BJ	53	TYR
35	BM	134	THR
38	BP	26	GLU
38	BP	112	ARG
42	BT	3	ARG
45	BW	74	LYS
49	B0	5	ASN
52	B3	35	LYS
53	B4	32	LYS
56	B5	220	ALA
8	AI	55	ASP
11	AL	116	TYR
20	AU	3	ILE
25	BC	191	LEU
26	BD	112	THR
27	BE	165	HIS
30	BH	94	ILE
31	BI	37	PHE
32	BJ	45	THR
38	BP	32	VAL
39	BQ	2	ARG
40	BR	51	VAL
42	BT	66	LYS
53	B4	2	LYS
2	AC	195	ILE
3	AD	138	PRO
4	AE	54	GLU
5	AF	98	GLU
7	AH	78	SER
9	AJ	92	LEU
11	AL	33	CYS
13	AN	100	SER
20	AU	12	ASP
25	BC	36	ASN
27	BE	94	GLN
29	BG	101	VAL
38	BP	109	ILE
45	BW	53	GLY
48	BZ	31	ILE
8	AI	25	GLY
15	AP	40	ASN

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Mol	Chain	Res	Type
27	BE	81	GLY
28	BF	12	VAL
28	BF	75	GLY
38	BP	69	VAL
49	B0	24	VAL
3	AD	199	ILE
12	AM	63	VAL
27	BE	148	ILE
2	AC	144	GLY
10	AK	77	GLY
11	AL	84	GLY
28	BF	140	ILE
29	BG	116	LEU
11	AL	43	LYS
20	AU	52	VAL
31	BI	97	VAL
36	BN	84	GLY
37	BO	27	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%)	63	83
2	AC	170/171 (99%)	170 (100%)	0	100	100
3	AD	172/173 (99%)	169 (98%)	3 (2%)	63	83
4	AE	113/113 (100%)	111 (98%)	2 (2%)	62	82
5	AF	87/87 (100%)	85 (98%)	2 (2%)	53	76
6	AG	123/123 (100%)	121 (98%)	2 (2%)	65	84
7	AH	104/105 (99%)	104 (100%)	0	100	100
8	AI	105/105 (100%)	102 (97%)	3 (3%)	45	70
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	89 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	AL	103/104 (99%)	102 (99%)	1 (1%)	78	89
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	82 (99%)	1 (1%)	74	87
14	AO	76/77 (99%)	74 (97%)	2 (3%)	49	73
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	73 (99%)	1 (1%)	69	85
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	69 (99%)	1 (1%)	69	85
19	AT	65/65 (100%)	64 (98%)	1 (2%)	67	85
20	AU	44/44 (100%)	41 (93%)	3 (7%)	17	48
25	BC	216/217 (100%)	213 (99%)	3 (1%)	69	85
26	BD	164/164 (100%)	160 (98%)	4 (2%)	52	75
27	BE	165/165 (100%)	162 (98%)	3 (2%)	62	82
28	BF	149/150 (99%)	147 (99%)	2 (1%)	71	86
29	BG	137/138 (99%)	134 (98%)	3 (2%)	55	77
30	BH	114/114 (100%)	112 (98%)	2 (2%)	62	82
31	BI	109/110 (99%)	108 (99%)	1 (1%)	81	90
32	BJ	116/116 (100%)	115 (99%)	1 (1%)	81	90
33	BK	103/103 (100%)	103 (100%)	0	100	100
34	BL	102/103 (99%)	100 (98%)	2 (2%)	58	79
35	BM	109/109 (100%)	107 (98%)	2 (2%)	62	82
36	BN	100/100 (100%)	99 (99%)	1 (1%)	78	89
37	BO	86/87 (99%)	86 (100%)	0	100	100
38	BP	99/100 (99%)	97 (98%)	2 (2%)	58	79
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	76	88
40	BR	84/84 (100%)	82 (98%)	2 (2%)	52	75
41	BS	93/93 (100%)	92 (99%)	1 (1%)	76	88
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	82 (99%)	1 (1%)	74	87
44	BV	78/78 (100%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	57 (97%)	2 (3%)	40	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	47 (98%)	1 (2%)	56	78
49	B0	47/48 (98%)	47 (100%)	0	100	100
50	B1	45/45 (100%)	44 (98%)	1 (2%)	55	77
51	B2	38/38 (100%)	35 (92%)	3 (8%)	13	43
52	B3	51/52 (98%)	51 (100%)	0	100	100
53	B4	34/34 (100%)	33 (97%)	1 (3%)	45	70
56	B5	173/181 (96%)	170 (98%)	3 (2%)	63	83
All	All	4842/4870 (99%)	4774 (99%)	68 (1%)	71	85

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	17	HIS
1	AB	106	VAL
1	AB	189	ASN
3	AD	50	TYR
3	AD	56	GLU
3	AD	181	PHE
4	AE	70	MET
4	AE	89	THR
5	AF	72	ASP
5	AF	97	THR
6	AG	12	LEU
6	AG	27	ASN
8	AI	53	LEU
8	AI	56	MET
8	AI	105	ARG
10	AK	100	ASN
11	AL	28	GLN
13	AN	81	ARG
14	AO	24	THR
14	AO	45	HIS
16	AQ	69	THR
18	AS	14	LEU
19	AT	30	PHE
20	AU	18	PHE
20	AU	20	ARG

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Mol	Chain	Res	Type
20	AU	27	VAL
25	BC	24	HIS
25	BC	86	ARG
25	BC	200	MET
26	BD	90	PHE
26	BD	91	THR
26	BD	103	ASP
26	BD	172	VAL
27	BE	122	GLU
27	BE	152	GLU
27	BE	163	ASN
28	BF	35	LEU
28	BF	134	GLN
29	BG	34	ARG
29	BG	154	GLU
29	BG	162	ARG
30	BH	68	ARG
30	BH	104	THR
31	BI	16	MET
32	BJ	30	THR
34	BL	77	ILE
34	BL	81	ASP
35	BM	1	MET
35	BM	126	ILE
36	BN	1	MET
38	BP	19	PHE
38	BP	75	THR
39	BQ	5	ARG
40	BR	31	GLU
40	BR	80	ARG
41	BS	81	SER
43	BU	8	ASP
45	BW	23	LYS
45	BW	39	GLN
48	BZ	37	ARG
50	B1	22	THR
51	B2	1	MET
51	B2	25	LYS
51	B2	34	ARG
53	B4	24	ARG
56	B5	12	ARG
56	B5	129	GLN

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Mol	Chain	Res	Type
56	B5	148	ASN

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

Mol	Chain	Res	Type
4	AE	96	GLN
10	AK	100	ASN
29	BG	110	HIS
44	BV	88	HIS
45	BW	56	HIS
46	BX	31	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	264 (17%)	77 (5%)
22	A1	74/76 (97%)	14 (18%)	6 (8%)
23	A2	14/15 (93%)	5 (35%)	2 (14%)
24	A3	76/77 (98%)	14 (18%)	7 (9%)
54	BA	2902/2903 (99%)	451 (15%)	146 (5%)
55	BB	116/118 (98%)	12 (10%)	3 (2%)
All	All	4711/4722 (99%)	760 (16%)	241 (5%)

All (760) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	51	A
21	AA	61	G
21	AA	65	A
21	AA	66	A

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Mol	Chain	Res	Type
21	AA	70	U
21	AA	71	A
21	AA	84	U
21	AA	85	U
21	AA	94	G
21	AA	95	C
21	AA	109	A
21	AA	110	C
21	AA	121	U
21	AA	122	G
21	AA	131	A
21	AA	144	G
21	AA	165	G
21	AA	173	U
21	AA	181	A
21	AA	182	A
21	AA	191	G
21	AA	197	A
21	AA	198	G
21	AA	204	G
21	AA	212	G
21	AA	214	C
21	AA	238	A
21	AA	239	U
21	AA	240	G
21	AA	245	U
21	AA	246	A
21	AA	247	G
21	AA	251	G
21	AA	252	U
21	AA	266	G
21	AA	267	C
21	AA	289	G
21	AA	308	C
21	AA	309	A
21	AA	321	A
21	AA	328	C
21	AA	329	A
21	AA	330	C
21	AA	335	C
21	AA	343	U
21	AA	344	A

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Mol	Chain	Res	Type
21	AA	346	G
21	AA	347	G
21	AA	348	G
21	AA	352	C
21	AA	354	G
21	AA	356	A
21	AA	358	U
21	AA	367	U
21	AA	372	C
21	AA	381	C
21	AA	397	A
21	AA	398	U
21	AA	406	G
21	AA	412	A
21	AA	413	G
21	AA	414	A
21	AA	415	A
21	AA	421	U
21	AA	422	C
21	AA	429	U
21	AA	437	U
21	AA	438	U
21	AA	448	A
21	AA	449	G
21	AA	452	A
21	AA	461	A
21	AA	467	U
21	AA	468	A
21	AA	474	G
21	AA	481	G
21	AA	484	G
21	AA	493	A
21	AA	494	G
21	AA	500	G
21	AA	501	C
21	AA	505	G
21	AA	506	G
21	AA	508	U
21	AA	509	A
21	AA	511	C
21	AA	527	G
21	AA	532	A

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Mol	Chain	Res	Type
21	AA	533	A
21	AA	534	U
21	AA	535	A
21	AA	547	A
21	AA	550	G
21	AA	553	A
21	AA	559	A
21	AA	564	C
21	AA	565	U
21	AA	566	G
21	AA	571	U
21	AA	572	A
21	AA	573	A
21	AA	575	G
21	AA	576	C
21	AA	619	U
21	AA	620	C
21	AA	625	U
21	AA	633	G
21	AA	654	G
21	AA	659	U
21	AA	660	C
21	AA	665	A
21	AA	671	G
21	AA	687	A
21	AA	700	G
21	AA	702	A
21	AA	718	A
21	AA	719	C
21	AA	724	G
21	AA	725	G
21	AA	755	G
21	AA	756	C
21	AA	761	G
21	AA	762	U
21	AA	777	A
21	AA	787	A
21	AA	793	U
21	AA	794	A
21	AA	808	C
21	AA	812	G
21	AA	817	C

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Mol	Chain	Res	Type
21	AA	819	A
21	AA	827	U
21	AA	828	U
21	AA	841	C
21	AA	843	U
21	AA	844	G
21	AA	846	G
21	AA	849	G
21	AA	885	G
21	AA	887	G
21	AA	889	A
21	AA	890	G
21	AA	914	A
21	AA	926	G
21	AA	927	G
21	AA	934	C
21	AA	939	G
21	AA	942	G
21	AA	945	G
21	AA	960	U
21	AA	961	U
21	AA	962	C
21	AA	968	A
21	AA	969	A
21	AA	972	C
21	AA	974	A
21	AA	976	G
21	AA	978	A
21	AA	979	C
21	AA	980	C
21	AA	993	G
21	AA	1004	A
21	AA	1006	G
21	AA	1031	C
21	AA	1033	G
21	AA	1042	A
21	AA	1050	G
21	AA	1053	G
21	AA	1054	C
21	AA	1055	A
21	AA	1056	U
21	AA	1065	U

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Mol	Chain	Res	Type
21	AA	1068	G
21	AA	1078	U
21	AA	1079	G
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1125	U
21	AA	1129	C
21	AA	1130	A
21	AA	1136	C
21	AA	1139	G
21	AA	1151	A
21	AA	1152	A
21	AA	1159	U
21	AA	1161	C
21	AA	1167	A
21	AA	1168	U
21	AA	1169	A
21	AA	1183	U
21	AA	1189	U
21	AA	1190	G
21	AA	1191	A
21	AA	1196	A
21	AA	1200	C
21	AA	1201	A
21	AA	1202	U
21	AA	1212	U
21	AA	1217	C
21	AA	1223	C
21	AA	1224	U
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1228	C
21	AA	1239	A
21	AA	1240	U
21	AA	1241	G
21	AA	1257	A
21	AA	1267	C
21	AA	1279	G
21	AA	1280	A

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Mol	Chain	Res	Type
21	AA	1281	C
21	AA	1282	C
21	AA	1285	A
21	AA	1287	A
21	AA	1301	U
21	AA	1303	C
21	AA	1305	G
21	AA	1308	U
21	AA	1309	G
21	AA	1319	A
21	AA	1320	C
21	AA	1322	C
21	AA	1336	C
21	AA	1337	G
21	AA	1338	G
21	AA	1345	U
21	AA	1360	A
21	AA	1363	A
21	AA	1364	U
21	AA	1378	C
21	AA	1382	C
21	AA	1383	C
21	AA	1432	G
21	AA	1446	A
21	AA	1453	G
21	AA	1466	C
21	AA	1471	U
21	AA	1484	C
21	AA	1492	A
21	AA	1493	A
21	AA	1494	G
21	AA	1499	A
21	AA	1503	A
21	AA	1504	G
21	AA	1505	G
21	AA	1506	U
21	AA	1529	G
21	AA	1530	G
21	AA	1533	C
21	AA	1534	A
22	A1	10	G
22	A1	17	U

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Mol	Chain	Res	Type
22	A1	20	G
22	A1	47	U
22	A1	48	C
22	A1	49	G
22	A1	56	C
22	A1	57	G
22	A1	58	A
22	A1	60	C
22	A1	62	C
22	A1	70	C
22	A1	75	C
22	A1	76	A
23	A2	80	C
23	A2	82	A
23	A2	89	U
23	A2	91	A
23	A2	92	U
24	A3	2	G
24	A3	9	G
24	A3	10	G
24	A3	18	U
24	A3	20	G
24	A3	22	A
24	A3	32	G
24	A3	49	C
24	A3	57	C
24	A3	58	A
24	A3	70	C
24	A3	75	C
24	A3	76	C
24	A3	77	A
54	BA	9	G
54	BA	14	A
54	BA	15	G
54	BA	20	C
54	BA	33	C
54	BA	34	U
54	BA	63	A
54	BA	71	A
54	BA	74	A
54	BA	75	G
54	BA	88	G

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Mol	Chain	Res	Type
54	BA	91	A
54	BA	92	U
54	BA	98	G
54	BA	100	U
54	BA	102	U
54	BA	110	G
54	BA	111	A
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	125	A
54	BA	126	A
54	BA	139	U
54	BA	140	C
54	BA	141	G
54	BA	142	A
54	BA	143	C
54	BA	145	C
54	BA	146	A
54	BA	147	C
54	BA	181	A
54	BA	196	A
54	BA	197	A
54	BA	199	A
54	BA	216	A
54	BA	222	A
54	BA	230	G
54	BA	233	A
54	BA	248	G
54	BA	250	G
54	BA	266	G
54	BA	278	A
54	BA	279	A
54	BA	294	A
54	BA	297	G
54	BA	299	A
54	BA	316	C
54	BA	323	C
54	BA	324	A
54	BA	330	A
54	BA	331	C

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Mol	Chain	Res	Type
54	BA	346	A
54	BA	370	G
54	BA	373	U
54	BA	374	A
54	BA	386	G
54	BA	387	U
54	BA	406	G
54	BA	411	G
54	BA	422	A
54	BA	428	A
54	BA	429	A
54	BA	430	A
54	BA	450	G
54	BA	451	U
54	BA	457	A
54	BA	473	G
54	BA	481	G
54	BA	491	G
54	BA	493	G
54	BA	504	A
54	BA	505	A
54	BA	507	A
54	BA	527	C
54	BA	528	A
54	BA	530	G
54	BA	531	C
54	BA	532	A
54	BA	533	G
54	BA	546	U
54	BA	547	A
54	BA	548	G
54	BA	549	G
54	BA	550	C
54	BA	573	U
54	BA	574	A
54	BA	588	U
54	BA	590	A
54	BA	603	A
54	BA	614	A
54	BA	627	A
54	BA	631	A
54	BA	637	A

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Mol	Chain	Res	Type
54	BA	645	C
54	BA	653	U
54	BA	655	A
54	BA	671	C
54	BA	686	U
54	BA	719	C
54	BA	727	A
54	BA	740	C
54	BA	747	U
54	BA	748	G
54	BA	750	A
54	BA	751	A
54	BA	752	A
54	BA	753	A
54	BA	763	G
54	BA	764	A
54	BA	775	G
54	BA	776	G
54	BA	782	A
54	BA	784	G
54	BA	791	C
54	BA	792	A
54	BA	805	G
54	BA	809	G
54	BA	812	C
54	BA	827	U
54	BA	828	U
54	BA	829	A
54	BA	830	G
54	BA	846	U
54	BA	858	G
54	BA	859	G
54	BA	866	A
54	BA	867	C
54	BA	889	C
54	BA	890	C
54	BA	891	G
54	BA	897	C
54	BA	910	A
54	BA	914	G
54	BA	915	C
54	BA	933	A

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Mol	Chain	Res	Type
54	BA	934	U
54	BA	941	A
54	BA	946	C
54	BA	959	A
54	BA	961	C
54	BA	974	G
54	BA	981	A
54	BA	982	C
54	BA	984	A
54	BA	989	G
54	BA	996	A
54	BA	1012	U
54	BA	1013	C
54	BA	1022	G
54	BA	1024	G
54	BA	1025	G
54	BA	1026	G
54	BA	1033	U
54	BA	1044	C
54	BA	1046	A
54	BA	1047	G
54	BA	1058	U
54	BA	1069	A
54	BA	1070	A
54	BA	1073	A
54	BA	1077	A
54	BA	1086	A
54	BA	1087	G
54	BA	1088	A
54	BA	1089	A
54	BA	1090	A
54	BA	1100	C
54	BA	1112	G
54	BA	1126	A
54	BA	1128	G
54	BA	1129	A
54	BA	1132	U
54	BA	1133	A
54	BA	1135	C
54	BA	1143	A
54	BA	1144	A
54	BA	1176	U

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Mol	Chain	Res	Type
54	BA	1204	A
54	BA	1205	A
54	BA	1206	G
54	BA	1237	A
54	BA	1242	U
54	BA	1253	A
54	BA	1256	G
54	BA	1265	A
54	BA	1266	G
54	BA	1271	G
54	BA	1272	A
54	BA	1276	A
54	BA	1288	G
54	BA	1289	C
54	BA	1300	G
54	BA	1301	A
54	BA	1302	A
54	BA	1313	U
54	BA	1317	G
54	BA	1325	U
54	BA	1326	U
54	BA	1327	A
54	BA	1341	G
54	BA	1342	A
54	BA	1350	C
54	BA	1365	A
54	BA	1379	U
54	BA	1385	A
54	BA	1388	G
54	BA	1390	U
54	BA	1396	U
54	BA	1416	G
54	BA	1417	C
54	BA	1419	A
54	BA	1420	A
54	BA	1428	C
54	BA	1440	U
54	BA	1452	G
54	BA	1454	C
54	BA	1455	G
54	BA	1458	U
54	BA	1459	G

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Mol	Chain	Res	Type
54	BA	1461	C
54	BA	1468	U
54	BA	1482	G
54	BA	1487	U
54	BA	1490	A
54	BA	1493	C
54	BA	1523	U
54	BA	1528	A
54	BA	1535	A
54	BA	1537	G
54	BA	1538	G
54	BA	1539	U
54	BA	1540	G
54	BA	1549	A
54	BA	1552	A
54	BA	1553	A
54	BA	1566	A
54	BA	1569	A
54	BA	1584	U
54	BA	1607	C
54	BA	1608	A
54	BA	1609	A
54	BA	1610	A
54	BA	1611	C
54	BA	1616	A
54	BA	1618	A
54	BA	1639	C
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1651	G
54	BA	1652	A
54	BA	1654	A
54	BA	1663	G
54	BA	1670	C
54	BA	1674	G
54	BA	1675	C
54	BA	1684	G
54	BA	1714	U
54	BA	1730	C
54	BA	1732	C
54	BA	1758	U

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Mol	Chain	Res	Type
54	BA	1761	C
54	BA	1764	C
54	BA	1773	A
54	BA	1779	U
54	BA	1782	U
54	BA	1784	A
54	BA	1800	C
54	BA	1801	A
54	BA	1808	A
54	BA	1810	A
54	BA	1815	A
54	BA	1816	C
54	BA	1821	A
54	BA	1834	U
54	BA	1835	G
54	BA	1847	A
54	BA	1848	A
54	BA	1855	U
54	BA	1873	G
54	BA	1906	G
54	BA	1912	A
54	BA	1914	C
54	BA	1929	G
54	BA	1937	A
54	BA	1938	A
54	BA	1939	U
54	BA	1940	U
54	BA	1945	G
54	BA	1953	A
54	BA	1955	U
54	BA	1956	U
54	BA	1962	C
54	BA	1963	U
54	BA	1964	G
54	BA	1966	A
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1981	A
54	BA	1982	U
54	BA	1993	U
54	BA	1997	C

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Mol	Chain	Res	Type
54	BA	2005	A
54	BA	2021	C
54	BA	2022	U
54	BA	2023	C
54	BA	2030	A
54	BA	2031	A
54	BA	2032	G
54	BA	2035	G
54	BA	2043	C
54	BA	2052	A
54	BA	2059	A
54	BA	2060	A
54	BA	2061	G
54	BA	2069	G
54	BA	2073	C
54	BA	2076	U
54	BA	2092	U
54	BA	2095	A
54	BA	2109	U
54	BA	2112	G
54	BA	2113	U
54	BA	2114	A
54	BA	2117	A
54	BA	2118	U
54	BA	2126	A
54	BA	2127	G
54	BA	2133	G
54	BA	2155	U
54	BA	2157	G
54	BA	2159	G
54	BA	2160	C
54	BA	2169	A
54	BA	2172	U
54	BA	2173	A
54	BA	2174	C
54	BA	2192	U
54	BA	2194	U
54	BA	2196	C
54	BA	2197	U
54	BA	2199	A
54	BA	2213	U
54	BA	2224	G

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Mol	Chain	Res	Type
54	BA	2225	A
54	BA	2230	G
54	BA	2238	G
54	BA	2239	G
54	BA	2246	G
54	BA	2251	G
54	BA	2267	A
54	BA	2268	A
54	BA	2269	G
54	BA	2283	C
54	BA	2296	U
54	BA	2297	A
54	BA	2308	G
54	BA	2309	A
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2325	G
54	BA	2334	U
54	BA	2335	A
54	BA	2347	C
54	BA	2361	G
54	BA	2383	G
54	BA	2385	C
54	BA	2403	C
54	BA	2406	A
54	BA	2407	A
54	BA	2419	U
54	BA	2425	A
54	BA	2427	C
54	BA	2428	G
54	BA	2429	G
54	BA	2430	A
54	BA	2432	A
54	BA	2433	A
54	BA	2441	U
54	BA	2448	A
54	BA	2452	C
54	BA	2455	G
54	BA	2473	U
54	BA	2488	G
54	BA	2491	U

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Mol	Chain	Res	Type
54	BA	2492	U
54	BA	2496	C
54	BA	2498	C
54	BA	2499	C
54	BA	2500	U
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2504	U
54	BA	2505	G
54	BA	2518	A
54	BA	2525	G
54	BA	2531	A
54	BA	2532	G
54	BA	2540	C
54	BA	2547	A
54	BA	2553	G
54	BA	2554	U
54	BA	2556	C
54	BA	2565	A
54	BA	2566	A
54	BA	2567	G
54	BA	2573	C
54	BA	2576	G
54	BA	2577	A
54	BA	2602	A
54	BA	2603	G
54	BA	2606	C
54	BA	2609	U
54	BA	2614	A
54	BA	2625	G
54	BA	2626	C
54	BA	2628	C
54	BA	2660	A
54	BA	2661	G
54	BA	2669	G
54	BA	2682	A
54	BA	2683	C
54	BA	2716	C
54	BA	2726	A
54	BA	2732	G
54	BA	2751	G

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Mol	Chain	Res	Type
54	BA	2755	C
54	BA	2756	U
54	BA	2765	A
54	BA	2766	A
54	BA	2777	G
54	BA	2778	A
54	BA	2780	G
54	BA	2797	U
54	BA	2808	G
54	BA	2816	G
54	BA	2817	U
54	BA	2821	A
54	BA	2830	C
54	BA	2833	U
54	BA	2850	A
54	BA	2858	C
54	BA	2859	G
54	BA	2884	U
54	BA	2894	G
54	BA	2895	G
55	BB	9	G
55	BB	13	G
55	BB	15	A
55	BB	25	U
55	BB	35	C
55	BB	42	C
55	BB	44	G
55	BB	45	A
55	BB	53	A
55	BB	64	G
55	BB	90	C
55	BB	109	A

All (241) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	60	A
21	AA	64	G
21	AA	65	A
21	AA	66	A
21	AA	70	U

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Mol	Chain	Res	Type
21	AA	172	A
21	AA	181	A
21	AA	190	A
21	AA	238	A
21	AA	244	U
21	AA	245	U
21	AA	246	A
21	AA	251	G
21	AA	281	G
21	AA	308	C
21	AA	320	A
21	AA	328	C
21	AA	343	U
21	AA	344	A
21	AA	346	G
21	AA	354	G
21	AA	357	G
21	AA	412	A
21	AA	448	A
21	AA	451	A
21	AA	481	G
21	AA	500	G
21	AA	505	G
21	AA	509	A
21	AA	532	A
21	AA	534	U
21	AA	571	U
21	AA	574	A
21	AA	575	G
21	AA	619	U
21	AA	632	U
21	AA	653	U
21	AA	659	U
21	AA	701	U
21	AA	718	A
21	AA	734	G
21	AA	761	G
21	AA	764	C
21	AA	777	A
21	AA	793	U
21	AA	818	G
21	AA	827	U

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Mol	Chain	Res	Type
21	AA	884	U
21	AA	913	A
21	AA	933	G
21	AA	960	U
21	AA	978	A
21	AA	1043	G
21	AA	1049	U
21	AA	1053	G
21	AA	1078	U
21	AA	1101	A
21	AA	1129	C
21	AA	1159	U
21	AA	1167	A
21	AA	1190	G
21	AA	1201	A
21	AA	1211	U
21	AA	1212	U
21	AA	1222	G
21	AA	1225	A
21	AA	1280	A
21	AA	1298	U
21	AA	1308	U
21	AA	1347	G
21	AA	1430	A
21	AA	1432	G
21	AA	1445	U
21	AA	1452	C
21	AA	1493	A
21	AA	1533	C
22	A1	1	G
22	A1	10	G
22	A1	32	C
22	A1	47	U
22	A1	61	C
22	A1	75	C
23	A2	81	U
23	A2	91	A
24	A3	9	G
24	A3	31	G
24	A3	47	G
24	A3	56	PSU
24	A3	69	C

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Mol	Chain	Res	Type
24	A3	75	C
24	A3	76	C
54	BA	33	C
54	BA	62	U
54	BA	74	A
54	BA	91	A
54	BA	118	A
54	BA	125	A
54	BA	143	C
54	BA	160	A
54	BA	196	A
54	BA	199	A
54	BA	215	G
54	BA	228	C
54	BA	247	G
54	BA	249	C
54	BA	278	A
54	BA	323	C
54	BA	329	G
54	BA	330	A
54	BA	345	A
54	BA	369	U
54	BA	372	G
54	BA	386	G
54	BA	421	C
54	BA	449	A
54	BA	476	G
54	BA	481	G
54	BA	526	A
54	BA	527	C
54	BA	530	G
54	BA	531	C
54	BA	532	A
54	BA	613	A
54	BA	659	G
54	BA	670	A
54	BA	750	A
54	BA	762	U
54	BA	775	G
54	BA	791	C
54	BA	809	G
54	BA	829	A

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Mol	Chain	Res	Type
54	BA	887	U
54	BA	988	A
54	BA	1069	A
54	BA	1086	A
54	BA	1087	G
54	BA	1089	A
54	BA	1128	G
54	BA	1143	A
54	BA	1206	G
54	BA	1210	G
54	BA	1224	U
54	BA	1236	G
54	BA	1254	A
54	BA	1273	U
54	BA	1288	G
54	BA	1300	G
54	BA	1312	U
54	BA	1325	U
54	BA	1340	U
54	BA	1397	U
54	BA	1427	A
54	BA	1451	C
54	BA	1458	U
54	BA	1509	A
54	BA	1597	A
54	BA	1608	A
54	BA	1609	A
54	BA	1610	A
54	BA	1617	C
54	BA	1618	A
54	BA	1674	G
54	BA	1713	A
54	BA	1731	G
54	BA	1800	C
54	BA	1834	U
54	BA	1847	A
54	BA	1857	G
54	BA	1913	A
54	BA	1936	A
54	BA	1937	A
54	BA	1945	G
54	BA	1952	A

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Mol	Chain	Res	Type
54	BA	1955	U
54	BA	1963	U
54	BA	1970	A
54	BA	1971	U
54	BA	1980	G
54	BA	1981	A
54	BA	2020	A
54	BA	2021	C
54	BA	2035	G
54	BA	2060	A
54	BA	2076	U
54	BA	2086	U
54	BA	2112	G
54	BA	2113	U
54	BA	2117	A
54	BA	2118	U
54	BA	2157	G
54	BA	2163	A
54	BA	2172	U
54	BA	2180	U
54	BA	2191	A
54	BA	2197	U
54	BA	2213	U
54	BA	2225	A
54	BA	2229	U
54	BA	2245	U
54	BA	2250	G
54	BA	2267	A
54	BA	2282	G
54	BA	2286	G
54	BA	2296	U
54	BA	2307	G
54	BA	2308	G
54	BA	2360	G
54	BA	2389	G
54	BA	2391	G
54	BA	2406	A
54	BA	2418	A
54	BA	2427	C
54	BA	2429	G
54	BA	2487	G
54	BA	2498	C

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Mol	Chain	Res	Type
54	BA	2500	U
54	BA	2503	A
54	BA	2504	U
54	BA	2531	A
54	BA	2553	G
54	BA	2563	U
54	BA	2565	A
54	BA	2576	G
54	BA	2581	G
54	BA	2585	U
54	BA	2602	A
54	BA	2605	U
54	BA	2625	G
54	BA	2668	G
54	BA	2681	C
54	BA	2682	A
54	BA	2689	U
54	BA	2751	G
54	BA	2755	C
54	BA	2780	G
54	BA	2858	C
54	BA	2887	A
55	BB	12	C
55	BB	15	A
55	BB	63	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CM0	A1	34	22,23	15,26,27	2.35	3 (20%)	15,37,40	3.63	4 (26%)
22	6MZ	A1	37	22	17,25,26	1.10	1 (5%)	15,36,39	1.61	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	7MG	A1	46	22	20,26,27	1.76	3 (15%)	24,39,42	1.54	2 (8%)
22	5MU	A1	54	22	13,22,23	1.33	2 (15%)	14,32,35	3.30	1 (7%)
22	PSU	A1	55	22	16,21,22	1.34	2 (12%)	20,30,33	4.75	5 (25%)
22	4SU	A1	7	22	13,21,22	1.23	1 (7%)	14,30,33	2.69	2 (14%)
24	H2U	A3	21	24	17,21,22	1.53	3 (17%)	20,30,33	1.15	2 (10%)
24	OMC	A3	33	24	15,22,23	1.38	2 (13%)	20,31,34	1.10	1 (5%)
24	5MU	A3	55	24	13,22,23	1.36	3 (23%)	14,32,35	3.45	1 (7%)
24	PSU	A3	56	24	16,21,22	1.39	3 (18%)	20,30,33	4.64	7 (35%)
24	4SU	A3	8	24	13,21,22	1.29	1 (7%)	14,30,33	2.97	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CM0	A1	34	22,23	-	2/6/30/31	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	7MG	A1	46	22	-	1/7/37/38	0/3/3/3
22	5MU	A1	54	22	-	0/3/25/26	0/2/2/2
22	PSU	A1	55	22	-	0/7/25/26	0/2/2/2
22	4SU	A1	7	22	-	0/3/25/26	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
24	OMC	A3	33	24	-	0/5/27/28	0/2/2/2
24	5MU	A3	55	24	-	0/3/25/26	0/2/2/2
24	PSU	A3	56	24	-	3/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/3/25/26	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	34	CM0	O5-C5	-7.22	1.23	1.37
22	A1	46	7MG	C8-N9	-5.55	1.32	1.45
24	A3	21	H2U	C2-N3	-3.65	1.31	1.38
22	A1	34	CM0	O5'-C5'	-3.50	1.39	1.44
24	A3	21	H2U	C4-N3	-3.37	1.32	1.37
24	A3	56	PSU	O4'-C1'	-3.16	1.39	1.44
22	A1	46	7MG	O5'-C5'	-3.03	1.40	1.44
22	A1	34	CM0	C4-C5	2.92	1.47	1.40
24	A3	33	OMC	C4-N3	-2.72	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	33	OMC	O5'-C5'	-2.69	1.41	1.44
24	A3	55	5MU	O5'-C5'	-2.60	1.41	1.44
24	A3	21	H2U	O4'-C4'	-2.59	1.39	1.45
22	A1	7	4SU	O5'-C5'	-2.59	1.41	1.44
22	A1	55	PSU	O4'-C1'	-2.55	1.40	1.44
24	A3	56	PSU	O5'-C5'	-2.52	1.41	1.44
22	A1	54	5MU	O5'-C5'	-2.47	1.41	1.44
22	A1	46	7MG	C6-N1	2.34	1.37	1.33
22	A1	37	6MZ	C8-N7	-2.32	1.30	1.34
22	A1	54	5MU	C4-N3	2.29	1.37	1.33
24	A3	8	4SU	C6-N1	2.28	1.38	1.35
22	A1	55	PSU	C4-N3	2.18	1.36	1.33
24	A3	55	5MU	C4-N3	2.15	1.36	1.33
24	A3	55	5MU	C6-C5	-2.08	1.34	1.40
24	A3	56	PSU	O4'-C4'	-2.02	1.40	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	55	PSU	N1-C2-N3	-14.43	116.96	128.43
24	A3	56	PSU	N1-C2-N3	-13.12	118.00	128.43
24	A3	55	5MU	C4-N3-C2	12.38	125.60	115.14
22	A1	54	5MU	C4-N3-C2	11.89	125.18	115.14
22	A1	55	PSU	C4-N3-C2	11.80	125.11	115.14
24	A3	56	PSU	C4-N3-C2	11.64	124.97	115.14
22	A1	34	CM0	C4-N3-C2	11.43	124.79	115.14
24	A3	56	PSU	C5-C4-N3	-8.23	114.75	125.36
24	A3	8	4SU	C2-N3-C4	8.21	127.05	115.15
22	A1	55	PSU	C5-C4-N3	-7.83	115.28	125.36
22	A1	7	4SU	C2-N3-C4	7.20	125.59	115.15
24	A3	8	4SU	C5-C4-N3	-6.64	115.21	123.81
22	A1	7	4SU	C5-C4-N3	-6.15	115.85	123.81
22	A1	34	CM0	C5-C4-N3	-5.68	115.10	122.74
22	A1	46	7MG	C6-N1-C2	5.19	123.45	116.06
22	A1	37	6MZ	C9-N6-C6	4.97	127.15	122.87
22	A1	55	PSU	C6-N1-C2	4.14	121.92	115.32
24	A3	56	PSU	C5-C6-N1	-4.10	119.30	124.44
24	A3	56	PSU	C6-N1-C2	4.06	121.80	115.32
22	A1	46	7MG	C6-C5-C4	3.96	119.45	115.20
22	A1	34	CM0	C4'-O4'-C1'	-3.88	105.78	109.83
24	A3	33	OMC	C2-N3-C4	3.47	119.58	116.26
22	A1	34	CM0	O5-C5-C4	3.34	119.58	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	55	PSU	C5-C6-N1	-3.24	120.38	124.44
24	A3	56	PSU	C4'-O4'-C1'	-2.54	106.29	109.42
24	A3	8	4SU	C4'-O4'-C1'	-2.52	107.20	109.83
24	A3	21	H2U	C5-C4-N3	2.47	119.45	116.65
22	A1	37	6MZ	C2-N1-C6	2.41	118.75	116.62
24	A3	56	PSU	O4'-C1'-C2'	2.26	108.32	104.66
24	A3	21	H2U	N3-C2-N1	2.04	118.81	116.65

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	34	CM0	C4-C5-O5-C7
22	A1	34	CM0	C6-C5-O5-C7
24	A3	56	PSU	O4'-C1'-C5-C6
24	A3	56	PSU	O4'-C1'-C5-C4
24	A3	56	PSU	C2'-C1'-C5-C6
22	A1	46	7MG	C3'-C4'-C5'-O5'

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
58	FME	BA	3001	57	9,9,10	0.85	1 (11%)	6,9,11	1.22	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	FME	BA	3001	57	-	0/6/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	3001	FME	CA-C	2.14	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	FME	O-C-CA	-2.58	119.20	125.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.